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Neutral and cationic yttrium alkyl complexes with linked 1,4,7- triazacyclononane-amide monoanionic ancillary ligands: synthesis and catalytic ethene polymerisation

de Araujo Bambirra, S.; van Leusen, D.; Meetsma, A.; Hessen, B.; Teuben, J.H

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1. SUBMISSION DETAILS

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Dr. B. Hessen

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3. TITLE AND AUTHOR LIST

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Neutral and cationic yttrium alkyl complexes with linked 1,4,7-
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synthesis and catalytic ethene polymerisation
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# The loop structure below should contain the names and addresses of all
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  _publ_author_address

'Bambirra, Sergio'
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'Leusen, Daan van'

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'Teuben, Jan H.'
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Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.
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Beurskens, P.T., Beurskens, G., Gelder, R. de
Garc\'ia-Granda, S., Gould, R.O., Israel, & Smits, J.M.M. (1999).
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University, The Netherlands.

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

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

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

Fig. 4. Perspective ORTEP drawing of the title compound.
 All non-hydrogen atoms are represented by thermal vibrational
 ellipsoids drawn to encompass 50% of the electron density.
 The hydrogen atoms are omitted for sake of clarity.

```

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data_c26h61n4

_database_code_CSD      157466

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# 5. CHEMICAL DATA

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_chemical_formula_moiety
'C26 H61 N4 Si2 Y'
_chemical_formula_structural      ?
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_sum
'C26 H61 N4 Si2 Y'
_chemical_formula_weight      574.87
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loop_
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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'
N   N     0.0061    0.0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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C   C     0.0033    0.0016
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# 6. CRYSTAL DATA

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_symmetry_space_group_name_H-M   'P -1'

loop_
_symmetry_equiv_pos_as_xyz
x,y,z

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-x,-y,-z

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_cell_length_b 9.859(1)
_cell_length_c 17.291(3)
_cell_angle_alpha 95.60(1)
_cell_angle_beta 90.68(1)
_cell_angle_gamma 98.63(1)
_cell_volume 1645.7(4)
_cell_formula_units_Z 2
_cell_measurement_temperature 130
_cell_measurement_reflns_used 22
_cell_measurement_theta_min 9.36
_cell_measurement_theta_max 16.17
_cell_special_details
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Unit cell parameters (Duisenberg, 1992) and orientation matrix were determined from a least-squares treatment of SET4 (de Boer & Duisenberg, 1984) setting. Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

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_diffrn_radiation_monochromator 'perpendicular mounted graphite'
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;
scintillation NaI crystal with photomultiplier
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Enraf Nonius CAD-4F diffractometer
;
_diffrn_measurement_method '\w/2\q'
_diffrn_special_details

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;
Crystal into the cold nitrogen stream of the low-temperature unit
(Bolhuis, 1971), on an Enraf-Nonius CAD-4F diffractometer.
Graphite-monochromated Mo K $\alpha$  radiation,
\w/2\q scan, \D\w = (1.05 + 0.34 tg \q)\%.
;
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_diffrn_standard_refl_index_l
2 2 2
1 -1 4

# number of measured reflections (redundant set)
_diffrn_reflns_number                 6832
_diffrn_reflns_av_R_equivalents       0.0653
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_diffrn_reflns_limit_l_max            21
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_diffrn_reflns_theta_max              26.00
_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization effects, scale
variation, but not for absorption and reduced to  $F_o^2$ 
;

# number of unique reflections
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_reflns_number_gt                     3940
_reflns_threshold_expression          >2sigma(I)

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_computing_cell_refinement             'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction              'HELENA (Spek, 1997)'
_computing_structure_solution
;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement        'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
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PLUTO (Meetsma, 1999)
ORTEP (Furrugia, 1998; Burnett et al., 1996)
PLATON (Spek, 1994, 1996)
;
_computing_publication_material        'PLATON (Spek, 1990)'

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# 8. REFINEMENT DATA

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Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ 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.

;

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_refine_ls_weighting_scheme
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_refine_ls_restrained_S_all 1.016
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_atom_site_fract_z

_atom_site_occupancy

_atom_site_U_iso_or_equiv

Y1	Y	Uani	0.11240(6)	0.34085(6)	0.24472(4)	1.000	0.0227(2)
Si1	Si	Uani	0.2811(2)	0.1473(2)	0.06587(11)	1.000	0.0340(6)
Si2	Si	Uani	0.3159(2)	0.1893(2)	0.41542(11)	1.000	0.0353(7)
N1	N	Uani	0.2226(5)	0.5532(5)	0.2799(3)	1.000	0.0258(17)
N2	N	Uani	-0.0410(5)	0.4621(5)	0.3368(3)	1.000	0.0246(17)
N3	N	Uani	-0.0922(5)	0.1666(5)	0.2897(3)	1.000	0.0273(17)
N4	N	Uani	-0.1330(5)	0.3786(5)	0.1792(3)	1.000	0.0261(17)
C1	C	Uani	0.3906(7)	0.5396(7)	0.1781(4)	1.000	0.044(3)
C2	C	Uani	0.3462(8)	0.7698(8)	0.2331(5)	1.000	0.058(3)
C3	C	Uani	0.4720(7)	0.6301(9)	0.3134(5)	1.000	0.055(3)
C4	C	Uani	0.3554(6)	0.6248(6)	0.2526(4)	1.000	0.032(2)
C5	C	Uani	0.1727(7)	0.6349(6)	0.3456(4)	1.000	0.032(2)
C6	C	Uani	0.0647(7)	0.5472(7)	0.3887(4)	1.000	0.033(2)
C7	C	Uani	-0.1353(7)	0.3685(6)	0.3816(4)	1.000	0.031(2)

C8	C	Uani	-0.1029(7)	0.2228(6)	0.3721(4)	1.000	0.032(2)
C9	C	Uani	-0.0533(8)	0.0238(7)	0.2882(4)	1.000	0.037(2)
C10	C	Uani	-0.1604(10)	-0.0812(8)	0.3233(5)	1.000	0.067(4)
C11	C	Uani	-0.0187(8)	-0.0307(7)	0.2079(4)	1.000	0.049(3)
C12	C	Uani	-0.2201(7)	0.1650(7)	0.2439(4)	1.000	0.039(2)
C13	C	Uani	-0.2013(7)	0.2344(7)	0.1697(4)	1.000	0.034(2)
C14	C	Uani	-0.1151(7)	0.4307(7)	0.1015(4)	1.000	0.035(2)
C15	C	Uani	-0.2481(7)	0.4286(8)	0.0530(4)	1.000	0.044(3)
C16	C	Uani	-0.0314(7)	0.5752(7)	0.1091(4)	1.000	0.041(3)
C17	C	Uani	-0.2107(6)	0.4669(7)	0.2302(4)	1.000	0.032(2)
C18	C	Uani	-0.1200(7)	0.5494(6)	0.2944(4)	1.000	0.032(2)
C19	C	Uani	0.1564(6)	0.2516(6)	0.1099(3)	1.000	0.0258(19)
C20	C	Uani	0.2007(8)	-0.0333(8)	0.0355(5)	1.000	0.064(3)
C21	C	Uani	0.3584(11)	0.2166(11)	-0.0226(5)	1.000	0.094(5)
C22	C	Uani	0.4267(8)	0.1304(9)	0.1318(5)	1.000	0.060(3)
C23	C	Uani	0.2623(7)	0.2235(7)	0.3180(4)	1.000	0.033(2)
C24	C	Uani	0.5018(8)	0.1670(10)	0.4230(5)	1.000	0.067(4)
C25	C	Uani	0.2148(9)	0.0276(8)	0.4473(5)	1.000	0.055(3)
C26	C	Uani	0.2949(9)	0.3318(8)	0.4910(4)	1.000	0.058(3)
H1	H	Uiso	0.39302	0.44429	0.18907	1.000	0.0655
H1'	H	Uiso	0.48091	0.57946	0.16035	1.000	0.0655
H1''	H	Uiso	0.32028	0.54079	0.13760	1.000	0.0655
H2	H	Uiso	0.26703	0.76783	0.19777	1.000	0.0861
H2'	H	Uiso	0.43091	0.80685	0.20808	1.000	0.0861
H2''	H	Uiso	0.33480	0.82849	0.28100	1.000	0.0861
H3	H	Uiso	0.45489	0.69070	0.35944	1.000	0.0830
H3'	H	Uiso	0.56013	0.66587	0.29137	1.000	0.0830
H3''	H	Uiso	0.47524	0.53708	0.32806	1.000	0.0830
H5	H	Uiso	0.13251	0.71214	0.32652	1.000	0.0388
H5'	H	Uiso	0.25093	0.67442	0.38156	1.000	0.0388
H6	H	Uiso	0.11072	0.48620	0.41914	1.000	0.0392
H6'	H	Uiso	0.01951	0.60815	0.42571	1.000	0.0392
H7	H	Uiso	-0.23151	0.36817	0.36369	1.000	0.0372
H7'	H	Uiso	-0.12733	0.40355	0.43731	1.000	0.0372
H8	H	Uiso	-0.01473	0.22062	0.39996	1.000	0.0386
H8'	H	Uiso	-0.17590	0.16226	0.39675	1.000	0.0386
H9	H	Uiso	0.03285	0.03284	0.32097	1.000	0.0446
H10	H	Uiso	-0.24794	-0.09110	0.29393	1.000	0.1004
H10'	H	Uiso	-0.17420	-0.04892	0.37768	1.000	0.1004
H10''	H	Uiso	-0.12751	-0.17052	0.32076	1.000	0.1004
H11	H	Uiso	-0.10091	-0.04210	0.17371	1.000	0.0738
H11'	H	Uiso	0.01288	-0.12006	0.20974	1.000	0.0738
H11''	H	Uiso	0.05438	0.03439	0.18768	1.000	0.0738
H12	H	Uiso	-0.28499	0.21109	0.27686	1.000	0.0463
H12'	H	Uiso	-0.26313	0.06797	0.23061	1.000	0.0463
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H15'	H	Uiso	-0.22531	0.46998	0.00457	1.000	0.0658
H15''	H	Uiso	-0.31052	0.48143	0.08267	1.000	0.0658
H16	H	Uiso	-0.00467	0.60066	0.05739	1.000	0.0613
H16'	H	Uiso	0.05145	0.57650	0.14146	1.000	0.0613
H16''	H	Uiso	-0.08745	0.64127	0.13324	1.000	0.0613
H17	H	Uiso	-0.28748	0.40845	0.25318	1.000	0.0384
H17'	H	Uiso	-0.25076	0.53063	0.19880	1.000	0.0384
H18	H	Uiso	-0.05499	0.62103	0.27205	1.000	0.0387
H18'	H	Uiso	-0.17801	0.59656	0.33146	1.000	0.0387
H19	H	Uiso	0.06599	0.19992	0.09091	1.000	0.0315
H19'	H	Uiso	0.16972	0.33523	0.08181	1.000	0.0315
H20	H	Uiso	0.16851	-0.07839	0.08144	1.000	0.0957
H20'	H	Uiso	0.26879	-0.08348	0.00925	1.000	0.0957
H20''	H	Uiso	0.12233	-0.03331	-0.00015	1.000	0.0957
H21	H	Uiso	0.28480	0.22569	-0.05973	1.000	0.1408

H21'	H	Uiso	0.41756	0.15342	-0.04653	1.000	0.1408
H21"	H	Uiso	0.41344	0.30719	-0.00826	1.000	0.1408
H22	H	Uiso	0.47535	0.22229	0.15028	1.000	0.0899
H22'	H	Uiso	0.49051	0.07715	0.10367	1.000	0.0899
H22"	H	Uiso	0.39130	0.08289	0.17631	1.000	0.0899
H23	H	Uiso	0.23858	0.12818	0.29269	1.000	0.0397
H23'	H	Uiso	0.35271	0.25784	0.29667	1.000	0.0397
H24	H	Uiso	0.52131	0.09702	0.38210	1.000	0.1009
H24'	H	Uiso	0.52101	0.13754	0.47400	1.000	0.1009
H24"	H	Uiso	0.56027	0.25483	0.41683	1.000	0.1009
H25	H	Uiso	0.11986	0.04254	0.45751	1.000	0.0823
H25'	H	Uiso	0.25752	0.00428	0.49471	1.000	0.0823
H25"	H	Uiso	0.21417	-0.04824	0.40609	1.000	0.0823
H26	H	Uiso	0.33063	0.42045	0.47208	1.000	0.0862
H26'	H	Uiso	0.34603	0.32110	0.53850	1.000	0.0862
H26"	H	Uiso	0.19695	0.32895	0.50228	1.000	0.0862

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

Y1	0.0210(3)	0.0231(3)	0.0240(3)	-0.0026(2)	0.0023(2)	0.0067(2)
Si1	0.0317(11)	0.0377(11)	0.0333(11)	-0.0067(9)	0.0040(9)	0.0142(9)
Si2	0.0293(11)	0.0449(12)	0.0358(11)	0.0087(9)	0.0053(9)	0.0157(9)
N1	0.023(3)	0.026(3)	0.028(3)	-0.005(2)	0.000(2)	0.007(2)
N2	0.031(3)	0.022(3)	0.021(3)	-0.002(2)	0.001(2)	0.007(2)
N3	0.022(3)	0.023(3)	0.038(3)	0.002(2)	0.010(2)	0.007(2)
N4	0.025(3)	0.031(3)	0.023(3)	-0.007(2)	0.001(2)	0.013(2)
C1	0.025(4)	0.051(5)	0.053(5)	0.002(4)	0.015(3)	0.000(3)
C2	0.046(5)	0.039(5)	0.087(7)	0.013(4)	0.022(5)	-0.002(4)
C3	0.025(4)	0.071(6)	0.064(5)	-0.010(4)	-0.003(4)	0.001(4)
C4	0.017(3)	0.028(4)	0.051(4)	-0.002(3)	0.003(3)	0.003(3)
C5	0.034(4)	0.026(3)	0.035(4)	-0.007(3)	-0.004(3)	0.005(3)
C6	0.036(4)	0.032(4)	0.030(4)	-0.009(3)	0.005(3)	0.014(3)
C7	0.030(4)	0.034(4)	0.029(4)	-0.003(3)	0.009(3)	0.007(3)
C8	0.036(4)	0.032(4)	0.030(4)	0.007(3)	0.005(3)	0.007(3)
C9	0.045(4)	0.027(4)	0.041(4)	0.004(3)	0.008(3)	0.008(3)
C10	0.081(7)	0.029(4)	0.091(7)	0.014(4)	0.033(6)	0.004(4)
C11	0.058(5)	0.032(4)	0.057(5)	-0.011(4)	0.015(4)	0.013(4)
C12	0.032(4)	0.031(4)	0.048(4)	-0.009(3)	0.001(3)	-0.003(3)
C13	0.027(4)	0.036(4)	0.036(4)	-0.008(3)	-0.004(3)	0.002(3)
C14	0.028(4)	0.047(4)	0.031(4)	-0.003(3)	-0.001(3)	0.012(3)
C15	0.037(4)	0.057(5)	0.041(4)	0.002(4)	-0.008(3)	0.022(4)
C16	0.037(4)	0.053(5)	0.037(4)	0.009(3)	-0.001(3)	0.017(4)
C17	0.023(4)	0.039(4)	0.035(4)	-0.001(3)	0.001(3)	0.012(3)
C18	0.035(4)	0.028(4)	0.035(4)	-0.004(3)	0.007(3)	0.012(3)
C19	0.020(3)	0.031(4)	0.027(3)	0.000(3)	0.004(3)	0.007(3)
C20	0.041(5)	0.057(5)	0.089(7)	-0.035(5)	-0.004(5)	0.019(4)
C21	0.126(9)	0.118(9)	0.066(6)	0.041(6)	0.078(7)	0.085(8)
C22	0.032(4)	0.067(6)	0.078(6)	-0.030(5)	-0.006(4)	0.022(4)
C23	0.036(4)	0.033(4)	0.031(4)	0.006(3)	0.001(3)	0.006(3)
C24	0.045(5)	0.109(8)	0.062(6)	0.035(5)	0.010(4)	0.041(5)
C25	0.063(6)	0.055(5)	0.051(5)	0.016(4)	0.001(4)	0.017(4)
C26	0.057(6)	0.064(6)	0.052(5)	-0.012(4)	-0.016(4)	0.021(4)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

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;
Bond distances, angles etc. have been calculated using the
rounded fractional coordinates. All esds are estimated
from the variances of the (full) variance-covariance matrix.
The cell esds are taken into account in the estimation of
distances, angles and torsion angles
;

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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
Y1      N1      2.231(5)      .      .      yes
Y1      N2      2.541(5)      .      .      yes
Y1      N3      2.618(5)      .      .      yes
Y1      N4      2.740(5)      .      .      yes
Y1      C19     2.476(5)      .      .      yes
Y1      C23     2.421(7)      .      .      yes
Si1     C19     1.839(6)      .      .      yes
Si1     C20     1.859(8)      .      .      yes
Si1     C21     1.860(10)     .      .      yes
Si1     C22     1.855(8)      .      .      yes
Si2     C23     1.836(7)      .      .      yes
Si2     C24     1.875(8)      .      .      yes
Si2     C25     1.881(8)      .      .      yes
Si2     C26     1.860(8)      .      .      yes
N1      C4      1.491(8)      .      .      yes
N1      C5      1.460(8)      .      .      yes
N2      C6      1.468(9)      .      .      yes
N2      C7      1.486(8)      .      .      yes
N2      C18     1.480(8)      .      .      yes
N3      C8      1.488(9)      .      .      yes
N3      C9      1.511(9)      .      .      yes
N3      C12     1.474(9)      .      .      yes
N4      C13     1.471(8)      .      .      yes
N4      C14     1.488(9)      .      .      yes
N4      C17     1.477(8)      .      .      yes
C1      C4      1.540(10)     .      .      no
C2      C4      1.516(10)     .      .      no
C3      C4      1.536(10)     .      .      no
C5      C6      1.515(10)     .      .      no
C7      C8      1.511(9)      .      .      no
C9      C10     1.535(11)     .      .      no
C9      C11     1.501(10)     .      .      no
C12     C13     1.512(10)     .      .      no
C14     C15     1.540(10)     .      .      no
C14     C16     1.527(10)     .      .      no
C17     C18     1.506(9)      .      .      no
C1      H1      0.9802      .      .      no
C1      H1'     0.9797      .      .      no
C1      H1"     0.9795      .      .      no
C2      H2      0.9794      .      .      no
C2      H2'     0.9798      .      .      no
C2      H2"     0.9805      .      .      no
C3      H3      0.9795      .      .      no
C3      H3'     0.9799      .      .      no
C3      H3"     0.9799      .      .      no
C5      H5      0.9902      .      .      no
C5      H5'     0.9897      .      .      no
C6      H6      0.9901      .      .      no
C6      H6'     0.9895      .      .      no

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C7	H7	0.9897	.	.	no
C7	H7'	0.9892	.	.	no
C8	H8	0.9895	.	.	no
C8	H8'	0.9899	.	.	no
C9	H9	1.0001	.	.	no
C10	H10	0.9800	.	.	no
C10	H10'	0.9805	.	.	no
C10	H10"	0.9796	.	.	no
C11	H11	0.9807	.	.	no
C11	H11'	0.9800	.	.	no
C11	H11"	0.9799	.	.	no
C12	H12	0.9909	.	.	no
C12	H12'	0.9899	.	.	no
C13	H13	0.9901	.	.	no
C13	H13'	0.9904	.	.	no
C14	H14	0.9996	.	.	no
C15	H15	0.9799	.	.	no
C15	H15'	0.9805	.	.	no
C15	H15"	0.9803	.	.	no
C16	H16	0.9802	.	.	no
C16	H16'	0.9794	.	.	no
C16	H16"	0.9804	.	.	no
C17	H17	0.9896	.	.	no
C17	H17'	0.9899	.	.	no
C18	H18	0.9895	.	.	no
C18	H18'	0.9904	.	.	no
C19	H19	0.9897	.	.	no
C19	H19'	0.9900	.	.	no
C20	H20	0.9804	.	.	no
C20	H20'	0.9798	.	.	no
C20	H20"	0.9800	.	.	no
C21	H21	0.9807	.	.	no
C21	H21'	0.9800	.	.	no
C21	H21"	0.9797	.	.	no
C22	H22	0.9803	.	.	no
C22	H22'	0.9801	.	.	no
C22	H22"	0.9800	.	.	no
C23	H23	0.9902	.	.	no
C23	H23'	0.9900	.	.	no
C24	H24	0.9800	.	.	no
C24	H24'	0.9798	.	.	no
C24	H24"	0.9802	.	.	no
C25	H25	0.9804	.	.	no
C25	H25'	0.9789	.	.	no
C25	H25"	0.9805	.	.	no
C26	H26	0.9800	.	.	no
C26	H26'	0.9801	.	.	no
C26	H26"	0.9800	.	.	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

N1	Y1	N2	72.38(17)	.	.	.	yes
N1	Y1	N3	139.45(17)	.	.	.	yes
N1	Y1	N4	104.95(17)	.	.	.	yes
N1	Y1	C19	113.81(19)	.	.	.	yes
N1	Y1	C23	95.9(2)	.	.	.	yes
N2	Y1	N3	68.77(16)	.	.	.	yes

N2	Y1	N4	65.54(16)	.	.	.	yes
N2	Y1	C19	147.91(18)	.	.	.	yes
N2	Y1	C23	109.8(2)	.	.	.	yes
N3	Y1	N4	68.88(15)	.	.	.	yes
N3	Y1	C19	105.26(18)	.	.	.	yes
N3	Y1	C23	86.7(2)	.	.	.	yes
N4	Y1	C19	82.74(17)	.	.	.	yes
N4	Y1	C23	155.3(2)	.	.	.	yes
C19	Y1	C23	101.1(2)	.	.	.	yes
C19	Si1	C20	112.1(3)	.	.	.	yes
C19	Si1	C21	112.5(4)	.	.	.	yes
C19	Si1	C22	114.3(3)	.	.	.	yes
C20	Si1	C21	106.3(4)	.	.	.	yes
C20	Si1	C22	104.4(4)	.	.	.	yes
C21	Si1	C22	106.6(4)	.	.	.	yes
C23	Si2	C24	113.4(4)	.	.	.	yes
C23	Si2	C25	112.4(4)	.	.	.	yes
C23	Si2	C26	112.5(3)	.	.	.	yes
C24	Si2	C25	105.8(4)	.	.	.	yes
C24	Si2	C26	105.3(4)	.	.	.	yes
C25	Si2	C26	106.8(4)	.	.	.	yes
Y1	N1	C4	129.8(4)	.	.	.	yes
Y1	N1	C5	119.0(4)	.	.	.	yes
C4	N1	C5	110.8(5)	.	.	.	yes
Y1	N2	C6	99.8(4)	.	.	.	yes
Y1	N2	C7	114.5(4)	.	.	.	yes
Y1	N2	C18	110.5(4)	.	.	.	yes
C6	N2	C7	110.4(5)	.	.	.	yes
C6	N2	C18	110.9(5)	.	.	.	yes
C7	N2	C18	110.3(5)	.	.	.	yes
Y1	N3	C8	100.9(3)	.	.	.	yes
Y1	N3	C9	110.8(4)	.	.	.	yes
Y1	N3	C12	112.3(4)	.	.	.	yes
C8	N3	C9	108.7(5)	.	.	.	yes
C8	N3	C12	112.4(5)	.	.	.	yes
C9	N3	C12	111.2(5)	.	.	.	yes
Y1	N4	C13	99.0(4)	.	.	.	yes
Y1	N4	C14	112.1(4)	.	.	.	yes
Y1	N4	C17	113.3(4)	.	.	.	yes
C13	N4	C14	109.4(5)	.	.	.	yes
C13	N4	C17	111.7(5)	.	.	.	yes
C14	N4	C17	110.8(5)	.	.	.	yes
N1	C4	C1	106.8(5)	.	.	.	yes
N1	C4	C2	112.8(5)	.	.	.	yes
N1	C4	C3	111.0(6)	.	.	.	yes
C1	C4	C2	108.3(6)	.	.	.	no
C1	C4	C3	108.6(5)	.	.	.	no
C2	C4	C3	109.2(6)	.	.	.	no
N1	C5	C6	110.9(5)	.	.	.	yes
N2	C6	C5	113.1(5)	.	.	.	yes
N2	C7	C8	111.9(5)	.	.	.	yes
N3	C8	C7	113.8(5)	.	.	.	yes
N3	C9	C10	114.3(6)	.	.	.	yes
N3	C9	C11	111.7(5)	.	.	.	yes
C10	C9	C11	110.4(6)	.	.	.	no
N3	C12	C13	114.8(6)	.	.	.	yes
N4	C13	C12	115.4(6)	.	.	.	yes
N4	C14	C15	116.1(6)	.	.	.	yes
N4	C14	C16	110.4(5)	.	.	.	yes
C15	C14	C16	110.0(6)	.	.	.	no
N4	C17	C18	111.7(5)	.	.	.	yes
N2	C18	C17	112.2(5)	.	.	.	yes
Y1	C19	Si1	134.2(3)	.	.	.	yes
Y1	C23	Si2	145.4(4)	.	.	.	yes

C4	C1	H1	109.42	.	.	.	no
C4	C1	H1'	109.43	.	.	.	no
C4	C1	H1"	109.46	.	.	.	no
H1	C1	H1'	109.48	.	.	.	no
H1	C1	H1"	109.49	.	.	.	no
H1'	C1	H1"	109.55	.	.	.	no
C4	C2	H2	109.50	.	.	.	no
C4	C2	H2'	109.46	.	.	.	no
C4	C2	H2"	109.41	.	.	.	no
H2	C2	H2'	109.53	.	.	.	no
H2	C2	H2"	109.48	.	.	.	no
H2'	C2	H2"	109.45	.	.	.	no
C4	C3	H3	109.43	.	.	.	no
C4	C3	H3'	109.43	.	.	.	no
C4	C3	H3"	109.44	.	.	.	no
H3	C3	H3'	109.51	.	.	.	no
H3	C3	H3"	109.52	.	.	.	no
H3'	C3	H3"	109.49	.	.	.	no
N1	C5	H5	109.40	.	.	.	no
N1	C5	H5'	109.45	.	.	.	no
C6	C5	H5	109.47	.	.	.	no
C6	C5	H5'	109.50	.	.	.	no
H5	C5	H5'	108.05	.	.	.	no
N2	C6	H6	108.92	.	.	.	no
N2	C6	H6'	108.98	.	.	.	no
C5	C6	H6	108.95	.	.	.	no
C5	C6	H6'	108.99	.	.	.	no
H6	C6	H6'	107.81	.	.	.	no
N2	C7	H7	109.19	.	.	.	no
N2	C7	H7'	109.23	.	.	.	no
C8	C7	H7	109.22	.	.	.	no
C8	C7	H7'	109.23	.	.	.	no
H7	C7	H7'	108.00	.	.	.	no
N3	C8	H8	108.78	.	.	.	no
N3	C8	H8'	108.79	.	.	.	no
C7	C8	H8	108.79	.	.	.	no
C7	C8	H8'	108.75	.	.	.	no
H8	C8	H8'	107.71	.	.	.	no
N3	C9	H9	106.61	.	.	.	no
C10	C9	H9	106.61	.	.	.	no
C11	C9	H9	106.67	.	.	.	no
C9	C10	H10	109.47	.	.	.	no
C9	C10	H10'	109.47	.	.	.	no
C9	C10	H10"	109.49	.	.	.	no
H10	C10	H10'	109.43	.	.	.	no
H10	C10	H10"	109.50	.	.	.	no
H10'	C10	H10"	109.47	.	.	.	no
C9	C11	H11	109.48	.	.	.	no
C9	C11	H11'	109.53	.	.	.	no
C9	C11	H11"	109.51	.	.	.	no
H11	C11	H11'	109.41	.	.	.	no
H11	C11	H11"	109.42	.	.	.	no
H11'	C11	H11"	109.48	.	.	.	no
N3	C12	H12	108.51	.	.	.	no
N3	C12	H12'	108.56	.	.	.	no
C13	C12	H12	108.56	.	.	.	no
C13	C12	H12'	108.63	.	.	.	no
H12	C12	H12'	107.49	.	.	.	no
N4	C13	H13	108.42	.	.	.	no
N4	C13	H13'	108.43	.	.	.	no
C12	C13	H13	108.43	.	.	.	no
C12	C13	H13'	108.46	.	.	.	no
H13	C13	H13'	107.44	.	.	.	no
N4	C14	H14	106.57	.	.	.	no

C15	C14	H14	106.65	.	.	.	no
C16	C14	H14	106.57	.	.	.	no
C14	C15	H15	109.51	.	.	.	no
C14	C15	H15'	109.48	.	.	.	no
C14	C15	H15"	109.52	.	.	.	no
H15	C15	H15'	109.44	.	.	.	no
H15	C15	H15"	109.46	.	.	.	no
H15'	C15	H15"	109.41	.	.	.	no
C14	C16	H16	109.43	.	.	.	no
C14	C16	H16'	109.52	.	.	.	no
C14	C16	H16"	109.46	.	.	.	no
H16	C16	H16'	109.51	.	.	.	no
H16	C16	H16"	109.42	.	.	.	no
H16'	C16	H16"	109.49	.	.	.	no
N4	C17	H17	109.30	.	.	.	no
N4	C17	H17'	109.27	.	.	.	no
C18	C17	H17	109.31	.	.	.	no
C18	C17	H17'	109.25	.	.	.	no
H17	C17	H17'	107.98	.	.	.	no
N2	C18	H18	109.18	.	.	.	no
N2	C18	H18'	109.11	.	.	.	no
C17	C18	H18	109.23	.	.	.	no
C17	C18	H18'	109.15	.	.	.	no
H18	C18	H18'	107.88	.	.	.	no
Y1	C19	H19	103.67	.	.	.	no
Y1	C19	H19'	103.66	.	.	.	no
Si1	C19	H19	103.65	.	.	.	no
Si1	C19	H19'	103.61	.	.	.	no
H19	C19	H19'	105.34	.	.	.	no
Si1	C20	H20	109.47	.	.	.	no
Si1	C20	H20'	109.49	.	.	.	no
Si1	C20	H20"	109.49	.	.	.	no
H20	C20	H20'	109.46	.	.	.	no
H20	C20	H20"	109.44	.	.	.	no
H20'	C20	H20"	109.49	.	.	.	no
Si1	C21	H21	109.47	.	.	.	no
Si1	C21	H21'	109.49	.	.	.	no
Si1	C21	H21"	109.50	.	.	.	no
H21	C21	H21'	109.42	.	.	.	no
H21	C21	H21"	109.44	.	.	.	no
H21'	C21	H21"	109.50	.	.	.	no
Si1	C22	H22	109.47	.	.	.	no
Si1	C22	H22'	109.49	.	.	.	no
Si1	C22	H22"	109.51	.	.	.	no
H22	C22	H22'	109.44	.	.	.	no
H22	C22	H22"	109.46	.	.	.	no
H22'	C22	H22"	109.46	.	.	.	no
Y1	C23	H23	100.46	.	.	.	no
Y1	C23	H23'	100.47	.	.	.	no
Si2	C23	H23	100.55	.	.	.	no
Si2	C23	H23'	100.58	.	.	.	no
H23	C23	H23'	104.30	.	.	.	no
Si2	C24	H24	109.46	.	.	.	no
Si2	C24	H24'	109.47	.	.	.	no
Si2	C24	H24"	109.47	.	.	.	no
H24	C24	H24'	109.49	.	.	.	no
H24	C24	H24"	109.45	.	.	.	no
H24'	C24	H24"	109.47	.	.	.	no
Si2	C25	H25	109.44	.	.	.	no
Si2	C25	H25'	109.51	.	.	.	no
Si2	C25	H25"	109.43	.	.	.	no
H25	C25	H25'	109.53	.	.	.	no
H25	C25	H25"	109.40	.	.	.	no
H25'	C25	H25"	109.51	.	.	.	no

Si2	C26	H26	109.50	.	.	.	no
Si2	C26	H26'	109.48	.	.	.	no
Si2	C26	H26''	109.47	.	.	.	no
H26	C26	H26'	109.46	.	.	.	no
H26	C26	H26''	109.46	.	.	.	no
H26'	C26	H26''	109.46	.	.	.	no

loop_

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 _geom_torsion_atom_site_label_3
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N2	Y1	N1	C4	-174.9(5)	.	.	.	.	no
N2	Y1	N1	C5	13.6(4)	.	.	.	.	no
N3	Y1	N1	C4	168.0(4)	.	.	.	.	no
N3	Y1	N1	C5	-3.6(6)	.	.	.	.	no
N4	Y1	N1	C4	-117.2(5)	.	.	.	.	no
N4	Y1	N1	C5	71.3(4)	.	.	.	.	no
C19	Y1	N1	C4	-28.6(5)	.	.	.	.	no
C19	Y1	N1	C5	159.8(4)	.	.	.	.	no
C23	Y1	N1	C4	76.2(5)	.	.	.	.	no
C23	Y1	N1	C5	-95.3(5)	.	.	.	.	no
N1	Y1	N2	C6	-34.3(4)	.	.	.	.	no
N1	Y1	N2	C7	-152.2(4)	.	.	.	.	no
N1	Y1	N2	C18	82.5(4)	.	.	.	.	no
N3	Y1	N2	C6	133.8(4)	.	.	.	.	no
N3	Y1	N2	C7	15.9(4)	.	.	.	.	no
N3	Y1	N2	C18	-109.4(4)	.	.	.	.	no
N4	Y1	N2	C6	-150.5(4)	.	.	.	.	no
N4	Y1	N2	C7	91.6(4)	.	.	.	.	no
N4	Y1	N2	C18	-33.7(4)	.	.	.	.	no
C19	Y1	N2	C6	-141.2(4)	.	.	.	.	no
C19	Y1	N2	C7	100.9(5)	.	.	.	.	no
C19	Y1	N2	C18	-24.4(6)	.	.	.	.	no
C23	Y1	N2	C6	55.7(4)	.	.	.	.	no
C23	Y1	N2	C7	-62.2(4)	.	.	.	.	no
C23	Y1	N2	C18	172.5(4)	.	.	.	.	no
N1	Y1	N3	C8	-19.9(5)	.	.	.	.	no
N1	Y1	N3	C9	-134.9(4)	.	.	.	.	no
N1	Y1	N3	C12	100.0(4)	.	.	.	.	no
N2	Y1	N3	C8	-37.4(3)	.	.	.	.	no
N2	Y1	N3	C9	-152.4(4)	.	.	.	.	no
N2	Y1	N3	C12	82.5(4)	.	.	.	.	no
N4	Y1	N3	C8	-108.4(4)	.	.	.	.	no
N4	Y1	N3	C9	136.6(4)	.	.	.	.	no
N4	Y1	N3	C12	11.5(4)	.	.	.	.	no
C19	Y1	N3	C8	175.8(3)	.	.	.	.	no
C19	Y1	N3	C9	60.9(4)	.	.	.	.	no
C19	Y1	N3	C12	-64.2(4)	.	.	.	.	no
C23	Y1	N3	C8	75.3(4)	.	.	.	.	no
C23	Y1	N3	C9	-39.7(4)	.	.	.	.	no
C23	Y1	N3	C12	-164.8(4)	.	.	.	.	no
N1	Y1	N4	C13	-172.2(4)	.	.	.	.	no
N1	Y1	N4	C14	72.5(4)	.	.	.	.	no
N1	Y1	N4	C17	-53.7(4)	.	.	.	.	no
N2	Y1	N4	C13	-109.9(4)	.	.	.	.	no
N2	Y1	N4	C14	134.8(4)	.	.	.	.	no
N2	Y1	N4	C17	8.5(4)	.	.	.	.	no

N3	Y1	N4	C13	-34.4(4)	.	.	.	.	no
N3	Y1	N4	C14	-149.7(4)	.	.	.	.	no
N3	Y1	N4	C17	84.0(4)	.	.	.	.	no
C19	Y1	N4	C13	75.0(4)	.	.	.	.	no
C19	Y1	N4	C14	-40.3(4)	.	.	.	.	no
C19	Y1	N4	C17	-166.5(4)	.	.	.	.	no
C23	Y1	N4	C13	-25.7(7)	.	.	.	.	no
C23	Y1	N4	C14	-141.0(5)	.	.	.	.	no
C23	Y1	N4	C17	92.7(6)	.	.	.	.	no
N1	Y1	C19	Si1	92.9(4)	.	.	.	.	no
N2	Y1	C19	Si1	-172.4(3)	.	.	.	.	no
N3	Y1	C19	Si1	-98.2(4)	.	.	.	.	no
N4	Y1	C19	Si1	-163.9(4)	.	.	.	.	no
C23	Y1	C19	Si1	-8.6(5)	.	.	.	.	no
N1	Y1	C23	Si2	70.5(6)	.	.	.	.	no
N2	Y1	C23	Si2	-2.8(7)	.	.	.	.	no
N3	Y1	C23	Si2	-68.9(6)	.	.	.	.	no
N4	Y1	C23	Si2	-77.1(8)	.	.	.	.	no
C19	Y1	C23	Si2	-173.8(6)	.	.	.	.	no
C20	Si1	C19	Y1	104.9(5)	.	.	.	.	no
C21	Si1	C19	Y1	-135.4(5)	.	.	.	.	no
C22	Si1	C19	Y1	-13.7(6)	.	.	.	.	no
C26	Si2	C23	Y1	-28.2(8)	.	.	.	.	no
C24	Si2	C23	Y1	-147.6(6)	.	.	.	.	no
C25	Si2	C23	Y1	92.4(7)	.	.	.	.	no
C5	N1	C4	C3	68.1(7)	.	.	.	.	no
Y1	N1	C5	C6	10.3(7)	.	.	.	.	no
C5	N1	C4	C2	-54.8(7)	.	.	.	.	no
Y1	N1	C4	C1	14.3(7)	.	.	.	.	no
Y1	N1	C4	C2	133.1(5)	.	.	.	.	no
Y1	N1	C4	C3	-104.0(6)	.	.	.	.	no
C4	N1	C5	C6	-162.8(5)	.	.	.	.	no
C5	N1	C4	C1	-173.6(5)	.	.	.	.	no
C7	N2	C6	C5	174.3(5)	.	.	.	.	no
C18	N2	C6	C5	-63.1(7)	.	.	.	.	no
Y1	N2	C6	C5	53.4(5)	.	.	.	.	no
C6	N2	C7	C8	-102.3(6)	.	.	.	.	no
C18	N2	C7	C8	134.7(6)	.	.	.	.	no
Y1	N2	C7	C8	9.3(6)	.	.	.	.	no
C7	N2	C18	C17	-68.0(7)	.	.	.	.	no
Y1	N2	C18	C17	59.7(6)	.	.	.	.	no
C6	N2	C18	C17	169.4(5)	.	.	.	.	no
Y1	N3	C9	C11	-60.9(6)	.	.	.	.	no
C12	N3	C9	C11	64.8(7)	.	.	.	.	no
Y1	N3	C12	C13	14.2(7)	.	.	.	.	no
C8	N3	C12	C13	127.2(6)	.	.	.	.	no
C9	N3	C12	C13	-110.6(6)	.	.	.	.	no
C8	N3	C9	C10	62.7(7)	.	.	.	.	no
C8	N3	C9	C11	-171.0(6)	.	.	.	.	no
C12	N3	C9	C10	-61.5(7)	.	.	.	.	no
Y1	N3	C8	C7	60.9(6)	.	.	.	.	no
C9	N3	C8	C7	177.4(5)	.	.	.	.	no
C12	N3	C8	C7	-59.0(7)	.	.	.	.	no
Y1	N3	C9	C10	172.8(5)	.	.	.	.	no
C17	N4	C14	C16	62.2(7)	.	.	.	.	no
Y1	N4	C17	C18	17.5(6)	.	.	.	.	no
C13	N4	C17	C18	128.2(6)	.	.	.	.	no
C14	N4	C17	C18	-109.5(6)	.	.	.	.	no
Y1	N4	C14	C15	168.5(5)	.	.	.	.	no
Y1	N4	C14	C16	-65.4(6)	.	.	.	.	no
C13	N4	C14	C15	59.7(7)	.	.	.	.	no
C13	N4	C14	C16	-174.2(5)	.	.	.	.	no
Y1	N4	C13	C12	59.7(6)	.	.	.	.	no
C14	N4	C13	C12	177.1(6)	.	.	.	.	no

C17	N4	C13	C12	-59.9(7)	.	.	.	.	no
C17	N4	C14	C15	-63.9(7)	.	.	.	.	no
N1	C5	C6	N2	-47.2(7)	.	.	.	.	no
N2	C7	C8	N3	-50.7(7)	.	.	.	.	no
N3	C12	C13	N4	-55.9(8)	.	.	.	.	no
N4	C17	C18	N2	-50.8(7)	.	.	.	.	no

loop_

_geom_contact_atom_site_label_1
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 _geom_contact_site_symmetry_2
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Y1	H1	2.9939	.	.	no
Y1	H1 "	3.3279	.	.	no
Y1	H3 "	3.9710	.	.	no
Y1	H11 "	3.0520	.	.	no
Y1	H16 '	3.1851	.	.	no
Si1	H1	3.4756	.	.	no
Si1	H11 "	3.2330	.	.	no
Si2	H8	3.3157	.	.	no
Si2	H9	3.2984	.	.	no
N1	H18	2.9059	.	.	no
C1	C19	3.473(9)	.	.	no
C11	C13	3.492(10)	.	.	no
C13	C11	3.492(10)	.	.	no
C16	C18	3.353(10)	.	.	no
C18	C16	3.353(10)	.	.	no
C19	C1	3.473(9)	.	.	no
C1	H19 '	3.0790	.	.	no
C2	H5 '	2.9347	.	.	no
C2	H5	2.6895	.	.	no
C3	H5 '	2.5559	.	.	no
C3	H26 '	3.0614	.	2_666	no
C5	H2 "	2.6398	.	.	no
C5	H18	2.5372	.	.	no
C5	H2	3.0748	.	.	no
C5	H3	2.7445	.	.	no
C6	H7 '	3.0407	.	2_566	no
C7	H17	2.7541	.	.	no
C7	H12	2.5595	.	.	no
C8	H10 '	2.6767	.	.	no
C9	H23	2.8925	.	.	no
C10	H12 '	2.5719	.	.	no
C10	H8 '	2.6300	.	.	no
C11	H20	2.9211	.	.	no
C11	H13	2.9700	.	.	no
C11	H12 '	2.7394	.	.	no
C11	H23	3.0425	.	.	no
C12	H7	2.7528	.	.	no
C12	H10	2.7245	.	.	no
C12	H17	2.5744	.	.	no
C12	H11	2.6977	.	.	no
C13	H19	3.0193	.	.	no
C13	H11	3.0411	.	.	no
C13	H15	2.7147	.	.	no
C14	H19	3.0838	.	.	no
C14	H16	3.0076	.	2_565	no
C14	H19 '	3.0930	.	.	no
C15	H17 '	2.6235	.	.	no
C15	H13 '	2.6182	.	.	no
C16	H18	2.8275	.	.	no
C16	H17 '	2.6763	.	.	no

C17	H7	2.5898	.	.	no
C17	H15"	2.7462	.	.	no
C17	H16"	2.6863	.	.	no
C17	H12	2.7207	.	.	no
C18	H10"	2.7666	.	1_565	no
C18	H16"	3.0190	.	.	no
C18	H5	2.7614	.	.	no
C19	H1	2.9949	.	.	no
C19	H1"	3.0470	.	.	no
C19	H11"	2.7107	.	.	no
C19	H13	2.9961	.	.	no
C19	H14	2.6642	.	.	no
C20	H11"	3.0768	.	.	no
C22	H13'	2.7786	.	1_655	no
C23	H8	3.0787	.	.	no
C23	H9	2.7127	.	.	no
C23	H22"	3.0765	.	.	no
C25	H9	2.8143	.	.	no
C25	H10'	3.0481	.	2_556	no
C26	H6	2.8759	.	.	no
H1	Y1	2.9939	.	.	no
H1	Si1	3.4756	.	.	no
H1	C19	2.9949	.	.	no
H1	H3"	2.5627	.	.	no
H1	H22	2.4800	.	.	no
H1'	H2'	2.4344	.	.	no
H1'	H3'	2.4177	.	.	no
H1"	Y1	3.3279	.	.	no
H1"	C19	3.0470	.	.	no
H1"	H2	2.5051	.	.	no
H1"	H19'	2.4305	.	.	no
H2	C5	3.0748	.	.	no
H2	H1"	2.5051	.	.	no
H2'	H1'	2.4344	.	.	no
H2'	H3'	2.5477	.	.	no
H2"	C5	2.6398	.	.	no
H2"	H3	2.4241	.	.	no
H2"	H5	2.3253	.	.	no
H2"	H5'	2.4865	.	.	no
H3	C5	2.7445	.	.	no
H3	H2"	2.4241	.	.	no
H3	H5'	2.0281	.	.	no
H3'	H1'	2.4177	.	.	no
H3'	H2'	2.5477	.	.	no
H3"	Y1	3.9710	.	.	no
H3"	H1	2.5627	.	.	no
H5	C2	2.6895	.	.	no
H5	C18	2.7614	.	.	no
H5	H2"	2.3253	.	.	no
H5	H18	2.0924	.	.	no
H5'	C2	2.9347	.	.	no
H5'	C3	2.5559	.	.	no
H5'	H2"	2.4865	.	.	no
H5'	H3	2.0281	.	.	no
H6	C26	2.8759	.	.	no
H6	H7'	2.3912	.	.	no
H6	H26	2.5309	.	.	no
H6	H26"	2.4467	.	.	no
H6'	H7'	2.3237	.	.	no
H6'	H18'	2.4999	.	.	no
H6'	H26"	2.5993	.	2_566	no
H7	C12	2.7528	.	.	no
H7	C17	2.5898	.	.	no
H7	H12	2.0522	.	.	no

H7	H17	2.0735	.	.	no
H7	H18'	2.3566	.	.	no
H7	H24"	2.4144	.	1_455	no
H7'	H6	2.3912	.	.	no
H7'	H6'	2.3237	.	.	no
H7'	C6	3.0407	.	2_566	no
H8	Si2	3.3157	.	.	no
H8	C23	3.0787	.	.	no
H8	H9	2.3004	.	.	no
H8'	C10	2.6300	.	.	no
H8'	H10'	2.0786	.	.	no
H8'	H12	2.4438	.	.	no
H9	Si2	3.2984	.	.	no
H9	C23	2.7127	.	.	no
H9	C25	2.8143	.	.	no
H9	H8	2.3004	.	.	no
H9	H23	2.1780	.	.	no
H9	H25	2.4892	.	.	no
H9	H25"	2.5626	.	.	no
H10	C12	2.7245	.	.	no
H10	H11	2.5875	.	.	no
H10	H12'	2.0204	.	.	no
H10'	C8	2.6767	.	.	no
H10'	H8'	2.0786	.	.	no
H10'	C25	3.0481	.	2_556	no
H10'	H25'	2.3859	.	2_556	no
H10"	C18	2.7666	.	1_545	no
H10"	H11'	2.4238	.	.	no
H10"	H18	2.3569	.	1_545	no
H10"	H18'	2.3015	.	1_545	no
H11	C12	2.6977	.	.	no
H11	C13	3.0411	.	.	no
H11	H10	2.5875	.	.	no
H11	H12'	2.2423	.	.	no
H11	H13	2.4654	.	.	no
H11'	H10"	2.4238	.	.	no
H11"	Y1	3.0520	.	.	no
H11"	Si1	3.2330	.	.	no
H11"	C19	2.7107	.	.	no
H11"	C20	3.0768	.	.	no
H11"	H19	2.4408	.	.	no
H11"	H20	2.4269	.	.	no
H11"	H23	2.5521	.	.	no
H12	C7	2.5595	.	.	no
H12	C17	2.7207	.	.	no
H12	H7	2.0522	.	.	no
H12	H8'	2.4438	.	.	no
H12	H17	2.0307	.	.	no
H12'	C10	2.5719	.	.	no
H12'	C11	2.7394	.	.	no
H12'	H10	2.0204	.	.	no
H12'	H11	2.2423	.	.	no
H13	C11	2.9700	.	.	no
H13	C19	2.9961	.	.	no
H13	H11	2.4654	.	.	no
H13	H14	2.3078	.	.	no
H13	H19	2.2123	.	.	no
H13'	C15	2.6182	.	.	no
H13'	C22	2.7786	.	1_455	no
H13'	H15	2.1415	.	.	no
H13'	H17	2.4320	.	.	no
H13'	H22	2.2649	.	1_455	no
H13'	H22'	2.4701	.	1_455	no
H14	C19	2.6642	.	.	no

H14	H13	2.3078	.	.	no
H14	H19	2.2608	.	.	no
H14	H19'	2.3222	.	.	no
H14	H16	2.3472	.	2_565	no
H15	C13	2.7147	.	.	no
H15	H13'	2.1415	.	.	no
H15	H20'	2.5752	.	2_555	no
H15'	H16	2.4637	.	.	no
H15'	H19'	2.5458	.	2_565	no
H15"	C17	2.7462	.	.	no
H15"	H16"	2.5868	.	.	no
H15"	H17'	2.0756	.	.	no
H16	H15'	2.4637	.	.	no
H16	C14	3.0076	.	2_565	no
H16	H14	2.3472	.	2_565	no
H16'	Y1	3.1851	.	.	no
H16'	H18	2.5265	.	.	no
H16"	C17	2.6863	.	.	no
H16"	C18	3.0190	.	.	no
H16"	H15"	2.5868	.	.	no
H16"	H17'	2.1918	.	.	no
H16"	H18	2.4488	.	.	no
H17	C7	2.7541	.	.	no
H17	C12	2.5744	.	.	no
H17	H7	2.0735	.	.	no
H17	H12	2.0307	.	.	no
H17	H13'	2.4320	.	.	no
H17'	C15	2.6235	.	.	no
H17'	C16	2.6763	.	.	no
H17'	H15"	2.0756	.	.	no
H17'	H16"	2.1918	.	.	no
H18	N1	2.9059	.	.	no
H18	C5	2.5372	.	.	no
H18	C16	2.8275	.	.	no
H18	H5	2.0924	.	.	no
H18	H10"	2.3569	.	1_565	no
H18	H16'	2.5265	.	.	no
H18	H16"	2.4488	.	.	no
H18'	H6'	2.4999	.	.	no
H18'	H7	2.3566	.	.	no
H18'	H10"	2.3015	.	1_565	no
H19	C13	3.0193	.	.	no
H19	C14	3.0838	.	.	no
H19	H11"	2.4408	.	.	no
H19	H13	2.2123	.	.	no
H19	H14	2.2608	.	.	no
H19'	C1	3.0790	.	.	no
H19'	C14	3.0930	.	.	no
H19'	H1"	2.4305	.	.	no
H19'	H14	2.3222	.	.	no
H19'	H15'	2.5458	.	2_565	no
H20	C11	2.9211	.	.	no
H20	H11"	2.4269	.	.	no
H20'	H15	2.5752	.	2_555	no
H20"	H20"	2.5828	.	2_555	no
H22	H1	2.4800	.	.	no
H22	H13'	2.2649	.	1_655	no
H22'	H13'	2.4701	.	1_655	no
H22"	C23	3.0765	.	.	no
H22"	H23	2.5676	.	.	no
H23	C9	2.8925	.	.	no
H23	C11	3.0425	.	.	no
H23	H9	2.1780	.	.	no
H23	H11"	2.5521	.	.	no

H23	H22"	2.5676	.	.	no
H24"	H7	2.4144	.	1_655	no
H25	H9	2.4892	.	.	no
H25'	H10'	2.3859	.	2_556	no
H25"	H9	2.5626	.	.	no
H26	H6	2.5309	.	.	no
H26'	C3	3.0614	.	2_666	no
H26"	H6	2.4467	.	.	no
H26"	H6'	2.5993	.	2_566	no

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