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Neutral and Cationic Rare Earth Metal Alkyl and Benzyl Compounds with the 1,4,6-Trimethyl-6-pyrrolidin-1-yl-1,4-diazepane Ligand and Their Performance in the Catalytic Hydroamination/Cyclization of Aminoalkenes

Ge, Shaozhong; Meetsma, Auke; Hessen, Bart

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2008-05-15 # Formatted by publCIF
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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 choice FI, CI or EI for Inorganic
#                               FM, CM or EM for Metal-organic
#                               FO, CO or EO for Organic
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_publ_requested_coeditor_name     ?

_publ_contact_letter              # Include date of submission
;
  Date of submission : 2008-05-15 11:25:01

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  (Our Compound_Identification_Code : Q1157)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_printers_final   ?
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_journal_page_last             ?

_journal_suppl_publ_number     ?
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#=====

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3. TITLE AND AUTHOR LIST

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Title (type here to add)
;
_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.

```

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_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

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(type here to add preparation details)
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_publ_section_exptl_refinement
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(type here to add refinement details)
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;
Allen, F. H. (2002). <i>Acta Cryst.</i> B58, 380--388.

Beurskens, P.T., Beurskens, G., Gelder, R. de, Garc'ia-Granda, S. Gould, R.O.,
Isra'el, & Smits, J.M.M. (1999). The <i>DIRDIF99</i> program system,
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Space-group symmetry, Kluwer Academic Publishers, Dordrecht, The Netherlands.

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```

Sheldrick, G. M. (1997). *SHELXL97*. Program for Crystal Structure Refinement. University of Göttingen, Germany.

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Wilson, A. J. C. (1992). *International Tables for Crystallography, Volume C*, Kluwer Academic Publishers, Dordrecht, The Netherlands.

;

_publ_section_figure_captions

;

Fig. 1. Perspective *PLUTO* drawing 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 are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.

;

#=====

5. CHEMICAL DATA

_chemical_name_systematic

;

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety

'C₂₄ H₅₈ N₃ Si₃ Y'

Ex: 'C₁₂ H₁₆ N₂ O₆, H₂ O' and '(Cd²⁺)₃, (C₆ N₆ Cr³⁻)₂, 2(H₂ O)'

_chemical_formula_structural ?

_chemical_formula_sum

'C₂₄ H₅₈ N₃ Si₃ Y'

_chemical_formula_iupac ?

_chemical_formula_weight 561.91

_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

```

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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
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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 b c a'
_symmetry_Int_Tables_number    61

```

```

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
  5 -x,-y,-z
  6 1/2+x,y,1/2-z
  7 1/2-x,1/2+y,z
  8 x,1/2-y,1/2+z

```

```

_cell_length_a              17.211(1)
_cell_length_b              17.984(2)
_cell_length_c              20.309(2)
_cell_angle_alpha           90
_cell_angle_beta            90
_cell_angle_gamma           90
_cell_volume                 6286.1(10)
_cell_formula_units_Z       8

```

```

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 6022
_cell_measurement_theta_min   2.48
_cell_measurement_theta_max   28.94
_cell_special_details

```

```
;
```

The final unit cell was obtained from the xyz centroids of 6022 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     0.41
_exptl_crystal_size_mid     0.33
_exptl_crystal_size_min     0.22
_exptl_crystal_size_rad     ?
_exptl_crystal_density_meas  ?
_exptl_crystal_density_diffn 1.187

```

```

_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             2432
_exptl_absorpt_coefficient_mu    1.985
_exptl_absorpt_correction_type   'Multi-Scan'
_exptl_absorpt_process_details   '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min  0.4831
_exptl_absorpt_correction_T_max  0.6461

```

``` # 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, 2000)).
;
_diffn_detector_area_resol_mean   '4096x4096 / 62x62 (binned 512)'

_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)
_diffn_reflns_number             49161
_diffn_reflns_av_R_equivalents   0.0527
_diffn_reflns_av_sigmaI/netI     0.0338
_diffn_reflns_limit_h_min        -21
_diffn_reflns_limit_h_max        21
_diffn_reflns_limit_k_min        -22
_diffn_reflns_limit_k_max        22
_diffn_reflns_limit_l_min        -25
_diffn_reflns_limit_l_max        25
_diffn_reflns_theta_min          2.26
_diffn_reflns_theta_max          26.73
_diffn_measured_fraction_theta_max 0.999
_diffn_reflns_theta_full         25.00

```

```

_diffn_measured_fraction_theta_full    0.999

_diffn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2001) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflns_number_total          6670
_reflns_number_gt             5151
_reflns_threshold_expression   I>2\sigma(I)

_computing_data_collection      'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement      'SAINTPLUS, Version 6.02A, (Bruker, 2001)'
_computing_data_reduction       'XPREP, Version 5.1/NT, (Bruker, 2001)'
_computing_structure_solution
;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2006)
PLATON (Spek, 2003)
;
_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/[\sigma^2(Fo^2)+(0.0322P)^2+2.1759P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary    heavy    # heavy,direct,difmap,geom
_atom_sites_solution_secondary  direct   # difmap
_atom_sites_solution_hydrogens  difmap   # geom
_refine_ls_hydrogen_treatment   refall   # none, undef, noref, refall,
                                         # refxyz, refU, constr or mixed

_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration '.'
_refine_ls_abs_structure_Flack   ?

```


_refine_ls_number_reflns	6670
_refine_ls_number_parameters	512
_refine_ls_number_restraints	0
_refine_ls_number_constraints	?
_refine_ls_R_factor_all	0.0475
_refine_ls_R_factor_gt	0.0289
_refine_ls_wR_factor_ref	0.0688
_refine_ls_wR_factor_gt	0.0624
_refine_ls_goodness_of_fit_ref	1.039
_refine_ls_restrained_S_all	1.039
_refine_ls_shift/su_max	0.001
_refine_ls_shift/su_mean	0.000
_refine_diff_density_max	0.450
_refine_diff_density_min	-0.291
_refine_diff_density_rms	0.069
_vrn_publ_code_frame_time_sec	10.0
_vrn_publ_code_meas_time_hour	9.0

#=====

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Y Y Uani 0.15930(1) 0.12534(1) 0.20778(1) 1.000 0.0118(1) . .
Si1 Si Uani 0.27469(3) 0.12011(3) 0.02908(3) 1.000 0.0155(2) . .
Si2 Si Uani 0.04561(3) -0.04060(3) 0.14201(3) 1.000 0.0177(2) . .
Si3 Si Uani 0.04405(3) 0.28125(3) 0.11961(3) 1.000 0.0177(2) . .
N1 N Uani 0.26211(9) 0.21805(9) 0.25868(8) 1.000 0.0155(5) . .
N2 N Uani 0.28900(9) 0.06842(9) 0.24419(8) 1.000 0.0152(5) . .
N3 N Uani 0.16651(9) 0.12186(9) 0.33920(8) 1.000 0.0149(5) . .
C1 C Uani 0.24561(14) 0.29811(12) 0.25035(12) 1.000 0.0223(7) . .
C2 C Uani 0.32870(12) 0.19926(12) 0.21554(11) 1.000 0.0191(6) . .
C3 C Uani 0.35241(12) 0.11757(12) 0.22049(10) 1.000 0.0189(6) . .
C4 C Uani 0.29980(14) -0.00632(12) 0.21512(12) 1.000 0.0215(7) . .
C5 C Uani 0.29119(12) 0.06222(12) 0.31686(10) 1.000 0.0168(6) . .
C6 C Uani 0.25247(11) 0.12691(11) 0.35294(10) 1.000 0.0158(6) . .
C7 C Uani 0.27437(14) 0.12075(14) 0.42604(10) 1.000 0.0216(7) . .
C8 C Uani 0.28169(12) 0.20213(12) 0.32855(10) 1.000 0.0166(6) . .
C9 C Uani 0.12924(13) 0.05531(12) 0.37045(11) 1.000 0.0202(7) . .
C10 C Uani 0.04540(14) 0.07659(14) 0.38546(13) 1.000 0.0293(8) . .
C11 C Uani 0.03737(13) 0.15692(13) 0.36250(11) 1.000 0.0235(7) . .
C12 C Uani 0.12031(12) 0.18579(12) 0.36448(11) 1.000 0.0197(7) . .
C13 C Uani 0.20461(12) 0.11868(13) 0.09681(10) 1.000 0.0177(6) . .
C14 C Uani 0.22809(15) 0.11411(14) -0.05481(11) 1.000 0.0233(7) . .
C15 C Uani 0.33242(14) 0.20842(13) 0.02906(12) 1.000 0.0250(7) . .
C16 C Uani 0.34531(14) 0.04083(13) 0.03367(11) 1.000 0.0224(7) . .
C17 C Uani 0.08510(13) 0.00966(12) 0.21327(10) 1.000 0.0189(6) . .
C18 C Uani -0.02559(17) -0.11639(15) 0.16331(14) 1.000 0.0329(8) . .
C19 C Uani -0.00788(14) 0.02606(14) 0.08724(12) 1.000 0.0261(7) . .

```

C20 C Uani 0.12461(17) -0.08780(15) 0.09376(14) 1.000 0.0317(8) . .
 C21 C Uani 0.05977(12) 0.22135(12) 0.19192(10) 1.000 0.0181(6) . .
 C22 C Uani -0.03448(16) 0.35303(14) 0.13183(13) 1.000 0.0306(8) . .
 C23 C Uani 0.01699(15) 0.22671(13) 0.04433(11) 1.000 0.0237(7) . .
 C24 C Uani 0.13239(15) 0.33611(14) 0.09593(13) 1.000 0.0289(8) . .
 H1 H Uiso 0.2017(13) 0.3105(12) 0.2769(10) 1.000 0.017(6) . .
 H1' H Uiso 0.2352(13) 0.3090(12) 0.2047(11) 1.000 0.024(6) . .
 H1" H Uiso 0.2906(13) 0.3282(12) 0.2636(10) 1.000 0.022(6) . .
 H2 H Uiso 0.3725(13) 0.2286(12) 0.2282(10) 1.000 0.020(6) . .
 H2' H Uiso 0.3143(12) 0.2105(11) 0.1742(11) 1.000 0.015(5) . .
 H3 H Uiso 0.3646(11) 0.1003(11) 0.1770(10) 1.000 0.011(5) . .
 H3' H Uiso 0.3953(13) 0.1100(11) 0.2493(11) 1.000 0.019(6) . .
 H4 H Uiso 0.3508(12) -0.0263(11) 0.2266(9) 1.000 0.011(5) . .
 H4' H Uiso 0.2971(12) -0.0030(12) 0.1692(12) 1.000 0.022(6) . .
 H4" H Uiso 0.2607(12) -0.0367(11) 0.2314(10) 1.000 0.012(5) . .
 H5 H Uiso 0.3432(12) 0.0561(11) 0.3310(10) 1.000 0.017(6) . .
 H5' H Uiso 0.2647(11) 0.0147(11) 0.3296(9) 1.000 0.009(5) . .
 H7 H Uiso 0.2404(14) 0.1508(14) 0.4531(12) 1.000 0.036(7) . .
 H7' H Uiso 0.3261(14) 0.1351(12) 0.4326(11) 1.000 0.023(6) . .
 H7" H Uiso 0.2687(12) 0.0695(12) 0.4411(10) 1.000 0.016(5) . .
 H8 H Uiso 0.2605(11) 0.2404(11) 0.3546(9) 1.000 0.008(5) . .
 H8' H Uiso 0.3376(12) 0.2050(12) 0.3344(10) 1.000 0.018(6) . .
 H9 H Uiso 0.1560(12) 0.0407(12) 0.4094(12) 1.000 0.025(6) . .
 H9' H Uiso 0.1328(12) 0.0143(12) 0.3437(11) 1.000 0.022(6) . .
 H10 H Uiso 0.0381(14) 0.0706(13) 0.4306(13) 1.000 0.036(7) . .
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 H12 H Uiso 0.1283(12) 0.2274(12) 0.3380(10) 1.000 0.016(5) . .
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 H16 H Uiso 0.3756(13) 0.0390(12) 0.0718(12) 1.000 0.029(6) . .
 H16' H Uiso 0.3804(14) 0.0414(13) -0.0034(12) 1.000 0.037(7) . .
 H16" H Uiso 0.3184(14) -0.0063(15) 0.0321(11) 1.000 0.034(7) . .
 H17 H Uiso 0.1147(13) -0.0270(12) 0.2376(11) 1.000 0.026(6) . .
 H17' H Uiso 0.0414(13) 0.0227(12) 0.2385(11) 1.000 0.027(6) . .
 H18 H Uiso -0.0007(16) -0.1503(15) 0.1863(14) 1.000 0.040(8) . .
 H18' H Uiso -0.0428(14) -0.1429(14) 0.1256(13) 1.000 0.036(7) . .
 H18" H Uiso -0.0687(18) -0.0959(16) 0.1834(14) 1.000 0.053(9) . .
 H19 H Uiso -0.0363(14) 0.0593(14) 0.1137(12) 1.000 0.036(7) . .
 H19' H Uiso -0.0426(15) 0.0021(14) 0.0579(12) 1.000 0.043(7) . .
 H19" H Uiso 0.0273(14) 0.0530(14) 0.0577(12) 1.000 0.040(7) . .
 H20 H Uiso 0.1636(15) -0.0516(16) 0.0772(13) 1.000 0.047(8) . .
 H20' H Uiso 0.1012(15) -0.1109(14) 0.0602(14) 1.000 0.039(7) . .
 H20" H Uiso 0.1500(16) -0.1214(15) 0.1179(15) 1.000 0.046(9) . .
 H21 H Uiso 0.0154(15) 0.1902(14) 0.1965(12) 1.000 0.041(7) . .
 H21' H Uiso 0.0583(13) 0.2515(14) 0.2291(11) 1.000 0.031(7) . .
 H22 H Uiso -0.0821(15) 0.3310(14) 0.1391(12) 1.000 0.034(7) . .
 H22' H Uiso -0.0356(14) 0.3863(13) 0.0940(12) 1.000 0.033(7) . .
 H22" H Uiso -0.0252(14) 0.3850(13) 0.1693(13) 1.000 0.032(7) . .
 H23 H Uiso 0.0546(15) 0.1943(14) 0.0314(12) 1.000 0.036(7) . .
 H23' H Uiso 0.0051(16) 0.2597(16) 0.0055(14) 1.000 0.055(8) . .
 H23" H Uiso -0.0297(15) 0.1989(14) 0.0507(12) 1.000 0.036(7) . .
 H24 H Uiso 0.1481(16) 0.3719(14) 0.1313(14) 1.000 0.046(8) . .

H24' H Uiso 0.1244(16) 0.3665(15) 0.0573(15) 1.000 0.052(8) . .
H24'' H Uiso 0.1748(14) 0.3070(13) 0.0876(11) 1.000 0.027(7) . .

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_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Y 0.0120(1) 0.0117(1) 0.0117(1) 0.0002(1) -0.0006(1) -0.0002(1)
Si1 0.0161(3) 0.0167(3) 0.0137(3) 0.0004(2) 0.0011(2) -0.0003(3)
Si2 0.0202(3) 0.0156(3) 0.0172(3) -0.0015(2) 0.0006(2) -0.0041(2)
Si3 0.0197(3) 0.0148(3) 0.0185(3) 0.0015(2) -0.0022(2) 0.0026(2)
N1 0.0174(8) 0.0135(9) 0.0155(9) 0.0006(7) -0.0004(7) -0.0006(7)
N2 0.0172(9) 0.0139(8) 0.0145(8) -0.0005(7) 0.0003(7) 0.0008(7)
N3 0.0151(8) 0.0157(8) 0.0138(8) 0.0001(7) -0.0005(6) -0.0007(7)
C1 0.0254(12) 0.0146(11) 0.0268(13) 0.0004(10) -0.0041(10) -0.0020(9)
C2 0.0165(11) 0.0221(11) 0.0186(11) 0.0001(9) -0.0004(9) -0.0059(9)
C3 0.0148(10) 0.0241(12) 0.0179(11) -0.0021(9) 0.0009(8) -0.0001(9)
C4 0.0236(12) 0.0163(11) 0.0245(12) -0.0024(9) -0.0013(10) 0.0033(9)
C5 0.0165(11) 0.0187(11) 0.0151(10) 0.0033(8) -0.0035(8) 0.0026(9)
C6 0.0142(9) 0.0188(10) 0.0144(10) 0.0000(9) -0.0028(8) -0.0006(8)
C7 0.0208(11) 0.0282(13) 0.0159(11) -0.0008(10) -0.0018(9) -0.0011(11)
C8 0.0158(11) 0.0197(11) 0.0144(10) -0.0032(8) -0.0012(8) -0.0012(9)
C9 0.0228(11) 0.0217(12) 0.0162(11) 0.0046(9) -0.0008(9) -0.0049(9)
C10 0.0231(12) 0.0375(14) 0.0273(13) 0.0038(11) 0.0060(10) -0.0070(11)
C11 0.0165(11) 0.0354(13) 0.0185(11) -0.0036(10) 0.0021(9) 0.0023(10)
C12 0.0203(11) 0.0239(12) 0.0150(11) -0.0033(9) 0.0014(9) 0.0020(9)
C13 0.0152(10) 0.0188(11) 0.0191(11) 0.0009(9) 0.0004(8) -0.0003(9)
C14 0.0254(12) 0.0266(14) 0.0180(11) 0.0025(10) -0.0014(10) 0.0001(11)
C15 0.0254(13) 0.0262(13) 0.0233(12) 0.0012(10) 0.0063(10) -0.0056(10)
C16 0.0237(12) 0.0262(12) 0.0174(11) -0.0029(9) 0.0000(10) 0.0065(10)
C17 0.0224(11) 0.0182(11) 0.0161(10) 0.0006(9) 0.0009(9) -0.0028(9)
C18 0.0400(16) 0.0279(14) 0.0308(14) -0.0012(12) -0.0003(12) -0.0148(12)
C19 0.0238(12) 0.0308(14) 0.0236(12) 0.0006(10) -0.0009(10) -0.0013(11)
C20 0.0358(15) 0.0252(14) 0.0341(14) -0.0102(12) 0.0011(12) 0.0015(12)
C21 0.0204(11) 0.0169(11) 0.0171(11) 0.0010(8) -0.0006(8) 0.0026(9)
C22 0.0373(16) 0.0247(13) 0.0299(14) 0.0003(11) -0.0042(12) 0.0123(11)
C23 0.0232(12) 0.0236(12) 0.0243(12) -0.0010(10) -0.0073(10) 0.0037(10)
C24 0.0323(14) 0.0219(13) 0.0325(14) 0.0090(11) -0.0041(11) -0.0051(11)
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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	N1	2.6419(16)	.	.	yes
Y	N2	2.5647(16)	.	.	yes
Y	N3	2.6726(17)	.	.	yes
Y	C13	2.388(2)	.	.	yes
Y	C17	2.444(2)	.	.	yes
Y	C21	2.454(2)	.	.	yes
Si1	C13	1.830(2)	.	.	yes
Si1	C14	1.886(2)	.	.	yes
Si1	C15	1.873(2)	.	.	yes
Si1	C16	1.876(2)	.	.	yes
Si2	C17	1.837(2)	.	.	yes
Si2	C18	1.883(3)	.	.	yes
Si2	C19	1.877(3)	.	.	yes
Si2	C20	1.879(3)	.	.	yes
Si3	C21	1.841(2)	.	.	yes
Si3	C22	1.885(3)	.	.	yes
Si3	C23	1.875(2)	.	.	yes
Si3	C24	1.875(3)	.	.	yes
N1	C1	1.477(3)	.	.	yes
N1	C2	1.482(3)	.	.	yes
N1	C8	1.486(3)	.	.	yes
N2	C3	1.485(3)	.	.	yes
N2	C4	1.480(3)	.	.	yes
N2	C5	1.481(3)	.	.	yes
N3	C6	1.508(2)	.	.	yes
N3	C9	1.499(3)	.	.	yes
N3	C12	1.489(3)	.	.	yes
C2	C3	1.528(3)	.	.	no
C5	C6	1.528(3)	.	.	no
C6	C7	1.536(3)	.	.	no
C6	C8	1.526(3)	.	.	no
C9	C10	1.524(3)	.	.	no
C10	C11	1.524(3)	.	.	no
C11	C12	1.520(3)	.	.	no
C1	H1	0.96(2)	.	.	no
C1	H1'	0.96(2)	.	.	no
C1	H1''	0.98(2)	.	.	no
C2	H2	0.96(2)	.	.	no
C2	H2'	0.90(2)	.	.	no
C3	H3	0.96(2)	.	.	no
C3	H3'	0.95(2)	.	.	no
C4	H4	0.98(2)	.	.	no
C4	H4'	0.94(2)	.	.	no
C4	H4''	0.93(2)	.	.	no
C5	H5	0.95(2)	.	.	no
C5	H5'	1.00(2)	.	.	no
C7	H7	0.97(2)	.	.	no
C7	H7'	0.94(2)	.	.	no
C7	H7''	0.98(2)	.	.	no
C8	H8	0.942(19)	.	.	no
C8	H8'	0.97(2)	.	.	no
C9	H9	0.95(2)	.	.	no
C9	H9'	0.92(2)	.	.	no
C10	H10	0.93(3)	.	.	no
C10	H10'	0.92(2)	.	.	no
C11	H11	0.96(2)	.	.	no
C11	H11'	0.92(2)	.	.	no
C12	H12	0.93(2)	.	.	no
C12	H12'	0.96(2)	.	.	no

C13	H13	0.95 (3)	.	.	no
C13	H13'	0.84 (3)	.	.	no
C14	H14	0.97 (2)	.	.	no
C14	H14'	0.94 (3)	.	.	no
C14	H14''	0.93 (3)	.	.	no
C15	H15	0.93 (2)	.	.	no
C15	H15'	0.93 (2)	.	.	no
C15	H15''	0.98 (2)	.	.	no
C16	H16	0.93 (2)	.	.	no
C16	H16'	0.97 (2)	.	.	no
C16	H16''	0.97 (3)	.	.	no
C17	H17	0.97 (2)	.	.	no
C17	H17'	0.94 (2)	.	.	no
C18	H18	0.88 (3)	.	.	no
C18	H18'	0.95 (3)	.	.	no
C18	H18''	0.92 (3)	.	.	no
C19	H19	0.94 (2)	.	.	no
C19	H19'	0.95 (2)	.	.	no
C19	H19''	0.98 (2)	.	.	no
C20	H20	0.99 (3)	.	.	no
C20	H20'	0.89 (3)	.	.	no
C20	H20''	0.89 (3)	.	.	no
C21	H21	0.95 (3)	.	.	no
C21	H21'	0.93 (2)	.	.	no
C22	H22	0.92 (3)	.	.	no
C22	H22'	0.97 (2)	.	.	no
C22	H22''	0.97 (3)	.	.	no
C23	H23	0.91 (3)	.	.	no
C23	H23'	1.01 (3)	.	.	no
C23	H23''	0.96 (3)	.	.	no
C24	H24	1.00 (3)	.	.	no
C24	H24'	0.97 (3)	.	.	no
C24	H24''	0.91 (2)	.	.	no
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N1	Y	N2	63.65 (5)	.	yes
N1	Y	N3	65.98 (5)	.	yes
N1	Y	C13	100.50 (6)	.	yes
N1	Y	C17	150.40 (6)	.	yes
N1	Y	C21	94.29 (6)	.	yes
N2	Y	N3	70.26 (5)	.	yes
N2	Y	C13	88.16 (6)	.	yes
N2	Y	C17	95.85 (6)	.	yes
N2	Y	C21	157.89 (6)	.	yes
N3	Y	C13	157.85 (6)	.	yes
N3	Y	C17	87.64 (6)	.	yes
N3	Y	C21	100.37 (6)	.	yes
C13	Y	C17	99.85 (7)	.	yes
C13	Y	C21	98.01 (7)	.	yes
C17	Y	C21	103.90 (7)	.	yes
C13	Si1	C14	113.45 (10)	.	yes
C13	Si1	C15	111.21 (11)	.	yes
C13	Si1	C16	112.28 (10)	.	yes

C14	Si1	C15	105.89 (11)	.	.	.	yes
C14	Si1	C16	106.08 (11)	.	.	.	yes
C15	Si1	C16	107.50 (11)	.	.	.	yes
C17	Si2	C18	114.58 (11)	.	.	.	yes
C17	Si2	C19	109.52 (10)	.	.	.	yes
C17	Si2	C20	111.44 (11)	.	.	.	yes
C18	Si2	C19	106.22 (12)	.	.	.	yes
C18	Si2	C20	105.29 (12)	.	.	.	yes
C19	Si2	C20	109.54 (12)	.	.	.	yes
C21	Si3	C22	113.64 (11)	.	.	.	yes
C21	Si3	C23	112.38 (10)	.	.	.	yes
C21	Si3	C24	113.16 (11)	.	.	.	yes
C22	Si3	C23	106.70 (11)	.	.	.	yes
C22	Si3	C24	104.76 (11)	.	.	.	yes
C23	Si3	C24	105.51 (11)	.	.	.	yes
Y	N1	C1	116.20 (12)	.	.	.	yes
Y	N1	C2	98.21 (11)	.	.	.	yes
Y	N1	C8	113.82 (12)	.	.	.	yes
C1	N1	C2	107.65 (16)	.	.	.	yes
C1	N1	C8	109.92 (16)	.	.	.	yes
C2	N1	C8	110.20 (15)	.	.	.	yes
Y	N2	C3	107.98 (11)	.	.	.	yes
Y	N2	C4	110.91 (12)	.	.	.	yes
Y	N2	C5	109.85 (11)	.	.	.	yes
C3	N2	C4	108.61 (16)	.	.	.	yes
C3	N2	C5	110.45 (15)	.	.	.	yes
C4	N2	C5	109.03 (16)	.	.	.	yes
Y	N3	C6	103.23 (11)	.	.	.	yes
Y	N3	C9	114.94 (12)	.	.	.	yes
Y	N3	C12	107.54 (12)	.	.	.	yes
C6	N3	C9	112.93 (15)	.	.	.	yes
C6	N3	C12	114.42 (15)	.	.	.	yes
C9	N3	C12	104.00 (15)	.	.	.	yes
N1	C2	C3	112.76 (17)	.	.	.	yes
N2	C3	C2	113.42 (17)	.	.	.	yes
N2	C5	C6	114.18 (17)	.	.	.	yes
N3	C6	C5	107.05 (16)	.	.	.	yes
N3	C6	C7	114.54 (17)	.	.	.	yes
N3	C6	C8	108.46 (16)	.	.	.	yes
C5	C6	C7	107.56 (17)	.	.	.	no
C5	C6	C8	112.06 (16)	.	.	.	no
C7	C6	C8	107.27 (17)	.	.	.	no
N1	C8	C6	113.95 (17)	.	.	.	yes
N3	C9	C10	106.83 (17)	.	.	.	yes
C9	C10	C11	105.23 (19)	.	.	.	no
C10	C11	C12	103.33 (18)	.	.	.	no
N3	C12	C11	103.22 (17)	.	.	.	yes
Y	C13	Si1	157.54 (11)	.	.	.	yes
Y	C17	Si2	125.20 (10)	.	.	.	yes
Y	C21	Si3	128.25 (10)	.	.	.	yes
N1	C1	H1	108.4 (13)	.	.	.	no
N1	C1	H1'	110.1 (13)	.	.	.	no
N1	C1	H1''	110.7 (13)	.	.	.	no
H1	C1	H1'	110.4 (18)	.	.	.	no
H1	C1	H1''	109.9 (18)	.	.	.	no
H1'	C1	H1''	107.3 (18)	.	.	.	no
N1	C2	H2	109.0 (13)	.	.	.	no
N1	C2	H2'	106.7 (13)	.	.	.	no
C3	C2	H2	107.6 (13)	.	.	.	no
C3	C2	H2'	110.6 (13)	.	.	.	no
H2	C2	H2'	110.2 (18)	.	.	.	no

N2	C3	H3	105.5 (12)	.	.	.	no
N2	C3	H3'	106.6 (13)	.	.	.	no
C2	C3	H3	108.0 (12)	.	.	.	no
C2	C3	H3'	112.7 (12)	.	.	.	no
H3	C3	H3'	110.5 (17)	.	.	.	no
N2	C4	H4	110.6 (12)	.	.	.	no
N2	C4	H4'	109.5 (13)	.	.	.	no
N2	C4	H4''	107.6 (13)	.	.	.	no
H4	C4	H4'	107.8 (17)	.	.	.	no
H4	C4	H4''	110.5 (17)	.	.	.	no
H4'	C4	H4''	110.9 (18)	.	.	.	no
N2	C5	H5	109.6 (12)	.	.	.	no
N2	C5	H5'	108.1 (11)	.	.	.	no
C6	C5	H5	110.8 (12)	.	.	.	no
C6	C5	H5'	109.1 (11)	.	.	.	no
H5	C5	H5'	104.6 (16)	.	.	.	no
C6	C7	H7	111.1 (14)	.	.	.	no
C6	C7	H7'	110.6 (14)	.	.	.	no
C6	C7	H7''	110.3 (12)	.	.	.	no
H7	C7	H7'	110 (2)	.	.	.	no
H7	C7	H7''	106.8 (19)	.	.	.	no
H7'	C7	H7''	108.1 (18)	.	.	.	no
N1	C8	H8	107.9 (11)	.	.	.	no
N1	C8	H8'	109.4 (12)	.	.	.	no
C6	C8	H8	109.8 (12)	.	.	.	no
C6	C8	H8'	109.5 (13)	.	.	.	no
H8	C8	H8'	106.0 (17)	.	.	.	no
N3	C9	H9	111.4 (13)	.	.	.	no
N3	C9	H9'	111.2 (14)	.	.	.	no
C10	C9	H9	111.2 (13)	.	.	.	no
C10	C9	H9'	112.5 (13)	.	.	.	no
H9	C9	H9'	103.8 (19)	.	.	.	no
C9	C10	H10	107.2 (15)	.	.	.	no
C9	C10	H10'	111.1 (15)	.	.	.	no
C11	C10	H10	113.5 (15)	.	.	.	no
C11	C10	H10'	112.8 (15)	.	.	.	no
H10	C10	H10'	107 (2)	.	.	.	no
C10	C11	H11	108.8 (12)	.	.	.	no
C10	C11	H11'	113.6 (14)	.	.	.	no
C12	C11	H11	109.4 (12)	.	.	.	no
C12	C11	H11'	113.6 (14)	.	.	.	no
H11	C11	H11'	108.0 (18)	.	.	.	no
N3	C12	H12	110.0 (13)	.	.	.	no
N3	C12	H12'	110.7 (13)	.	.	.	no
C11	C12	H12	113.4 (13)	.	.	.	no
C11	C12	H12'	109.5 (13)	.	.	.	no
H12	C12	H12'	109.9 (18)	.	.	.	no
Y	C13	H13	91.0 (16)	.	.	.	no
Y	C13	H13'	87 (2)	.	.	.	no
Si1	C13	H13	104.3 (16)	.	.	.	no
Si1	C13	H13'	105 (2)	.	.	.	no
H13	C13	H13'	104 (3)	.	.	.	no
Si1	C14	H14	110.0 (13)	.	.	.	no
Si1	C14	H14'	113.0 (16)	.	.	.	no
Si1	C14	H14''	111.6 (15)	.	.	.	no
H14	C14	H14'	107.1 (19)	.	.	.	no
H14	C14	H14''	104 (2)	.	.	.	no
H14'	C14	H14''	111 (2)	.	.	.	no
Si1	C15	H15	109.3 (15)	.	.	.	no
Si1	C15	H15'	110.7 (14)	.	.	.	no
Si1	C15	H15''	111.6 (14)	.	.	.	no

H15	C15	H15'	108(2)	.	.	.	no
H15	C15	H15"	111(2)	.	.	.	no
H15'	C15	H15"	107(2)	.	.	.	no
Si1	C16	H16	115.4(14)	.	.	.	no
Si1	C16	H16'	111.0(14)	.	.	.	no
Si1	C16	H16"	110.8(15)	.	.	.	no
H16	C16	H16'	107(2)	.	.	.	no
H16	C16	H16"	105.3(19)	.	.	.	no
H16'	C16	H16"	107(2)	.	.	.	no
Y	C17	H17	109.1(13)	.	.	.	no
Y	C17	H17'	103.3(13)	.	.	.	no
Si2	C17	H17	105.2(13)	.	.	.	no
Si2	C17	H17'	104.9(14)	.	.	.	no
H17	C17	H17'	108.2(19)	.	.	.	no
Si2	C18	H18	107.9(18)	.	.	.	no
Si2	C18	H18'	112.4(16)	.	.	.	no
Si2	C18	H18"	109.6(18)	.	.	.	no
H18	C18	H18'	103(2)	.	.	.	no
H18	C18	H18"	116(3)	.	.	.	no
H18'	C18	H18"	108(2)	.	.	.	no
Si2	C19	H19	108.8(15)	.	.	.	no
Si2	C19	H19'	113.1(16)	.	.	.	no
Si2	C19	H19"	112.1(14)	.	.	.	no
H19	C19	H19'	109(2)	.	.	.	no
H19	C19	H19"	111(2)	.	.	.	no
H19'	C19	H19"	103(2)	.	.	.	no
Si2	C20	H20	111.7(16)	.	.	.	no
Si2	C20	H20'	106.3(17)	.	.	.	no
Si2	C20	H20"	112.0(19)	.	.	.	no
H20	C20	H20'	111(2)	.	.	.	no
H20	C20	H20"	107(2)	.	.	.	no
H20'	C20	H20"	109(2)	.	.	.	no
Y	C21	H21	97.7(16)	.	.	.	no
Y	C21	H21'	108.8(14)	.	.	.	no
Si3	C21	H21	107.7(15)	.	.	.	no
Si3	C21	H21'	107.6(15)	.	.	.	no
H21	C21	H21'	104(2)	.	.	.	no
Si3	C22	H22	111.4(16)	.	.	.	no
Si3	C22	H22'	109.3(14)	.	.	.	no
Si3	C22	H22"	113.1(14)	.	.	.	no
H22	C22	H22'	112(2)	.	.	.	no
H22	C22	H22"	106(2)	.	.	.	no
H22'	C22	H22"	105(2)	.	.	.	no
Si3	C23	H23	113.2(16)	.	.	.	no
Si3	C23	H23'	112.4(16)	.	.	.	no
Si3	C23	H23"	111.9(15)	.	.	.	no
H23	C23	H23'	107(2)	.	.	.	no
H23	C23	H23"	108(2)	.	.	.	no
H23'	C23	H23"	104(2)	.	.	.	no
Si3	C24	H24	111.9(16)	.	.	.	no
Si3	C24	H24'	113.0(16)	.	.	.	no
Si3	C24	H24"	113.2(15)	.	.	.	no
H24	C24	H24'	105(2)	.	.	.	no
H24	C24	H24"	107(2)	.	.	.	no
H24'	C24	H24"	107(2)	.	.	.	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


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_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
N2      Y      N1      C1      167.63(15)      .      .      .      .      no
N2      Y      N1      C2      53.27(11)      .      .      .      .      no
N2      Y      N1      C8      -63.15(12)      .      .      .      .      no
N3      Y      N1      C1      -113.43(15)      .      .      .      .      no
N3      Y      N1      C2      132.21(12)      .      .      .      .      no
N3      Y      N1      C8      15.79(12)      .      .      .      .      no
C13     Y      N1      C1      85.00(15)      .      .      .      .      no
C13     Y      N1      C2      -29.36(13)      .      .      .      .      no
C13     Y      N1      C8      -145.78(13)      .      .      .      .      no
C17     Y      N1      C1      -142.29(16)      .      .      .      .      no
C17     Y      N1      C2      103.35(16)      .      .      .      .      no
C17     Y      N1      C8      -13.1(2)      .      .      .      .      no
C21     Y      N1      C1      -13.98(15)      .      .      .      .      no
C21     Y      N1      C2      -128.34(12)      .      .      .      .      no
C21     Y      N1      C8      115.24(13)      .      .      .      .      no
N1      Y      N2      C3      -44.85(11)      .      .      .      .      no
N1      Y      N2      C4      -163.74(14)      .      .      .      .      no
N1      Y      N2      C5      75.66(12)      .      .      .      .      no
N3      Y      N2      C3      -117.10(12)      .      .      .      .      no
N3      Y      N2      C4      124.01(14)      .      .      .      .      no
N3      Y      N2      C5      3.41(12)      .      .      .      .      no
C13     Y      N2      C3      57.82(13)      .      .      .      .      no
C13     Y      N2      C4      -61.07(14)      .      .      .      .      no
C13     Y      N2      C5      178.33(13)      .      .      .      .      no
C17     Y      N2      C3      157.54(12)      .      .      .      .      no
C17     Y      N2      C4      38.64(14)      .      .      .      .      no
C17     Y      N2      C5      -81.96(13)      .      .      .      .      no
C21     Y      N2      C3      -49.1(2)      .      .      .      .      no
C21     Y      N2      C4      -168.01(16)      .      .      .      .      no
C21     Y      N2      C5      71.4(2)      .      .      .      .      no
N1      Y      N3      C6      -40.69(11)      .      .      .      .      no
N1      Y      N3      C9      -164.10(14)      .      .      .      .      no
N1      Y      N3      C12     80.63(12)      .      .      .      .      no
N2      Y      N3      C6      28.43(11)      .      .      .      .      no
N2      Y      N3      C9      -94.98(13)      .      .      .      .      no
N2      Y      N3      C12     149.75(13)      .      .      .      .      no
C13     Y      N3      C6      14.9(2)      .      .      .      .      no
C13     Y      N3      C9      -108.6(2)      .      .      .      .      no
C13     Y      N3      C12     136.17(18)      .      .      .      .      no
C17     Y      N3      C6      125.51(12)      .      .      .      .      no
C17     Y      N3      C9      2.10(13)      .      .      .      .      no
C17     Y      N3      C12     -113.18(12)      .      .      .      .      no
C21     Y      N3      C6      -130.79(11)      .      .      .      .      no
C21     Y      N3      C9      105.80(13)      .      .      .      .      no
C21     Y      N3      C12     -9.47(13)      .      .      .      .      no
N1      Y      C13     Si1      30.2(3)      .      .      .      .      no
N2      Y      C13     Si1      -32.6(3)      .      .      .      .      no
N3      Y      C13     Si1      -19.8(5)      .      .      .      .      no
C17     Y      C13     Si1      -128.2(3)      .      .      .      .      no
C21     Y      C13     Si1      126.1(3)      .      .      .      .      no
N1      Y      C17     Si2      -154.91(9)      .      .      .      .      no
N2      Y      C17     Si2      -111.21(13)      .      .      .      .      no
N3      Y      C17     Si2      178.91(13)      .      .      .      .      no
C13     Y      C17     Si2      -22.07(14)      .      .      .      .      no
C21     Y      C17     Si2      78.81(14)      .      .      .      .      no

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N1	Y	C21	Si3	89.63 (13)	.	.	.	.	no
N2	Y	C21	Si3	93.46 (19)	.	.	.	.	no
N3	Y	C21	Si3	155.97 (12)	.	.	.	.	no
C13	Y	C21	Si3	-11.62 (14)	.	.	.	.	no
C17	Y	C21	Si3	-113.91 (13)	.	.	.	.	no
C14	Si1	C13	Y	-174.4 (3)	.	.	.	.	no
C15	Si1	C13	Y	-55.2 (4)	.	.	.	.	no
C16	Si1	C13	Y	65.3 (4)	.	.	.	.	no
C18	Si2	C17	Y	-168.03 (13)	.	.	.	.	no
C19	Si2	C17	Y	-48.82 (16)	.	.	.	.	no
C20	Si2	C17	Y	72.55 (16)	.	.	.	.	no
C22	Si3	C21	Y	-175.14 (12)	.	.	.	.	no
C23	Si3	C21	Y	63.56 (16)	.	.	.	.	no
C24	Si3	C21	Y	-55.83 (16)	.	.	.	.	no
Y	N1	C2	C3	-59.92 (17)	.	.	.	.	no
C1	N1	C2	C3	179.14 (17)	.	.	.	.	no
C8	N1	C2	C3	59.3 (2)	.	.	.	.	no
Y	N1	C8	C6	12.2 (2)	.	.	.	.	no
C1	N1	C8	C6	144.51 (17)	.	.	.	.	no
C2	N1	C8	C6	-97.00 (19)	.	.	.	.	no
Y	N2	C3	C2	29.74 (19)	.	.	.	.	no
C4	N2	C3	C2	150.08 (18)	.	.	.	.	no
C5	N2	C3	C2	-90.4 (2)	.	.	.	.	no
Y	N2	C5	C6	-37.10 (19)	.	.	.	.	no
C3	N2	C5	C6	81.9 (2)	.	.	.	.	no
C4	N2	C5	C6	-158.83 (17)	.	.	.	.	no
Y	N3	C6	C5	-56.92 (15)	.	.	.	.	no
Y	N3	C6	C7	-176.05 (14)	.	.	.	.	no
Y	N3	C6	C8	64.18 (15)	.	.	.	.	no
C9	N3	C6	C5	67.8 (2)	.	.	.	.	no
C9	N3	C6	C7	-51.3 (2)	.	.	.	.	no
C9	N3	C6	C8	-171.08 (16)	.	.	.	.	no
C12	N3	C6	C5	-173.46 (16)	.	.	.	.	no
C12	N3	C6	C7	67.4 (2)	.	.	.	.	no
C12	N3	C6	C8	-52.4 (2)	.	.	.	.	no
Y	N3	C9	C10	-91.84 (17)	.	.	.	.	no
C6	N3	C9	C10	150.08 (17)	.	.	.	.	no
C12	N3	C9	C10	25.5 (2)	.	.	.	.	no
Y	N3	C12	C11	81.89 (15)	.	.	.	.	no
C6	N3	C12	C11	-164.08 (16)	.	.	.	.	no
C9	N3	C12	C11	-40.4 (2)	.	.	.	.	no
N1	C2	C3	N2	23.1 (2)	.	.	.	.	no
N2	C5	C6	N3	68.1 (2)	.	.	.	.	no
N2	C5	C6	C7	-168.33 (17)	.	.	.	.	no
N2	C5	C6	C8	-50.7 (2)	.	.	.	.	no
N3	C6	C8	N1	-53.5 (2)	.	.	.	.	no
C5	C6	C8	N1	64.5 (2)	.	.	.	.	no
C7	C6	C8	N1	-177.68 (16)	.	.	.	.	no
N3	C9	C10	C11	-0.7 (2)	.	.	.	.	no
C9	C10	C11	C12	-23.8 (2)	.	.	.	.	no
C10	C11	C12	N3	39.8 (2)	.	.	.	.	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	H11	3.34 (2)	.	.	.	.	no
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Si1	H2'	3.43 (2)	.	.	.	.	no
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Si1	H3	3.40 (2)	.	.	no
Si2	H13	3.23 (3)	.	.	no
Si3	H13 '	3.27 (3)	.	.	no
N1	N2	2.746 (2)	.	.	no
N1	N3	2.894 (2)	.	.	no
N1	C3	2.507 (3)	.	.	no
N1	C5	3.082 (3)	.	.	no
N1	C6	2.526 (3)	.	.	no
N1	C12	3.303 (3)	.	.	no
N2	C2	2.518 (3)	.	.	no
N2	N1	2.746 (2)	.	.	no
N2	N3	3.015 (2)	.	.	no
N2	C13	3.448 (3)	.	.	no
N2	C6	2.526 (3)	.	.	no
N2	C8	2.955 (3)	.	.	no
N3	N1	2.894 (2)	.	.	no
N3	C8	2.462 (3)	.	.	no
N3	N2	3.015 (2)	.	.	no
N3	C5	2.442 (3)	.	.	no
N1	H12	2.82 (2)	.	.	no
C13	N2	3.448 (3)	.	.	no
C13	C2	3.532 (3)	.	.	no
C13	C3	3.575 (3)	.	.	no
C17	C9	3.383 (3)	.	.	no
C1	H12	2.98 (2)	.	.	no
C1	H4 "	3.00 (2)	.	7_555	no
C3	H11	3.054 (19)	.	6_555	no
C3	H8 '	2.81 (2)	.	.	no
C4	H24	2.92 (3)	.	7_545	no
C5	H9	3.02 (2)	.	.	no
C5	H9 '	2.91 (2)	.	.	no
C7	H9	2.52 (2)	.	.	no
C7	H12 '	2.79 (2)	.	.	no
C8	H12	2.69 (2)	.	.	no
C8	H3 '	3.03 (2)	.	.	no
C8	H12 '	3.02 (2)	.	.	no
C9	H7 "	2.81 (2)	.	.	no
C9	H7	3.07 (2)	.	.	no
C9	H17	3.09 (2)	.	.	no
C9	H5 '	2.580 (19)	.	.	no
C12	H7	2.81 (2)	.	.	no
C12	H8	2.613 (19)	.	.	no
C13	H2 '	2.96 (2)	.	.	no
C13	H4 '	3.08 (2)	.	.	no
C15	H2 '	2.96 (2)	.	.	no
C16	H4 '	2.98 (2)	.	.	no
C16	H9	2.92 (2)	.	2_554	no
C17	H9 '	2.77 (2)	.	.	no
C20	H13	3.06 (3)	.	.	no
C21	H11	2.89 (2)	.	.	no
C23	H15 '	3.00 (2)	.	3_455	no
C24	H1 '	2.87 (2)	.	.	no
H1	H8	2.26 (3)	.	.	no
H1	H12	2.32 (3)	.	.	no
H1 '	C24	2.87 (2)	.	.	no
H1 '	H2 '	2.32 (3)	.	.	no
H1 '	H24	2.40 (4)	.	.	no
H1 '	H24 "	2.60 (3)	.	.	no
H1 "	H2	2.39 (3)	.	.	no
H1 "	H8	2.49 (3)	.	.	no
H2	H1 "	2.39 (3)	.	.	no

H2	H8'	2.28 (3)	.	.	no
H2'	Si1	3.43 (2)	.	.	no
H2'	C13	2.96 (2)	.	.	no
H2'	C15	2.96 (2)	.	.	no
H2'	H1'	2.32 (3)	.	.	no
H2'	H15"	2.45 (3)	.	.	no
H3	Si1	3.40 (2)	.	.	no
H3	H4	2.50 (3)	.	.	no
H3	H4'	2.20 (3)	.	.	no
H3	H16	2.41 (3)	.	.	no
H3'	C8	3.03 (2)	.	.	no
H3'	H5	2.12 (3)	.	.	no
H4	H3	2.50 (3)	.	.	no
H4	H5	2.59 (3)	.	.	no
H4'	C13	3.08 (2)	.	.	no
H4'	C16	2.98 (2)	.	.	no
H4'	H3	2.20 (3)	.	.	no
H4'	H16	2.51 (3)	.	.	no
H4'	H24	2.56 (3)	.	7_545	no
H4"	H5'	2.20 (3)	.	.	no
H4"	H17	2.52 (3)	.	.	no
H4"	C1	3.00 (2)	.	7_545	no
H5	H3'	2.12 (3)	.	.	no
H5	H4	2.59 (3)	.	.	no
H5	H7'	2.52 (3)	.	.	no
H5	H7"	2.59 (3)	.	.	no
H5	H19	2.36 (3)	.	6_555	no
H5'	C9	2.580 (19)	.	.	no
H5'	H4"	2.20 (3)	.	.	no
H5'	H7"	2.47 (3)	.	.	no
H5'	H9	2.52 (3)	.	.	no
H5'	H9'	2.29 (3)	.	.	no
H7	C9	3.07 (2)	.	.	no
H7	C12	2.81 (2)	.	.	no
H7	H8	2.59 (3)	.	.	no
H7	H12'	2.20 (3)	.	.	no
H7'	H5	2.52 (3)	.	.	no
H7'	H8'	2.37 (3)	.	.	no
H7"	C9	2.81 (2)	.	.	no
H7"	H5	2.59 (3)	.	.	no
H7"	H5'	2.47 (3)	.	.	no
H7"	H9	2.11 (3)	.	.	no
H7"	H14	2.59 (3)	.	2_555	no
H8	C12	2.613 (19)	.	.	no
H8	H1	2.26 (3)	.	.	no
H8	H1"	2.49 (3)	.	.	no
H8	H7	2.59 (3)	.	.	no
H8	H12	2.31 (3)	.	.	no
H8	H12'	2.56 (3)	.	.	no
H8'	C3	2.81 (2)	.	.	no
H8'	H2	2.28 (3)	.	.	no
H8'	H7'	2.37 (3)	.	.	no
H9	C5	3.02 (2)	.	.	no
H9	C7	2.52 (2)	.	.	no
H9	H5'	2.52 (3)	.	.	no
H9	H7"	2.11 (3)	.	.	no
H9	C16	2.92 (2)	.	2_555	no
H9	H16'	2.39 (3)	.	2_555	no
H9'	C5	2.91 (2)	.	.	no
H9'	C17	2.77 (2)	.	.	no
H9'	H5'	2.29 (3)	.	.	no

H9'	H17	2.30 (3)	.	.	no
H11	Y	3.34 (2)	.	.	no
H11	C21	2.89 (2)	.	.	no
H11	H21	2.53 (3)	.	.	no
H11	H21'	2.57 (3)	.	.	no
H11	C3	3.054 (19)	.	6_455	no
H11'	H15"	2.50 (3)	.	6_455	no
H12	N1	2.82 (2)	.	.	no
H12	C1	2.98 (2)	.	.	no
H12	C8	2.69 (2)	.	.	no
H12	H1	2.32 (3)	.	.	no
H12	H8	2.31 (3)	.	.	no
H12	H21'	2.56 (3)	.	.	no
H12'	C7	2.79 (2)	.	.	no
H12'	C8	3.02 (2)	.	.	no
H12'	H7	2.20 (3)	.	.	no
H12'	H8	2.56 (3)	.	.	no
H13	Si2	3.23 (3)	.	.	no
H13	C20	3.06 (3)	.	.	no
H13	H20	2.30 (4)	.	.	no
H13'	Si3	3.27 (3)	.	.	no
H13'	H23	2.47 (4)	.	.	no
H14	H7"	2.59 (3)	.	2_554	no
H15'	C23	3.00 (2)	.	3_555	no
H15'	H23'	2.56 (4)	.	3_555	no
H15"	H2'	2.45 (3)	.	.	no
H15"	H11'	2.50 (3)	.	6_555	no
H16	H3	2.41 (3)	.	.	no
H16	H4'	2.51 (3)	.	.	no
H16'	H9	2.39 (3)	.	2_554	no
H16"	H24'	2.54 (4)	.	7_545	no
H17	C9	3.09 (2)	.	.	no
H17	H4"	2.52 (3)	.	.	no
H17	H9'	2.30 (3)	.	.	no
H19	H5	2.36 (3)	.	6_455	no
H19'	H19"	2.56 (3)	.	5_555	no
H19"	H19'	2.56 (3)	.	5_555	no
H20	H13	2.30 (4)	.	.	no
H21	H11	2.53 (3)	.	.	no
H21'	H11	2.57 (3)	.	.	no
H21'	H12	2.56 (3)	.	.	no
H23	H13'	2.47 (4)	.	.	no
H23'	H15'	2.56 (4)	.	3_455	no
H24	H1'	2.40 (4)	.	.	no
H24	C4	2.92 (3)	.	7_555	no
H24	H4'	2.56 (3)	.	7_555	no
H24'	H16"	2.54 (4)	.	7_555	no
H24"	H1'	2.60 (3)	.	.	no

#===END of Crystallographic Information File