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Thermolysis of Half-Sandwich Vanadium(V) Imido Complexes to Generate Vanadium(III) Imido Species via a Vanadium(IV) Intermediate

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;
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2010-05-20 # 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 choose 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 : 2010-05-11 18:03:26

  Consider this CIF submission for deposition of the (first)
  X-ray structure of a manuscript to be submitted to : Organometallics
  (Our Compound_Identification_Code : Q1070)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_accepted          ?

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_journal_volume                   ?
_journal_issue                    ?
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_journal_page_last                ?

_journal_suppl_publ_number        ?
_journal_suppl_publ_pages         ?

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3. TITLE AND AUTHOR LIST

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Title (type here to add)
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_publ_section_title_footnote
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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.
;

```

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#=====
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4. TEXT

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Insert blank lines between paragraphs

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;

_publ_section_exptl_prep

;

(type here to add preparation details)

;

_publ_section_exptl_refinement

;

The structure was solved by Patterson methods and extension of the model was accomplished by direct methods applied to difference structure factors using the program *DIRDIF*. The positional and anisotropic displacement parameters for the non-hydrogen atoms were refined. Some atoms (C8, C9 & C10) showed unrealistic displacement parameters when allowed to vary anisotropically, suggesting dynamic disorder (dynamic means that the smeared electron density is due to fluctuations of the atomic positions within each unit cell. The disorder is compensated by the larger the displacement parameters). The smeared electron density for the C-positions have been described by two site occupancy factors with separately refined displacement parameters. The s.o.f. of the major fraction of the component of the disorder model refined to a value of 0.528(12).

A subsequent difference Fourier synthesis resulted in the location of the hydrogen atoms, which coordinates and isotropic displacement parameters were refined. The hydrogen atoms of the disordered C-positions were generated by geometrical considerations, constrained to idealized geometries, and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms.

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Insert blank lines between references

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Beurskens, P.T., Beurskens, G., Gelder, R. de, Garcia-Granda, S. Gould, R.O., Israel, & Smits, J.M.M. (1999). The *DIRDIF99* program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

Bruker, (2000). *SMART*, *SAINTPLUS* and *XPREP*. Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

Meetsma, A. (2005). Extended version of the program *PLUTO*. Groningen University, The Netherlands. (unpublished).

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

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

;

_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
'C15 H30 N P2 V'
# 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
'C15 H30 N P2 V'
_chemical_formula_iupac         ?
_chemical_formula_weight        337.30
_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
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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
P      P      0.1023    0.0942
'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'
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#=====

6. CRYSTAL DATA

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_symmetry_space_group_name_H-M  'P 21/c'
_symmetry_Int_Tables_number     14
```

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

```

_cell_length_a          15.132(1)
_cell_length_b          8.9402(6)
_cell_length_c          13.711(1)
_cell_angle_alpha       90
_cell_angle_beta        102.480(1)
_cell_angle_gamma       90
_cell_volume            1811.0(2)
_cell_formula_units_Z    4

```

```

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 5597
_cell_measurement_theta_min   2.66
_cell_measurement_theta_max   29.17
_cell_special_details

```

```
;
```

The final unit cell was obtained from the xyz centroids of 5597 reflections after integration using the SAINT software package (Bruker, 2000).

```
;
```

```

_exptl_crystal_description 'platelet'
_exptl_crystal_colour      'green'
_exptl_crystal_size_max    0.29
_exptl_crystal_size_mid    0.23
_exptl_crystal_size_min    0.11
_exptl_crystal_size_rad    ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 1.237
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000       720
_exptl_absorpt_coefficient_mu 0.714
_exptl_absorpt_correction_type 'Multi-Scan'
_exptl_absorpt_process_details 'SADABS (Bruker, 2000)'
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_exptl_absorpt_correction_T_max 0.9256

```

```
#=====
```

7. EXPERIMENTAL DATA

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; ?
;
_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 66.06

_diffn_standards_number      0
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```

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_diffrn_standards_interval_time      ?
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loop_
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_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number                14394
_diffrn_reflns_av_R_equivalents      0.0426
_diffrn_reflns_av_sigmaI/netI       0.0442
_diffrn_reflns_limit_h_min           -17
_diffrn_reflns_limit_h_max           19
_diffrn_reflns_limit_k_min           -10
_diffrn_reflns_limit_k_max           11
_diffrn_reflns_limit_l_min           -17
_diffrn_reflns_limit_l_max           17
_diffrn_reflns_theta_min              2.74
_diffrn_reflns_theta_max             26.73
_diffrn_measured_fraction_theta_max  0.995
_diffrn_reflns_theta_full             25.00
_diffrn_measured_fraction_theta_full 0.998

_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2000) and SADABS (Bruker, 2000)
;

# number of unique reflections
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_reflns_number_gt                     3028
_reflns_threshold_expression           $I > 2\sigma(I)$ 

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_computing_cell_refinement            'SAINTPLUS (Bruker, 2000)'
_computing_data_reduction             'XPREP (Bruker, 2000)'
_computing_structure_solution
;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement        'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2005)
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/[\s^2^(Fo^2^)+(0.0451P)^2^+0.8399P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     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          3840
_refine_ls_number_parameters      294
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0558
_refine_ls_R_factor_gt            0.0399
_refine_ls_wR_factor_ref          0.0950
_refine_ls_wR_factor_gt           0.0883
_refine_ls_goodness_of_fit_ref    1.021
_refine_ls_restrained_S_all       1.021
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          0.808
_refine_diff_density_min          -0.313
_refine_diff_density_rms          0.066

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_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
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P1 P Uani 0.22024(4) 0.01193(7) 0.19252(4) 1.000 0.0233(2) . .
P2 P Uani 0.22195(5) 0.01066(7) 0.41556(4) 1.000 0.0308(2) . .
N N Uani 0.32655(12) 0.24901(18) 0.32923(14) 1.000 0.0176(5) . .
C1 C Uani 0.14434(17) 0.4243(3) 0.33819(19) 1.000 0.0294(8) . .
C2 C Uani 0.09341(18) 0.3001(3) 0.3583(2) 1.000 0.0375(9) . .
C3 C Uani 0.06072(17) 0.2256(3) 0.2671(2) 1.000 0.0374(9) . .
C4 C Uani 0.09291(18) 0.3015(3) 0.1913(2) 1.000 0.0364(8) . .
C5 C Uani 0.14370(17) 0.4248(3) 0.23587(18) 1.000 0.0299(8) . .
C6 C Uani 0.29629(18) 0.0159(3) 0.1050(2) 1.000 0.0269(8) . .
C7 C Uani 0.1157(3) -0.0508(5) 0.1081(3) 1.000 0.0597(16) . .
C8A C Uani 0.2405(7) -0.1726(9) 0.2552(6) 0.528(12) 0.035(2) . .
C9A C Uani 0.2902(6) -0.1441(6) 0.3638(4) 0.528(12) 0.0260(18) . .
```



```

C10A C Uani 0.1304(5) -0.0804(10) 0.4373(6) 0.528(12) 0.036(3) . .
C11 C Uani 0.2956(2) 0.0124(3) 0.54046(19) 1.000 0.0326(9) . .
C12 C Uani 0.41919(14) 0.3028(3) 0.35282(17) 1.000 0.0224(7) . .
C13 C Uani 0.4666(2) 0.2643(4) 0.2687(2) 1.000 0.0415(10) . .
C14 C Uani 0.41614(18) 0.4723(3) 0.3660(2) 1.000 0.0300(8) . .
C15 C Uani 0.47028(19) 0.2312(3) 0.4508(2) 1.000 0.0359(9) . .
C9B C Uani 0.2334(8) -0.1720(7) 0.3597(5) 0.472(12) 0.040(3) . .
C10B C Uani 0.1040(7) -0.0330(10) 0.4561(7) 0.472(12) 0.032(2) . .
C8B C Uani 0.2803(8) -0.1454(10) 0.2757(7) 0.472(12) 0.034(3) . .
H101" H Uiso 0.14966 -0.17345 0.47345 0.528(12) 0.0533 . .
H3 H Uiso 0.0258(18) 0.141(3) 0.255(2) 1.000 0.039(8) . .
H2 H Uiso 0.0809(19) 0.270(3) 0.420(2) 1.000 0.042(8) . .
H5 H Uiso 0.1832(18) 0.491(3) 0.202(2) 1.000 0.035(7) . .
H6 H Uiso 0.356(2) 0.036(3) 0.140(2) 1.000 0.043(8) . .
H4 H Uiso 0.0817(19) 0.276(3) 0.125(2) 1.000 0.045(8) . .
H6" H Uiso 0.2939(17) -0.081(3) 0.0708(19) 1.000 0.036(7) . .
H7 H Uiso 0.069(2) -0.063(4) 0.142(2) 1.000 0.062(10) . .
H7' H Uiso 0.132(2) -0.141(4) 0.084(3) 1.000 0.067(10) . .
H7" H Uiso 0.096(5) 0.007(7) 0.053(5) 1.000 0.20(3) . .
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H14 H Uiso 0.3848(18) 0.497(3) 0.418(2) 1.000 0.030(7) . .
H14' H Uiso 0.4796(17) 0.512(3) 0.3844(18) 1.000 0.024(6) . .
H14" H Uiso 0.3829(18) 0.521(3) 0.303(2) 1.000 0.037(7) . .
H15 H Uiso 0.4723(19) 0.124(4) 0.438(2) 1.000 0.051(9) . .
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H15" H Uiso 0.533(2) 0.266(3) 0.463(2) 1.000 0.043(8) . .
H81 H Uiso 0.18231 -0.22413 0.25350 0.528(12) 0.0414 . .
H81' H Uiso 0.27785 -0.23631 0.22082 0.528(12) 0.0414 . .
H91 H Uiso 0.35296 -0.11005 0.36627 0.528(12) 0.0313 . .
H91' H Uiso 0.29251 -0.23668 0.40380 0.528(12) 0.0313 . .
H101 H Uiso 0.08920 -0.10365 0.37354 0.528(12) 0.0533 . .
H11" H Uiso 0.2918(17) -0.082(3) 0.5726(19) 1.000 0.037(7) . .
H1 H Uiso 0.1859(17) 0.492(3) 0.3920(19) 1.000 0.031(7) . .
H101' H Uiso 0.09923 -0.01695 0.47747 0.528(12) 0.0533 . .
H102' H Uiso 0.08860 0.05067 0.49555 0.472(12) 0.0473 . .
H102" H Uiso 0.11014 -0.12462 0.49627 0.472(12) 0.0473 . .
H82 H Uiso 0.27942 -0.23803 0.23595 0.472(12) 0.0399 . .
H82' H Uiso 0.34421 -0.11753 0.30283 0.472(12) 0.0399 . .
H92 H Uiso 0.26945 -0.24038 0.40967 0.472(12) 0.0483 . .
H92' H Uiso 0.17309 -0.21727 0.33425 0.472(12) 0.0483 . .
H102 H Uiso 0.05584 -0.04628 0.39620 0.472(12) 0.0473 . .

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_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
V 0.0110(2) 0.0147(2) 0.0173(2) 0.0002(1) 0.0031(1) 0.0009(2)
P1 0.0318(4) 0.0170(3) 0.0236(3) -0.0033(2) 0.0114(3) -0.0017(2)
P2 0.0542(5) 0.0170(3) 0.0204(3) 0.0022(2) 0.0063(3) -0.0014(3)
N 0.0133(9) 0.0106(9) 0.0282(10) -0.0017(7) 0.0030(7) 0.0007(7)
C1 0.0279(14) 0.0234(13) 0.0362(13) -0.0040(11) 0.0052(10) 0.0130(10)
C2 0.0298(14) 0.0412(16) 0.0490(16) 0.0037(14) 0.0249(12) 0.0146(12)
C3 0.0115(12) 0.0333(15) 0.0650(19) -0.0051(14) 0.0029(11) 0.0034(11)
C4 0.0316(15) 0.0364(15) 0.0333(14) -0.0008(12) -0.0104(11) 0.0174(12)
C5 0.0306(14) 0.0224(13) 0.0363(14) 0.0068(10) 0.0066(11) 0.0123(11)
C6 0.0262(14) 0.0277(14) 0.0278(13) -0.0085(11) 0.0082(10) 0.0005(11)
C7 0.042(2) 0.071(3) 0.076(3) -0.053(2) 0.0346(19) -0.0362(19)

```

```

C8A 0.062(6) 0.010(3) 0.028(3) -0.004(2) 0.002(4) -0.002(3)
C9A 0.036(4) 0.013(2) 0.028(3) 0.0047(18) 0.005(2) 0.004(2)
C10A 0.027(4) 0.042(5) 0.039(4) 0.014(3) 0.009(3) -0.007(3)
C11 0.0348(16) 0.0357(16) 0.0280(13) 0.0108(12) 0.0085(11) 0.0044(12)
C12 0.0145(11) 0.0211(12) 0.0314(12) -0.0052(9) 0.0048(9) -0.0025(9)
C13 0.0206(14) 0.057(2) 0.0498(18) -0.0252(16) 0.0139(12) -0.0113(14)
C14 0.0240(14) 0.0227(13) 0.0446(16) -0.0049(11) 0.0106(12) -0.0079(11)
C15 0.0204(14) 0.0324(16) 0.0486(17) 0.0015(12) -0.0062(12) -0.0049(12)
C9B 0.063(7) 0.017(3) 0.049(4) 0.006(3) 0.032(4) 0.009(3)
C10B 0.031(4) 0.034(4) 0.035(4) 0.000(3) 0.017(3) -0.011(3)
C8B 0.051(6) 0.014(4) 0.042(6) -0.002(3) 0.023(4) 0.007(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
```

V	P1	2.3507(7)	.	.	yes
V	P2	2.3522(7)	.	.	yes
V	N	1.6903(19)	.	.	yes
V	C1	2.284(3)	.	.	yes
V	C2	2.273(3)	.	.	yes
V	C3	2.275(3)	.	.	yes
V	C4	2.272(3)	.	.	yes
V	C5	2.284(3)	.	.	yes
P1	C6	1.834(3)	.	.	yes
P1	C7	1.835(4)	.	.	yes
P1	C8A	1.855(8)	.	.	yes
P1	C8B	1.912(10)	.	.	yes
P2	C9A	1.950(7)	.	.	yes
P2	C10A	1.688(8)	.	.	yes
P2	C11	1.830(3)	.	.	yes
P2	C9B	1.828(7)	.	.	yes
P2	C10B	2.019(11)	.	.	yes
N	C12	1.451(3)	.	.	yes
C1	C2	1.412(4)	.	.	no
C1	C5	1.401(4)	.	.	no
C2	C3	1.409(4)	.	.	no
C3	C4	1.413(4)	.	.	no
C4	C5	1.406(4)	.	.	no
C8A	C9A	1.537(10)	.	.	no
C8B	C9B	1.497(14)	.	.	no
C12	C14	1.528(4)	.	.	no
C12	C15	1.537(4)	.	.	no
C12	C13	1.524(4)	.	.	no
C1	H1	1.05(3)	.	.	no
C2	H2	0.95(3)	.	.	no
C3	H3	0.92(3)	.	.	no
C4	H4	0.92(3)	.	.	no
C5	H5	1.02(3)	.	.	no
C6	H6	0.94(3)	.	.	no

C6	H6'	0.88(3)	.	.	no
C6	H6"	0.98(3)	.	.	no
C7	H7	0.93(3)	.	.	no
C7	H7'	0.93(4)	.	.	no
C7	H7"	0.91(7)	.	.	no
C8A	H81	0.9900	.	.	no
C8A	H81'	0.9900	.	.	no
C8B	H82'	0.9900	.	.	no
C8B	H82	0.9900	.	.	no
C9A	H91'	0.9900	.	.	no
C9A	H91	0.9900	.	.	no
C9B	H92	0.9900	.	.	no
C9B	H92'	0.9900	.	.	no
C10A	H101	0.9800	.	.	no
C10A	H101'	0.9800	.	.	no
C10A	H101"	0.9800	.	.	no
C10B	H102'	0.9800	.	.	no
C10B	H102"	0.9800	.	.	no
C10B	H102	0.9800	.	.	no
C11	H11"	0.96(3)	.	.	no
C11	H11	0.90(3)	.	.	no
C11	H11'	0.99(3)	.	.	no
C13	H13'	0.99(3)	.	.	no
C13	H13	0.93(3)	.	.	no
C13	H13"	0.99(4)	.	.	no
C14	H14	0.96(3)	.	.	no
C14	H14'	1.00(3)	.	.	no
C14	H14"	1.00(3)	.	.	no
C15	H15	0.98(4)	.	.	no
C15	H15'	1.00(3)	.	.	no
C15	H15"	0.98(3)	.	.	no

loop_

_geom_angle_atom_site_label_1

_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

_geom_angle

_geom_angle_site_symmetry_1

_geom_angle_site_symmetry_2

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

P1	V	P2	80.95(2)	.	.	.	yes
P1	V	N	96.56(6)	.	.	.	yes
P1	V	C1	148.45(7)	.	.	.	yes
P1	V	C2	128.69(7)	.	.	.	yes
P1	V	C3	94.75(7)	.	.	.	yes
P1	V	C4	88.46(7)	.	.	.	yes
P1	V	C5	116.99(6)	.	.	.	yes
P2	V	N	96.26(6)	.	.	.	yes
P2	V	C1	117.09(7)	.	.	.	yes
P2	V	C2	88.59(7)	.	.	.	yes
P2	V	C3	95.00(7)	.	.	.	yes
P2	V	C4	129.08(7)	.	.	.	yes
P2	V	C5	148.57(7)	.	.	.	yes
N	V	C1	106.14(9)	.	.	.	yes
N	V	C2	134.61(9)	.	.	.	yes
N	V	C3	165.15(9)	.	.	.	yes
N	V	C4	134.53(9)	.	.	.	yes
N	V	C5	106.23(9)	.	.	.	yes
C1	V	C2	36.11(10)	.	.	.	yes
C1	V	C3	59.86(9)	.	.	.	yes
C1	V	C4	60.00(9)	.	.	.	yes
C1	V	C5	35.72(9)	.	.	.	yes
C2	V	C3	36.09(10)	.	.	.	yes
C2	V	C4	60.45(10)	.	.	.	yes
C2	V	C5	60.00(9)	.	.	.	yes

C3	V	C4	36.21(10)	.	.	.	yes
C3	V	C5	59.79(9)	.	.	.	yes
C4	V	C5	35.94(9)	.	.	.	yes
V	P1	C6	121.51(9)	.	.	.	yes
V	P1	C7	119.40(14)	.	.	.	yes
V	P1	C8A	113.6(3)	.	.	.	yes
V	P1	C8B	104.6(3)	.	.	.	yes
C6	P1	C7	99.82(16)	.	.	.	yes
C6	P1	C8A	104.8(3)	.	.	.	yes
C6	P1	C8B	96.9(4)	.	.	.	yes
C7	P1	C8A	93.1(3)	.	.	.	yes
C7	P1	C8B	112.7(3)	.	.	.	yes
V	P2	C9A	104.81(17)	.	.	.	yes
V	P2	C10A	124.0(3)	.	.	.	yes
V	P2	C11	122.75(9)	.	.	.	yes
V	P2	C9B	113.6(2)	.	.	.	yes
V	P2	C10B	114.1(3)	.	.	.	yes
C9A	P2	C10A	104.0(4)	.	.	.	yes
C9A	P2	C11	94.8(2)	.	.	.	yes
C10A	P2	C11	101.3(3)	.	.	.	yes
C9B	P2	C11	107.8(3)	.	.	.	yes
C10B	P2	C11	98.0(3)	.	.	.	yes
C9B	P2	C10B	96.4(4)	.	.	.	yes
V	N	C12	172.15(16)	.	.	.	yes
V	C1	C2	71.53(16)	.	.	.	yes
V	C1	C5	72.16(15)	.	.	.	yes
C2	C1	C5	108.2(2)	.	.	.	no
V	C2	C1	72.36(16)	.	.	.	yes
V	C2	C3	72.04(15)	.	.	.	yes
C1	C2	C3	107.5(2)	.	.	.	no
V	C3	C2	71.87(16)	.	.	.	yes
V	C3	C4	71.78(15)	.	.	.	yes
C2	C3	C4	108.4(2)	.	.	.	no
V	C4	C3	72.02(15)	.	.	.	yes
V	C4	C5	72.50(15)	.	.	.	yes
C3	C4	C5	107.5(2)	.	.	.	no
V	C5	C1	72.13(15)	.	.	.	yes
V	C5	C4	71.56(15)	.	.	.	yes
C1	C5	C4	108.5(2)	.	.	.	no
P1	C8A	C9A	107.4(5)	.	.	.	yes
P1	C8B	C9B	109.4(7)	.	.	.	yes
P2	C9A	C8A	106.5(5)	.	.	.	yes
P2	C9B	C8B	106.5(5)	.	.	.	yes
N	C12	C14	107.62(19)	.	.	.	yes
N	C12	C15	109.6(2)	.	.	.	yes
C13	C12	C15	109.7(2)	.	.	.	no
C14	C12	C15	109.4(2)	.	.	.	no
C13	C12	C14	110.2(2)	.	.	.	no
N	C12	C13	110.3(2)	.	.	.	yes
V	C1	H1	113.2(14)	.	.	.	no
C2	C1	H1	125.8(14)	.	.	.	no
C5	C1	H1	125.1(14)	.	.	.	no
V	C2	H2	122.1(18)	.	.	.	no
C1	C2	H2	128.5(17)	.	.	.	no
C3	C2	H2	124.1(17)	.	.	.	no
V	C3	H3	121.0(18)	.	.	.	no
C2	C3	H3	129.0(17)	.	.	.	no
C4	C3	H3	122.7(17)	.	.	.	no
V	C4	H4	121.9(18)	.	.	.	no
C3	C4	H4	126.2(18)	.	.	.	no
C5	C4	H4	126.4(18)	.	.	.	no
V	C5	H5	113.5(15)	.	.	.	no
C1	C5	H5	125.4(15)	.	.	.	no
C4	C5	H5	125.1(15)	.	.	.	no
P1	C6	H6	109.8(17)	.	.	.	no
P1	C6	H6'	109.5(19)	.	.	.	no

P1	C6	H6"	109.4(15)	.	.	.	no
H6	C6	H6'	107(2)	.	.	.	no
H6	C6	H6"	110(2)	.	.	.	no
H6'	C6	H6"	111(2)	.	.	.	no
P1	C7	H7	111.4(18)	.	.	.	no
P1	C7	H7'	103(2)	.	.	.	no
P1	C7	H7"	116(5)	.	.	.	no
H7	C7	H7'	111(3)	.	.	.	no
H7	C7	H7"	109(5)	.	.	.	no
H7'	C7	H7"	105(5)	.	.	.	no
P1	C8A	H81	110.00	.	.	.	no
P1	C8A	H81'	110.00	.	.	.	no
C9A	C8A	H81	110.00	.	.	.	no
C9A	C8A	H81'	110.00	.	.	.	no
H81	C8A	H81'	109.00	.	.	.	no
C9B	C8B	H82'	110.00	.	.	.	no
H82	C8B	H82'	108.00	.	.	.	no
P1	C8B	H82'	110.00	.	.	.	no
C9B	C8B	H82	110.00	.	.	.	no
P1	C8B	H82	110.00	.	.	.	no
C8A	C9A	H91	110.00	.	.	.	no
C8A	C9A	H91'	110.00	.	.	.	no
P2	C9A	H91	110.00	.	.	.	no
P2	C9A	H91'	110.00	.	.	.	no
H91	C9A	H91'	109.00	.	.	.	no
P2	C9B	H92	110.00	.	.	.	no
C8B	C9B	H92	110.00	.	.	.	no
C8B	C9B	H92'	110.00	.	.	.	no
P2	C9B	H92'	110.00	.	.	.	no
H92	C9B	H92'	109.00	.	.	.	no
P2	C10A	H101"	109.00	.	.	.	no
P2	C10A	H101	109.00	.	.	.	no
P2	C10A	H101'	109.00	.	.	.	no
H101'	C10A	H101	109.00	.	.	.	no
H101"	C10A	H101	109.00	.	.	.	no
H101'	C10A	H101"	110.00	.	.	.	no
P2	C10B	H102'	110.00	.	.	.	no
P2	C10B	H102"	110.00	.	.	.	no
P2	C10B	H102	110.00	.	.	.	no
H102'	C10B	H102"	109.00	.	.	.	no
H102'	C10B	H102	109.00	.	.	.	no
H102"	C10B	H102	109.00	.	.	.	no
P2	C11	H11	113.2(17)	.	.	.	no
P2	C11	H11'	110.6(16)	.	.	.	no
P2	C11	H11"	109.7(15)	.	.	.	no
H11	C11	H11'	106(2)	.	.	.	no
H11	C11	H11"	109(2)	.	.	.	no
H11'	C11	H11"	108(2)	.	.	.	no
C12	C13	H13	114.8(17)	.	.	.	no
C12	C13	H13'	108.3(17)	.	.	.	no
H13	C13	H13'	103(2)	.	.	.	no
H13	C13	H13"	105(2)	.	.	.	no
H13'	C13	H13"	115(2)	.	.	.	no
C12	C13	H13"	110.7(17)	.	.	.	no
C12	C14	H14	110.3(16)	.	.	.	no
C12	C14	H14'	109.2(15)	.	.	.	no
H14	C14	H14'	109(2)	.	.	.	no
H14	C14	H14"	108(2)	.	.	.	no
C12	C14	H14"	110.6(15)	.	.	.	no
H14'	C14	H14"	110(2)	.	.	.	no
C12	C15	H15'	113.2(16)	.	.	.	no
C12	C15	H15"	107.6(16)	.	.	.	no
C12	C15	H15	106.3(16)	.	.	.	no
H15	C15	H15"	106(2)	.	.	.	no
H15'	C15	H15"	110(2)	.	.	.	no
H15	C15	H15'	113(2)	.	.	.	no

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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
P2      V      P1      C6      -133.42(11)      .      .      .      .      no
P2      V      P1      C7      101.48(16)      .      .      .      .      no
P2      V      P1      C8A     -6.8(4)         .      .      .      .      no
N       V      P1      C6      -38.09(12)      .      .      .      .      no
N       V      P1      C7     -163.20(17)      .      .      .      .      no
N       V      P1      C8A     88.5(4)         .      .      .      .      no
C1      V      P1      C6      98.13(17)      .      .      .      .      no
C1      V      P1      C7     -27.0(2)        .      .      .      .      no
C1      V      P1      C8A    -135.3(4)        .      .      .      .      no
C2      V      P1      C6     145.77(13)      .      .      .      .      no
C2      V      P1      C7     20.66(18)       .      .      .      .      no
C2      V      P1      C8A    -87.7(4)         .      .      .      .      no
C3      V      P1      C6     132.26(12)      .      .      .      .      no
C3      V      P1      C7      7.16(17)        .      .      .      .      no
C3      V      P1      C8A   -101.2(4)        .      .      .      .      no
C4      V      P1      C6     96.58(13)       .      .      .      .      no
C4      V      P1      C7    -28.53(17)       .      .      .      .      no
C4      V      P1      C8A   -136.8(4)        .      .      .      .      no
C5      V      P1      C6     73.89(13)       .      .      .      .      no
C5      V      P1      C7    -51.21(17)       .      .      .      .      no
C5      V      P1      C8A   -159.5(4)        .      .      .      .      no
P1      V      P2      C9A     29.9(2)         .      .      .      .      no
P1      V      P2     C10A    -88.8(3)         .      .      .      .      no
P1      V      P2     C11    135.68(12)       .      .      .      .      no
N       V      P2      C9A    -65.8(2)         .      .      .      .      no
N       V      P2     C10A    175.6(4)         .      .      .      .      no
N       V      P2     C11     40.01(13)        .      .      .      .      no
C1      V      P2      C9A   -177.5(2)        .      .      .      .      no
C1      V      P2     C10A     63.8(4)         .      .      .      .      no
C1      V      P2     C11    -71.73(14)       .      .      .      .      no
C2      V      P2      C9A    159.4(2)         .      .      .      .      no
C2      V      P2     C10A     40.8(4)         .      .      .      .      no
C2      V      P2     C11    -94.75(13)       .      .      .      .      no
C3      V      P2      C9A    123.9(2)         .      .      .      .      no
C3      V      P2     C10A      5.3(4)          .      .      .      .      no
C3      V      P2     C11   -130.29(13)      .      .      .      .      no
C4      V      P2      C9A    110.4(3)         .      .      .      .      no
C4      V      P2     C10A     -8.2(4)          .      .      .      .      no
C4      V      P2     C11   -143.79(14)      .      .      .      .      no
C5      V      P2      C9A    158.2(3)         .      .      .      .      no
C5      V      P2     C10A     39.6(4)         .      .      .      .      no
C5      V      P2     C11    -95.96(17)       .      .      .      .      no
P1      V      C1      C2      78.14(19)       .      .      .      .      no
P1      V      C1      C5     -38.8(2)         .      .      .      .      no
P2      V      C1      C2    -41.55(16)       .      .      .      .      no
P2      V      C1      C5   -158.50(13)      .      .      .      .      no
N       V      C1      C2   -147.55(15)      .      .      .      .      no
N       V      C1      C5     95.51(16)       .      .      .      .      no
C2      V      C1      C5    -116.9(2)        .      .      .      .      no
C3      V      C1      C2     37.85(15)       .      .      .      .      no
C3      V      C1      C5    -79.10(17)       .      .      .      .      no
C4      V      C1      C2     79.93(17)       .      .      .      .      no
C4      V      C1      C5    -37.01(15)       .      .      .      .      no
C5      V      C1      C2    116.9(2)         .      .      .      .      no

```

P1	V	C2	C1	-139.00(13)	.	.	.	.	no
P1	V	C2	C3	-23.27(19)	.	.	.	.	no
P2	V	C2	C1	143.79(14)	.	.	.	.	no
P2	V	C2	C3	-100.48(15)	.	.	.	.	no
N	V	C2	C1	46.4(2)	.	.	.	.	no
N	V	C2	C3	162.12(15)	.	.	.	.	no
C1	V	C2	C3	115.7(2)	.	.	.	.	no
C3	V	C2	C1	-115.7(2)	.	.	.	.	no
C4	V	C2	C1	-78.58(16)	.	.	.	.	no
C4	V	C2	C3	37.16(15)	.	.	.	.	no
C5	V	C2	C1	-36.94(15)	.	.	.	.	no
C5	V	C2	C3	78.80(17)	.	.	.	.	no
P1	V	C3	C2	161.98(15)	.	.	.	.	no
P1	V	C3	C4	-80.84(15)	.	.	.	.	no
P2	V	C3	C2	80.67(15)	.	.	.	.	no
P2	V	C3	C4	-162.14(14)	.	.	.	.	no
C1	V	C3	C2	-37.87(15)	.	.	.	.	no
C1	V	C3	C4	79.31(17)	.	.	.	.	no
C2	V	C3	C4	117.2(2)	.	.	.	.	no
C4	V	C3	C2	-117.2(2)	.	.	.	.	no
C5	V	C3	C2	-79.43(16)	.	.	.	.	no
C5	V	C3	C4	37.76(15)	.	.	.	.	no
P1	V	C4	C3	100.19(15)	.	.	.	.	no
P1	V	C4	C5	-144.16(15)	.	.	.	.	no
P2	V	C4	C3	23.17(19)	.	.	.	.	no
P2	V	C4	C5	138.82(13)	.	.	.	.	no
N	V	C4	C3	-162.12(15)	.	.	.	.	no
N	V	C4	C5	-46.5(2)	.	.	.	.	no
C1	V	C4	C3	-78.87(17)	.	.	.	.	no
C1	V	C4	C5	36.78(15)	.	.	.	.	no
C2	V	C4	C3	-37.03(15)	.	.	.	.	no
C2	V	C4	C5	78.62(16)	.	.	.	.	no
C3	V	C4	C5	115.7(2)	.	.	.	.	no
C5	V	C4	C3	-115.7(2)	.	.	.	.	no
P1	V	C5	C1	158.41(13)	.	.	.	.	no
P1	V	C5	C4	41.06(17)	.	.	.	.	no
P2	V	C5	C1	38.7(2)	.	.	.	.	no
P2	V	C5	C4	-78.60(19)	.	.	.	.	no
N	V	C5	C1	-95.23(16)	.	.	.	.	no
N	V	C5	C4	147.43(15)	.	.	.	.	no
C1	V	C5	C4	-117.3(2)	.	.	.	.	no
C2	V	C5	C1	37.35(15)	.	.	.	.	no
C2	V	C5	C4	-80.00(17)	.	.	.	.	no
C3	V	C5	C1	79.31(17)	.	.	.	.	no
C3	V	C5	C4	-38.04(15)	.	.	.	.	no
C4	V	C5	C1	117.3(2)	.	.	.	.	no
N	V	C2	H2	-78(2)	.	.	.	.	no
C1	V	C2	H2	-125(2)	.	.	.	.	no
C3	V	C2	H2	120(2)	.	.	.	.	no
C4	V	C2	H2	157(2)	.	.	.	.	no
C5	V	C2	H2	-162(2)	.	.	.	.	no
P1	V	C3	H3	37(2)	.	.	.	.	no
P2	V	C3	H3	-44(2)	.	.	.	.	no
C1	V	C3	H3	-163(2)	.	.	.	.	no
C2	V	C3	H3	-125(2)	.	.	.	.	no
C4	V	C3	H3	118(2)	.	.	.	.	no
C5	V	C3	H3	156(2)	.	.	.	.	no
P1	V	C4	H4	-22(2)	.	.	.	.	no
P2	V	C4	H4	-99(2)	.	.	.	.	no
N	V	C4	H4	76(2)	.	.	.	.	no
C1	V	C4	H4	159(2)	.	.	.	.	no
C2	V	C4	H4	-159(2)	.	.	.	.	no
C3	V	C4	H4	-122(2)	.	.	.	.	no
C5	V	C4	H4	122(2)	.	.	.	.	no
P1	V	C5	H5	-80.0(17)	.	.	.	.	no
P2	V	C5	H5	160.3(16)	.	.	.	.	no

N	V	C5	H5	26.3(17)	.	.	.	.	no
C1	V	C5	H5	121.6(17)	.	.	.	.	no
P1	V	C1	H1	-160.1(15)	.	.	.	.	no
P2	V	C1	H1	80.3(15)	.	.	.	.	no
N	V	C1	H1	-25.7(15)	.	.	.	.	no
C2	V	C1	H1	121.8(15)	.	.	.	.	no
C3	V	C1	H1	159.7(15)	.	.	.	.	no
C4	V	C1	H1	-158.3(15)	.	.	.	.	no
C5	V	C1	H1	-121.2(15)	.	.	.	.	no
P1	V	C2	H2	96(2)	.	.	.	.	no
P2	V	C2	H2	19(2)	.	.	.	.	no
C2	V	C5	H5	158.9(17)	.	.	.	.	no
C3	V	C5	H5	-159.1(17)	.	.	.	.	no
C4	V	C5	H5	-121.1(17)	.	.	.	.	no
C7	P1	C8A	C9A	-149.4(6)	.	.	.	.	no
V	P1	C8A	C9A	-25.3(7)	.	.	.	.	no
C6	P1	C8A	C9A	109.6(6)	.	.	.	.	no
V	P2	C9A	C8A	-55.4(5)	.	.	.	.	no
C10A	P2	C9A	C8A	76.0(6)	.	.	.	.	no
C11	P2	C9A	C8A	178.9(5)	.	.	.	.	no
C2	C1	C5	V	-62.87(19)	.	.	.	.	no
C2	C1	C5	C4	-0.2(3)	.	.	.	.	no
V	C1	C2	C3	-63.95(19)	.	.	.	.	no
C5	C1	C2	V	63.27(19)	.	.	.	.	no
C5	C1	C2	C3	-0.7(3)	.	.	.	.	no
V	C1	C5	C4	62.71(19)	.	.	.	.	no
C1	C2	C3	V	64.15(19)	.	.	.	.	no
C1	C2	C3	C4	1.3(3)	.	.	.	.	no
V	C2	C3	C4	-62.91(19)	.	.	.	.	no
V	C3	C4	C5	-64.31(19)	.	.	.	.	no
C2	C3	C4	V	62.97(19)	.	.	.	.	no
C2	C3	C4	C5	-1.3(3)	.	.	.	.	no
C3	C4	C5	V	64.00(19)	.	.	.	.	no
C3	C4	C5	C1	0.9(3)	.	.	.	.	no
V	C4	C5	C1	-63.07(19)	.	.	.	.	no
P1	C8A	C9A	P2	49.5(7)	.	.	.	.	no

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_geom_contact_atom_site_label_2

_geom_contact_distance

_geom_contact_site_symmetry_1

_geom_contact_site_symmetry_2

_geom_contact_publ_flag

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P1	C3	3.404(3)	.	.	.	no
P1	C4	3.225(3)	.	.	.	no
P1	C9A	2.740(6)	.	.	.	no
P1	C9B	2.793(7)	.	.	.	no
P2	N	3.0425(19)	.	.	.	no
P2	P1	3.0526(8)	.	.	.	no
P2	C8A	2.804(8)	.	.	.	no
P2	C2	3.230(3)	.	.	.	no
P2	C3	3.412(3)	.	.	.	no
P2	C8B	2.671(10)	.	.	.	no
P1	H4	3.16(3)	.	.	.	no
P2	H2	3.16(3)	.	.	.	no
N	P1	3.0481(19)	.	.	.	no
N	P2	3.0425(19)	.	.	.	no
N	C1	3.197(3)	.	.	.	no
N	C5	3.199(3)	.	.	.	no
C1	N	3.197(3)	.	.	.	no
C1	C3	2.275(4)	.	.	.	no
C1	C4	2.278(4)	.	.	.	no
C2	C4	2.288(4)	.	.	.	no

C2	C10B	3.256(9)	.	.	no
C2	P2	3.230(3)	.	.	no
C2	C5	2.279(4)	.	.	no
C2	C10A	3.577(9)	.	.	no
C2	C7	3.554(5)	.	2_555	no
C3	C5	2.272(4)	.	.	no
C3	P2	3.412(3)	.	.	no
C3	C7	3.512(5)	.	.	no
C3	P1	3.404(3)	.	.	no
C3	C1	2.275(4)	.	.	no
C3	C10B	3.429(10)	.	.	no
C4	C7	3.393(5)	.	.	no
C4	C2	2.288(4)	.	.	no
C4	P1	3.225(3)	.	.	no
C4	C10B	3.543(10)	.	2_555	no
C4	C1	2.278(4)	.	.	no
C5	N	3.199(3)	.	.	no
C5	C2	2.279(4)	.	.	no
C5	C3	2.272(4)	.	.	no
C7	C2	3.554(5)	.	2_545	no
C10B	C4	3.543(10)	.	2_545	no
C1	H5	2.16(3)	.	.	no
C1	H2	2.13(3)	.	.	no
C2	H1	2.20(3)	.	.	no
C2	H7	2.75(3)	.	2_555	no
C2	H3	2.11(3)	.	.	no
C2	H102'	2.9300	.	.	no
C3	H101	3.0500	.	2_555	no
C3	H102	3.0200	.	.	no
C3	H2	2.09(3)	.	.	no
C3	H4	2.09(3)	.	.	no
C4	H102'	2.9800	.	4_554	no
C4	H102	2.6800	.	2_555	no
C4	H5	2.16(3)	.	.	no
C4	H101	2.8400	.	2_555	no
C4	H3	2.06(3)	.	.	no
C5	H1	2.18(3)	.	.	no
C5	H4	2.08(3)	.	.	no
C6	H1	3.04(3)	.	4_554	no
C7	H4	2.98(3)	.	.	no
C10A	H81	3.0800	.	.	no
C10B	H2	2.76(3)	.	.	no
C11	H5	3.07(3)	.	4_555	no
C13	H6	2.97(3)	.	.	no
C15	H11	2.95(3)	.	.	no
H1	H6'	2.56(4)	.	4_555	no
H1	C6	3.04(3)	.	4_555	no
H2	C10B	2.76(3)	.	.	no
H2	H102'	2.2100	.	.	no
H101"	H7'	2.3000	.	4_545	no
H101"	H11"	2.4200	.	.	no
H3	H102	2.5300	.	.	no
H3	H7	2.57(4)	.	.	no
H102'	H2	2.2100	.	.	no
H102'	C4	2.9800	.	4_555	no
H102'	C2	2.9300	.	.	no
H102'	H4	2.3800	.	4_555	no
H4	C7	2.98(3)	.	.	no
H4	H102'	2.3800	.	4_554	no
H4	H102	2.5800	.	2_555	no
H102"	H7'	2.4000	.	4_545	no
H5	H11'	2.50(4)	.	4_554	no
H5	C11	3.07(3)	.	4_554	no
H6	C13	2.97(3)	.	.	no
H6	H13"	2.41(4)	.	.	no
H6	H14'	2.59(4)	.	2_645	no

H6'	H1	2.56(4)	.	4_554	no
H6"	H7'	2.55(4)	.	.	no
H6"	H81'	2.5400	.	.	no
H7	H3	2.57(4)	.	.	no
H7	H81	2.4900	.	.	no
H7	C2	2.75(3)	.	2_545	no
H7'	H6"	2.55(4)	.	.	no
H7'	H81	2.4000	.	.	no
H7'	H102"	2.4000	.	4_544	no
H7'	H101"	2.3000	.	4_544	no
H11	C15	2.95(3)	.	.	no
H11	H15'	2.49(4)	.	.	no
H11'	H5	2.50(4)	.	4_555	no
H11"	H101"	2.4200	.	.	no
H13	H14'	2.58(4)	.	.	no
H13	H15"	2.55(4)	.	.	no
H13	H82'	2.5700	.	2_655	no
H13'	H14"	2.48(4)	.	.	no
H13"	H6	2.41(4)	.	.	no
H13"	H15	2.42(4)	.	.	no
H14	H15'	2.56(4)	.	.	no
H14'	H6	2.59(4)	.	2_655	no
H14'	H13	2.58(4)	.	.	no
H14'	H15"	2.51(4)	.	.	no
H14"	H13'	2.48(4)	.	.	no
H15	H13"	2.42(4)	.	.	no
H15'	H14	2.56(4)	.	.	no
H15'	H11	2.49(4)	.	.	no
H15"	H13	2.55(4)	.	.	no
H15"	H14'	2.51(4)	.	.	no
H81	C10A	3.0800	.	.	no
H81	H7	2.4900	.	.	no
H81	H7'	2.4000	.	.	no
H81'	H6"	2.5400	.	.	no
H82'	H13	2.5700	.	2_645	no
H101	C3	3.0500	.	2_545	no
H101	C4	2.8400	.	2_545	no
H102	C3	3.0200	.	.	no
H102	H3	2.5300	.	.	no
H102	C4	2.6800	.	2_545	no
H102	H4	2.5800	.	2_545	no

Loop Mechanism for Extra Tables(s)

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#_publ_manuscript_incl_extra_item
#'_geom_extra_tableA_col_1'
#'_geom_extra_tableA_col_2'
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#'_geom_extra_table_head_A'
#'_geom_table_footnote_A'
#'_geom_extra_tableB_col_1'
#'_geom_extra_tableB_col_2'
#'_geom_extra_tableB_col_3'
#'_geom_extra_table_head_B'
#'_geom_table_footnote_B'
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#
#loop_
#_geom_extra_tableA_col_1
#_geom_extra_tableA_col_2
#_geom_extra_tableA_col_3
# ? ? ?
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#loop_
#_geom_extra_tableB_col_1
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#_geom_table_footnote_A
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# ?
#;
```

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#
#_geom_table_footnote_B
#;
# ?
#;
```

```
#
#_geom_table_footnote_A
#;
# ?
#;
```

```
#
#_geom_table_footnote_B
#;
# ?
#;
```

===END of Crystallographic Information File

```
# CIF-file generated for C18H28NP2V P21/c q1075
```

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#=====
data_global
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# 0. AUDIT DETAILS
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_audit_creation_date '2010-06-04 15:46:12'
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_audit_creation_method
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PLATON <TABLE ACC> option (version :: 310310)
SHELXL97-2 & Manual Editing
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_audit_update_record
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?
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;
```

```
#=====
```

```
# 1. SUBMISSION DETAILS
```

```
_publ_contact_author_name
```

```
# Name of author for correspondence
```

```
;
```

```
Drs. A. Meetsma
```

```
;
_publ_contact_author_address      # Address of author for correspondence
;
```

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

```
;
_publ_contact_author_email        A.Meetsma@rug.nl
_publ_contact_author_fax          '+31 50 3634441'
_publ_contact_author_phone        '+31 50 3634368'
```

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

```
_publ_contact_letter              # Include date of submission
```

```
;
Dat of submission :    2010-06-04  15:46:12
```

```
Consider this CIF submission for deposition of the first
X-ray structure of a manuscript to be submitted to : Organometallics
(Our Compound_Identification_Code : q1075)
```

```
;
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```
#=====
```

2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_recd_electronic      ?
_journal_date_to_coeditor           ?
_journal_date_from_coeditor         ?
_journal_date_accepted              ?
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_journal_date_printers_first       ?
_journal_date_printers_final        ?
_journal_date_proofs_out            ?
_journal_date_proofs_in             ?
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_journal_coeditor_name             ?
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_journal_volume                     ?
_journal_issue                      ?
_journal_page_first                 ?
_journal_page_last                  ?
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_journal_suppl_publ_number         ?
_journal_suppl_publ_pages          ?
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#=====

# 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
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?
;
_publ_section_abstract
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?
;

# Insert blank lines between paragraphs

_publ_section_comment
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;
_publ_section_exptl_prep
;
;
_publ_section_exptl_refinement
;

The structure was solved by Patterson methods and extension of the model was
accomplished by direct methods applied to difference structure factors using
the program <i>DIRDIF</i>. The positional and anisotropic displacement
parameters for the non-hydrogen atoms were refined. A few atoms showed

```

unrealistic displacement parameters when allowed to vary anisotropically, suggesting dynamic disorder (dynamic means that the smeared electron density is due to fluctuations of the atomic positions within each unit cell). The smeared electron density for C5, C9 and C10 has been described by two site occupancy factors with separately refined displacement parameters. The s.o.f. of the major fraction of the component of the disorder model refined to a value of 0.560(9).

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 $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(\text{methyl } C)$.

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

Assigned values of bond distances for secondary C-H₂ = 0.99 Å, methyl C-H₃ = 0.98 Å and aromatic C-H = 0.95 Å.

;

_publ_section_related_literature

;

;

Insert blank lines between references

_publ_section_references

;

Beurskens, P.T., Beurskens, G., Gelder, R. de, Smits, J.M.M., Garc'ia-Granda, S. & Gould, R.O. (2008).

The DIRDIF08 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

Bruker, (2007). SMART (Version 5.632), SAINT-Plus (Version 7.46a) and SADABS (Version 2.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Meetsma, A. (2010). Extended version of the program PLUTO. University of Groningen, The Netherlands. (unpublished).

Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

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

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_publ_section_figure_captions

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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.

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_publ_section_acknowledgements

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5. CHEMICAL DATA

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_chemical_formula_sum
'C18 H28 N P2 V'
_chemical_formula_iupac              ?
_chemical_formula_weight              371.32
_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
V   V   0.3005   0.5294
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
P   P   0.1023   0.0942
'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                monoclinic
_symmetry_space_group_name_Hall      '-P 2ybc'
_symmetry_space_group_name_H-M       'P 21/c'
_symmetry_Int_Tables_number          14

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

_cell_length_a                       10.404(1)
_cell_length_b                       10.939(1)
_cell_length_c                       17.404(2)
_cell_angle_alpha                     90
_cell_angle_beta                      95.317(2)
_cell_angle_gamma                     90
_cell_volume                          1972.2(3)
_cell_formula_units_Z                 4

_cell_measurement_temperature        100(1)
_cell_measurement_reflns_used        6591
_cell_measurement_theta_min          2.71
_cell_measurement_theta_max          29.25
_cell_special_details

;
The final unit cell was obtained from the xyz centroids of
6591 reflections after integration using the SAINT software

```

```

package (Bruker, 2000).
;

_exptl_crystal_description      'block'
_exptl_crystal_colour           'brown'
_exptl_crystal_size_max        0.49
_exptl_crystal_size_mid        0.33
_exptl_crystal_size_min        0.13
_exptl_crystal_size_rad        ?
_exptl_crystal_density_meas     ?
_exptl_crystal_density_diffn    1.250
_exptl_crystal_density_method   'not measured'
_exptl_crystal_F_000            784
_exptl_absorpt_coefficient_mu   0.662
_exptl_absorpt_correction_type  'multi-scan'
_exptl_absorpt_process_details  '(SADABS, (Bruker, 2007))'
_exptl_absorpt_correction_T_min 0.7005
_exptl_absorpt_correction_T_max 0.9189

#=====

# 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, 2007)).
;
_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)
_diffn_reflns_number            17426
_diffn_reflns_av_R_equivalents 0.0503
_diffn_reflns_av_sigmaI/netI   0.0527
_diffn_reflns_limit_h_min      -13
_diffn_reflns_limit_h_max      13
_diffn_reflns_limit_k_min      -14

```



```

_diffrn_reflms_limit_k_max      14
_diffrn_reflms_limit_l_min     -22
_diffrn_reflms_limit_l_max      23
_diffrn_reflms_theta_min       2.71
_diffrn_reflms_theta_max       28.28
_diffrn_measured_fraction_theta_max 0.984
_diffrn_reflms_theta_full      25.00
_diffrn_measured_fraction_theta_full 0.993

_diffrn_reflms_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
_reflms_number_total            4821
_reflms_number_gt               3837
_reflms_threshold_expression    I>2\sigma(I)

_computing_data_collection      'SMART (Bruker, 2007)'
_computing_cell_refinement      'SAINT-Plus (Bruker, 2007)'
_computing_data_reduction       'SAINT-Plus (Bruker, 2007)'
_computing_structure_solution
;
DIRDIF-08 (Beurskens et al., 2008)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics
;
PLATON (Spek, 2003)
PLUTO (Meetsma, 2010)
;
_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)+(0.0460P)^2+1.4740P] 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  ?
_chemical_absolute_configuration '.'

```

```
# choose from: rm (reference molecule of known chirality),
# ad (anomalous dispersion - Flack), rmad (rm and ad),
# syn (from synthesis), unk (unknown) or . (not applicable).
```

```
_refine_ls_abs_structure_Flack      ?
_refine_ls_number_reflns            4821
_refine_ls_number_parameters         233
_refine_ls_number_restraints         0
_refine_ls_number_constraints        ?
_refine_ls_R_factor_all              0.0656
_refine_ls_R_factor_gt               0.0489
_refine_ls_wR_factor_ref             0.1150
_refine_ls_wR_factor_gt             0.1086
_refine_ls_goodness_of_fit_ref       1.054
_refine_ls_restrained_S_all          1.054
_refine_ls_shift/su_max              0.000
_refine_ls_shift/su_mean             0.000

_refine_diff_density_max             0.491
_refine_diff_density_min            -0.458
_refine_diff_density_rms             0.073
```

```
#=====
```

``` # 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
V V Uani 0.22347(3) 0.25684(3) 0.19099(2) 1.0 0.0173(1) . .
P1 P Uani 0.16270(6) 0.09864(5) 0.27242(4) 1.0 0.0215(2) . .
P2 P Uani 0.25154(6) 0.08939(6) 0.10922(4) 1.0 0.0259(2) . .
N N Uani 0.07117(18) 0.27471(16) 0.14493(11) 1.0 0.0188(5) . .
C1 C Uani 0.4181(3) 0.3336(4) 0.17191(19) 1.0 0.0538(13) . .
C2 C Uani 0.4361(3) 0.2649(3) 0.24014(19) 1.0 0.0383(9) . .
C3 C Uani 0.3657(3) 0.3178(3) 0.29427(18) 1.0 0.0431(10) . .
C4 C Uani 0.3036(3) 0.4185(3) 0.2635(3) 1.0 0.0574(13) . .
C5A C Uani 0.3205(12) 0.4395(11) 0.1981(7) 0.565(9) 0.035(3) . .
C6 C Uani 0.2786(3) 0.0412(3) 0.35046(19) 1.0 0.0439(10) . .
C7 C Uani 0.0191(2) 0.1164(2) 0.32483(15) 1.0 0.0296(8) . .
C8 C Uani 0.1253(4) -0.0414(3) 0.21481(18) 1.0 0.0536(13) . .
C9A C Uani 0.1296(5) -0.0218(4) 0.1314(3) 0.565(9) 0.0262(16) . .
C10A C Uani 0.2027(8) 0.1161(7) 0.0036(4) 0.565(9) 0.033(2) . .
C11 C Uani 0.4063(3) 0.0203(3) 0.0982(2) 1.0 0.0625(13) . .
C12 C Uani -0.0452(2) 0.27905(19) 0.10009(13) 1.0 0.0175(6) . .
C13 C Uani -0.1553(2) 0.2169(2) 0.12002(15) 1.0 0.0285(7) . .
C14 C Uani -0.2725(2) 0.2261(2) 0.07463(16) 1.0 0.0292(8) . .
C15 C Uani -0.2861(2) 0.2978(2) 0.00844(14) 1.0 0.0231(7) . .
C16 C Uani -0.1761(2) 0.3565(2) -0.01236(14) 1.0 0.0272(7) . .
C17 C Uani -0.0581(2) 0.3474(2) 0.03153(14) 1.0 0.0235(7) . .
C18 C Uani -0.4156(2) 0.3155(3) -0.03755(16) 1.0 0.0327(8) . .
C10B C Uani 0.1660(10) 0.0735(11) 0.0179(7) 0.435(9) 0.048(3) . .
C9B C Uani 0.2073(8) -0.0646(6) 0.1579(5) 0.435(9) 0.038(3) . .
C5B C Uani 0.3520(15) 0.4204(12) 0.1736(11) 0.435(9) 0.041(5) . .
H2 H Uiso 0.48826 0.19382 0.24763 1.0 0.0460 . .
```

H101' H Uiso 0.26559 0.17017 -0.01766 0.565(9) 0.0489 . .
 H6 H Uiso 0.29045 0.10258 0.39150 1.0 0.0661 . .
 H101" H Uiso 0.11712 0.15433 -0.00252 0.565(9) 0.0489 . .
 H3 H Uiso 0.36106 0.28855 0.34533 1.0 0.0517 . .
 H7 H Uiso -0.00313 0.03744 0.34675 1.0 0.0443 . .
 H7' H Uiso -0.05319 0.14510 0.28930 1.0 0.0443 . .
 H7" H Uiso 0.03673 0.17601 0.36649 1.0 0.0443 . .
 H11 H Uiso 0.39408 -0.05276 0.06571 1.0 0.0937 . .
 H11' H Uiso 0.44774 -0.00272 0.14897 1.0 0.0937 . .
 H6' H Uiso 0.36155 0.02483 0.33004 1.0 0.0661 . .
 H6" H Uiso 0.24537 -0.03451 0.37138 1.0 0.0661 . .
 H1 H Uiso 0.45285 0.32186 0.12388 1.0 0.0646 . .
 H16 H Uiso -0.18180 0.40442 -0.05807 1.0 0.0327 . .
 H17 H Uiso 0.01518 0.38798 0.01489 1.0 0.0282 . .
 H18 H Uiso -0.47907 0.26002 -0.01806 1.0 0.0491 . .
 H18' H Uiso -0.40741 0.29757 -0.09205 1.0 0.0491 . .
 H18" H Uiso -0.44412 0.40018 -0.03230 1.0 0.0491 . .
 H41 H Uiso 0.25067 0.46846 0.29220 1.0 0.0687 . .
 H51 H Uiso 0.28442 0.50479 0.16731 0.565(9) 0.0423 . .
 H81 H Uiso 0.18793 -0.10599 0.23220 1.0 0.0644 . .
 H81' H Uiso 0.03811 -0.07057 0.22442 1.0 0.0644 . .
 H91 H Uiso 0.04388 0.00667 0.109 0.565(9) 0.0313 . .
 H91' H Uiso 0.14778 -0.10076 0.10676 0.565(9) 0.0313 . .
 H101 H Uiso 0.19985 0.03785 -0.02383 0.565(9) 0.0489 . .
 H11" H Uiso 0.46116 0.07884 0.07380 1.0 0.0937 . .
 H13 H Uiso -0.14993 0.16776 0.16520 1.0 0.0342 . .
 H14 H Uiso -0.34512 0.18217 0.08933 1.0 0.0351 . .
 H102' H Uiso 0.07321 0.07991 0.02293 0.435(9) 0.0709 . .
 H102" H Uiso 0.185 -0.00646 -0.00375 0.435(9) 0.0709 . .
 H52 H Uiso 0.33080 0.47823 0.13367 0.435(9) 0.0494 . .
 H92 H Uiso 0.16448 -0.12022 0.11858 0.435(9) 0.0462 . .
 H92' H Uiso 0.28689 -0.105 0.18099 0.435(9) 0.0462 . .
 H102 H Uiso 0.19212 0.13822 -0.01633 0.435(9) 0.0709 . .

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

V 0.0170(2) 0.0153(2) 0.0185(2) 0.0035(1) -0.0038(1) -0.0026(1)
 P1 0.0270(3) 0.0181(3) 0.0198(3) 0.0040(2) 0.0037(3) 0.0002(2)
 P2 0.0247(3) 0.0314(3) 0.0223(3) -0.0055(3) 0.0061(3) -0.0094(3)
 N 0.0202(9) 0.0161(8) 0.0189(10) 0.0022(7) -0.0047(8) -0.0018(7)
 C1 0.051(2) 0.076(3) 0.0353(18) -0.0064(17) 0.0085(15) -0.048(2)
 C2 0.0227(12) 0.0317(14) 0.057(2) -0.0021(13) -0.0150(13) -0.0015(11)
 C3 0.0473(17) 0.0460(17) 0.0333(17) -0.0065(13) -0.0100(14) -0.0195(14)
 C4 0.0324(16) 0.0420(18) 0.094(3) -0.036(2) -0.0141(19) -0.0031(14)
 C5A 0.042(6) 0.014(3) 0.044(6) 0.004(3) -0.024(4) -0.010(3)
 C6 0.0330(14) 0.0494(18) 0.049(2) 0.0311(15) 0.0018(13) 0.0052(13)
 C7 0.0292(13) 0.0343(13) 0.0258(14) 0.0088(11) 0.0061(11) 0.0024(11)
 C8 0.100(3) 0.0250(14) 0.0403(18) -0.0071(12) 0.0312(19) -0.0277(16)
 C9A 0.027(3) 0.023(2) 0.028(3) -0.0032(18) 0.000(2) -0.006(2)
 C10A 0.048(5) 0.033(3) 0.018(3) -0.003(2) 0.007(3) 0.004(3)
 C11 0.0432(18) 0.0466(19) 0.092(3) -0.0337(19) -0.0244(18) 0.0217(15)
 C12 0.0195(10) 0.0142(9) 0.0182(12) -0.0023(8) -0.0011(9) 0.0008(8)
 C13 0.0279(12) 0.0264(12) 0.0297(14) 0.0112(10) -0.0055(11) -0.0079(10)
 C14 0.0238(12) 0.0247(12) 0.0377(16) 0.0049(11) -0.0051(11) -0.0076(9)
 C15 0.0226(11) 0.0253(11) 0.0202(12) -0.0068(9) -0.0049(10) 0.0044(9)
 C16 0.0274(12) 0.0391(14) 0.0148(12) 0.0064(10) 0.0003(10) 0.0085(11)
 C17 0.0215(11) 0.0298(12) 0.0195(12) 0.0046(10) 0.0036(9) 0.0017(9)
 C18 0.0265(13) 0.0389(15) 0.0302(15) -0.0037(12) -0.0111(11) 0.0034(11)
 C10B 0.035(5) 0.061(7) 0.043(6) -0.023(5) -0.015(4) 0.015(5)
 C9B 0.049(5) 0.017(3) 0.054(5) -0.008(3) 0.032(4) -0.013(3)

C5B 0.039(7) 0.015(6) 0.063(10) 0.020(5) -0.030(6) -0.014(5)

#=====

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

V	P1	2.3599(7)	.	.	yes
V	P2	2.3543(8)	.	.	yes
V	N	1.7193(19)	.	.	yes
V	C1	2.245(3)	.	.	yes
V	C2	2.298(3)	.	.	yes
V	C3	2.318(3)	.	.	yes
V	C4	2.285(4)	.	.	yes
V	C5A	2.237(12)	.	.	yes
V	C5B	2.271(14)	.	.	yes
P1	C6	1.841(3)	.	.	yes
P1	C7	1.832(2)	.	.	yes
P1	C8	1.852(3)	.	.	yes
P2	C9A	1.825(5)	.	.	yes
P2	C10A	1.884(7)	.	.	yes
P2	C11	1.805(3)	.	.	yes
P2	C9B	1.960(7)	.	.	yes
P2	C10B	1.757(12)	.	.	yes
N	C12	1.379(3)	.	.	yes
C1	C2	1.403(5)	.	.	no
C1	C5A	1.633(13)	.	.	no
C1	C5B	1.174(15)	.	.	no
C2	C3	1.374(5)	.	.	no
C3	C4	1.361(5)	.	.	no
C4	C5A	1.190(13)	.	.	no
C4	C5B	1.688(19)	.	.	no
C8	C9A	1.472(6)	.	.	no
C8	C9B	1.389(9)	.	.	no
C12	C13	1.403(3)	.	.	no
C12	C17	1.404(3)	.	.	no
C13	C14	1.394(3)	.	.	no
C14	C15	1.390(4)	.	.	no
C15	C16	1.389(3)	.	.	no
C15	C18	1.514(3)	.	.	no
C16	C17	1.388(3)	.	.	no
C1	H1	0.95	.	.	no
C2	H2	0.95	.	.	no
C3	H3	0.95	.	.	no
C4	H41	0.95	.	.	no
C5A	H51	0.95	.	.	no
C5B	H52	0.95	.	.	no
C6	H6	0.98	.	.	no
C6	H6"	0.98	.	.	no
C6	H6'	0.98	.	.	no
C7	H7	0.98	.	.	no

C7	H7'	0.98	.	.	no
C7	H7"	0.98	.	.	no
C8	H81	0.99	.	.	no
C8	H81'	0.99	.	.	no
C9A	H91'	0.99	.	.	no
C9A	H91	0.99	.	.	no
C9B	H92'	0.99	.	.	no
C9B	H92	0.99	.	.	no
C9B	H81	1.40	.	.	no
C10A	H101	0.98	.	.	no
C10A	H101'	0.98	.	.	no
C10A	H101"	0.98	.	.	no
C10B	H102	0.98	.	.	no
C10B	H102"	0.98	.	.	no
C10B	H102'	0.98	.	.	no
C11	H11"	0.98	.	.	no
C11	H11	0.98	.	.	no
C11	H11'	0.98	.	.	no
C13	H13	0.95	.	.	no
C14	H14	0.95	.	.	no
C16	H16	0.95	.	.	no
C17	H17	0.95	.	.	no
C18	H18	0.98	.	.	no
C18	H18'	0.98	.	.	no
C18	H18"	0.98	.	.	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

P1	V	P2	81.24(2)	.	.	.	yes
P1	V	N	94.40(6)	.	.	.	yes
P1	V	C1	131.19(10)	.	.	.	yes
P1	V	C2	96.13(8)	.	.	.	yes
P1	V	C3	86.13(8)	.	.	.	yes
P1	V	C4	109.89(12)	.	.	.	yes
P1	V	C5A	140.0(3)	.	.	.	yes
P1	V	C5B	148.4(5)	.	.	.	yes
P2	V	N	88.12(6)	.	.	.	yes
P2	V	C1	92.15(10)	.	.	.	yes
P2	V	C2	94.92(8)	.	.	.	yes
P2	V	C3	125.91(8)	.	.	.	yes
P2	V	C4	151.25(9)	.	.	.	yes
P2	V	C5A	130.4(3)	.	.	.	yes
P2	V	C5B	115.2(4)	.	.	.	yes
N	V	C1	133.90(11)	.	.	.	yes
N	V	C2	169.37(10)	.	.	.	yes
N	V	C3	145.43(10)	.	.	.	yes
N	V	C4	116.29(10)	.	.	.	yes
N	V	C5A	108.4(3)	.	.	.	yes
N	V	C5B	112.1(4)	.	.	.	yes
C1	V	C2	35.95(12)	.	.	.	yes
C1	V	C3	59.16(11)	.	.	.	yes
C1	V	C4	60.28(14)	.	.	.	yes
C1	V	C5A	42.7(3)	.	.	.	yes
C1	V	C5B	30.1(4)	.	.	.	yes
C2	V	C3	34.62(11)	.	.	.	yes
C2	V	C4	58.36(11)	.	.	.	yes
C2	V	C5A	62.1(3)	.	.	.	yes
C2	V	C5B	57.4(4)	.	.	.	yes
C3	V	C4	34.40(13)	.	.	.	yes

C3	V	C5A	56.5(3)	.	.	.	yes
C3	V	C5B	62.3(5)	.	.	.	yes
C4	V	C5A	30.5(3)	.	.	.	yes
C4	V	C5B	43.5(5)	.	.	.	yes
V	P1	C6	119.98(10)	.	.	.	yes
V	P1	C7	119.84(8)	.	.	.	yes
V	P1	C8	109.63(11)	.	.	.	yes
C6	P1	C7	100.23(13)	.	.	.	yes
C6	P1	C8	101.97(15)	.	.	.	yes
C7	P1	C8	102.54(15)	.	.	.	yes
V	P2	C9A	105.26(16)	.	.	.	yes
V	P2	C10A	115.6(2)	.	.	.	yes
V	P2	C11	123.50(11)	.	.	.	yes
V	P2	C9B	111.1(2)	.	.	.	yes
V	P2	C10B	122.9(4)	.	.	.	yes
C9A	P2	C10A	100.4(3)	.	.	.	yes
C9A	P2	C11	112.83(19)	.	.	.	yes
C10A	P2	C11	97.1(3)	.	.	.	yes
C9B	P2	C11	86.2(3)	.	.	.	yes
C10B	P2	C11	104.2(4)	.	.	.	yes
C9B	P2	C10B	100.8(5)	.	.	.	yes
V	N	C12	172.11(17)	.	.	.	yes
V	C1	C2	74.1(2)	.	.	.	yes
V	C1	C5A	68.4(4)	.	.	.	yes
V	C1	C5B	76.1(7)	.	.	.	yes
C2	C1	C5A	100.5(5)	.	.	.	no
C2	C1	C5B	116.4(10)	.	.	.	no
V	C2	C1	69.95(18)	.	.	.	yes
V	C2	C3	73.47(19)	.	.	.	yes
C1	C2	C3	108.5(3)	.	.	.	no
V	C3	C2	71.92(19)	.	.	.	yes
V	C3	C4	71.5(2)	.	.	.	yes
C2	C3	C4	109.6(3)	.	.	.	no
V	C4	C3	74.1(2)	.	.	.	yes
V	C4	C5A	72.5(6)	.	.	.	yes
V	C4	C5B	67.8(5)	.	.	.	yes
C3	C4	C5A	115.2(7)	.	.	.	no
C3	C4	C5B	101.7(5)	.	.	.	no
V	C5A	C1	68.9(4)	.	.	.	yes
V	C5A	C4	77.0(6)	.	.	.	yes
C1	C5A	C4	106.3(8)	.	.	.	no
C1	C5B	C4	103.8(11)	.	.	.	no
V	C5B	C4	68.7(5)	.	.	.	yes
V	C5B	C1	73.7(7)	.	.	.	yes
P1	C8	C9A	112.9(3)	.	.	.	yes
P1	C8	C9B	115.2(4)	.	.	.	yes
P2	C9A	C8	113.0(3)	.	.	.	yes
P2	C9B	C8	109.6(4)	.	.	.	yes
N	C12	C17	120.60(19)	.	.	.	yes
C13	C12	C17	116.9(2)	.	.	.	no
N	C12	C13	122.5(2)	.	.	.	yes
C12	C13	C14	121.1(2)	.	.	.	no
C13	C14	C15	121.8(2)	.	.	.	no
C14	C15	C16	117.0(2)	.	.	.	no
C16	C15	C18	121.2(2)	.	.	.	no
C14	C15	C18	121.8(2)	.	.	.	no
C15	C16	C17	122.1(2)	.	.	.	no
C12	C17	C16	121.1(2)	.	.	.	no
V	C1	H1	120	.	.	.	no
C2	C1	H1	130	.	.	.	no
C5A	C1	H1	130	.	.	.	no
C5B	C1	H1	114	.	.	.	no
V	C2	H2	123	.	.	.	no
C1	C2	H2	126	.	.	.	no
C3	C2	H2	126	.	.	.	no
V	C3	H3	123	.	.	.	no

C2	C3	H3	125	.	.	.	no
C4	C3	H3	125	.	.	.	no
V	C4	H41	122	.	.	.	no
C3	C4	H41	122	.	.	.	no
C5A	C4	H41	122	.	.	.	no
C5B	C4	H41	136	.	.	.	no
V	C5A	H51	119	.	.	.	no
C1	C5A	H51	127	.	.	.	no
C4	C5A	H51	127	.	.	.	no
C4	C5B	H52	128	.	.	.	no
V	C5B	H52	121	.	.	.	no
C1	C5B	H52	128	.	.	.	no
P1	C6	H6	109	.	.	.	no
P1	C6	H6'	109	.	.	.	no
P1	C6	H6"	109	.	.	.	no
H6	C6	H6'	110	.	.	.	no
H6'	C6	H6"	109	.	.	.	no
H6	C6	H6"	109	.	.	.	no
P1	C7	H7"	109	.	.	.	no
P1	C7	H7'	109	.	.	.	no
H7'	C7	H7"	110	.	.	.	no
H7	C7	H7'	109	.	.	.	no
H7	C7	H7"	109	.	.	.	no
P1	C7	H7	109	.	.	.	no
C9A	C8	H81'	109	.	.	.	no
H81	C8	H81'	108	.	.	.	no
C9B	C8	H81	70	.	.	.	no
C9B	C8	H81'	134	.	.	.	no
P1	C8	H81	109	.	.	.	no
P1	C8	H81'	109	.	.	.	no
C9A	C8	H81	109	.	.	.	no
C8	C9A	H91'	109	.	.	.	no
H91	C9A	H91'	108	.	.	.	no
C8	C9A	H91	109	.	.	.	no
P2	C9A	H91	109	.	.	.	no
P2	C9A	H91'	109	.	.	.	no
P2	C9B	H92'	110	.	.	.	no
C8	C9B	H81	42	.	.	.	no
C8	C9B	H92	110	.	.	.	no
C8	C9B	H92'	110	.	.	.	no
P2	C9B	H81	137	.	.	.	no
P2	C9B	H92	110	.	.	.	no
H81	C9B	H92'	71	.	.	.	no
H92	C9B	H92'	108	.	.	.	no
H81	C9B	H92	110	.	.	.	no
P2	C10A	H101'	109	.	.	.	no
P2	C10A	H101"	109	.	.	.	no
H101"	C10A	H101	109	.	.	.	no
P2	C10A	H101	109	.	.	.	no
H101'	C10A	H101"	109	.	.	.	no
H101'	C10A	H101	110	.	.	.	no
P2	C10B	H102"	109	.	.	.	no
P2	C10B	H102	109	.	.	.	no
H102'	C10B	H102"	109	.	.	.	no
P2	C10B	H102'	109	.	.	.	no
H102'	C10B	H102	109	.	.	.	no
H102"	C10B	H102	110	.	.	.	no
P2	C11	H11	109	.	.	.	no
H11	C11	H11'	109	.	.	.	no
P2	C11	H11'	110	.	.	.	no
P2	C11	H11"	109	.	.	.	no
H11'	C11	H11"	109	.	.	.	no
H11	C11	H11"	109	.	.	.	no
C12	C13	H13	119	.	.	.	no
C14	C13	H13	119	.	.	.	no
C15	C14	H14	119	.	.	.	no

C13	C14	H14	119	.	.	.	no
C15	C16	H16	119	.	.	.	no
C17	C16	H16	119	.	.	.	no
C12	C17	H17	119	.	.	.	no
C16	C17	H17	119	.	.	.	no
C15	C18	H18"	110	.	.	.	no
H18	C18	H18"	109	.	.	.	no
H18'	C18	H18"	110	.	.	.	no
H18	C18	H18'	109	.	.	.	no
C15	C18	H18	109	.	.	.	no
C15	C18	H18'	109	.	.	.	no

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P2	V	P1	C6	99.89(12)	.	.	.	.	no
P2	V	P1	C7	-135.55(10)	.	.	.	.	no
P2	V	P1	C8	-17.49(14)	.	.	.	.	no
N	V	P1	C6	-172.69(14)	.	.	.	.	no
N	V	P1	C7	-48.14(11)	.	.	.	.	no
N	V	P1	C8	69.92(15)	.	.	.	.	no
C1	V	P1	C6	14.74(18)	.	.	.	.	no
C1	V	P1	C7	139.30(16)	.	.	.	.	no
C1	V	P1	C8	-102.64(19)	.	.	.	.	no
C2	V	P1	C6	5.84(15)	.	.	.	.	no
C2	V	P1	C7	130.39(12)	.	.	.	.	no
C2	V	P1	C8	-111.55(16)	.	.	.	.	no
C3	V	P1	C6	-27.36(14)	.	.	.	.	no
C3	V	P1	C7	97.20(12)	.	.	.	.	no
C3	V	P1	C8	-144.74(16)	.	.	.	.	no
C4	V	P1	C6	-52.68(15)	.	.	.	.	no
C4	V	P1	C7	71.87(13)	.	.	.	.	no
C4	V	P1	C8	-170.07(16)	.	.	.	.	no
C5A	V	P1	C6	-46.9(5)	.	.	.	.	no
C5A	V	P1	C7	77.7(5)	.	.	.	.	no
C5A	V	P1	C8	-164.3(5)	.	.	.	.	no
P1	V	P2	C9A	32.28(17)	.	.	.	.	no
P1	V	P2	C10A	142.0(3)	.	.	.	.	no
P1	V	P2	C11	-99.23(14)	.	.	.	.	no
N	V	P2	C9A	-62.46(18)	.	.	.	.	no
N	V	P2	C10A	47.3(3)	.	.	.	.	no
N	V	P2	C11	166.03(15)	.	.	.	.	no
C1	V	P2	C9A	163.67(19)	.	.	.	.	no
C1	V	P2	C10A	-86.6(3)	.	.	.	.	no
C1	V	P2	C11	32.16(16)	.	.	.	.	no
C2	V	P2	C9A	127.75(19)	.	.	.	.	no
C2	V	P2	C10A	-122.5(3)	.	.	.	.	no
C2	V	P2	C11	-3.76(16)	.	.	.	.	no
C3	V	P2	C9A	110.99(19)	.	.	.	.	no
C3	V	P2	C10A	-139.3(3)	.	.	.	.	no
C3	V	P2	C11	-20.52(17)	.	.	.	.	no
C4	V	P2	C9A	148.1(3)	.	.	.	.	no
C4	V	P2	C10A	-102.2(4)	.	.	.	.	no
C4	V	P2	C11	16.5(3)	.	.	.	.	no
C5A	V	P2	C9A	-175.2(4)	.	.	.	.	no
C5A	V	P2	C10A	-65.5(5)	.	.	.	.	no
C5A	V	P2	C11	53.3(4)	.	.	.	.	no
P1	V	C1	C2	-15.2(3)	.	.	.	.	no

P1	V	C1	C5A	-123.6(5)	.	.	.	.	no
P2	V	C1	C2	-95.4(2)	.	.	.	.	no
P2	V	C1	C5A	156.2(5)	.	.	.	.	no
N	V	C1	C2	175.12(17)	.	.	.	.	no
N	V	C1	C5A	66.7(5)	.	.	.	.	no
C2	V	C1	C5A	-108.4(5)	.	.	.	.	no
C3	V	C1	C2	35.97(19)	.	.	.	.	no
C3	V	C1	C5A	-72.4(5)	.	.	.	.	no
C4	V	C1	C2	76.0(2)	.	.	.	.	no
C4	V	C1	C5A	-32.4(5)	.	.	.	.	no
C5A	V	C1	C2	108.4(5)	.	.	.	.	no
P1	V	C2	C1	168.6(2)	.	.	.	.	no
P1	V	C2	C3	-74.04(19)	.	.	.	.	no
P2	V	C2	C1	86.9(2)	.	.	.	.	no
P2	V	C2	C3	-155.73(18)	.	.	.	.	no
C1	V	C2	C3	117.4(3)	.	.	.	.	no
C3	V	C2	C1	-117.4(3)	.	.	.	.	no
C4	V	C2	C1	-81.8(3)	.	.	.	.	no
C4	V	C2	C3	35.6(2)	.	.	.	.	no
C5A	V	C2	C1	-46.8(4)	.	.	.	.	no
C5A	V	C2	C3	70.6(4)	.	.	.	.	no
P1	V	C3	C2	106.64(19)	.	.	.	.	no
P1	V	C3	C4	-134.6(2)	.	.	.	.	no
P2	V	C3	C2	30.4(2)	.	.	.	.	no
P2	V	C3	C4	149.1(2)	.	.	.	.	no
N	V	C3	C2	-161.21(19)	.	.	.	.	no
N	V	C3	C4	-42.5(3)	.	.	.	.	no
C1	V	C3	C2	-37.4(2)	.	.	.	.	no
C1	V	C3	C4	81.4(2)	.	.	.	.	no
C2	V	C3	C4	118.8(3)	.	.	.	.	no
C4	V	C3	C2	-118.8(3)	.	.	.	.	no
C5A	V	C3	C2	-88.3(4)	.	.	.	.	no
C5A	V	C3	C4	30.5(4)	.	.	.	.	no
P1	V	C4	C3	49.1(2)	.	.	.	.	no
P1	V	C4	C5A	172.7(6)	.	.	.	.	no
P2	V	C4	C3	-59.8(4)	.	.	.	.	no
P2	V	C4	C5A	63.8(7)	.	.	.	.	no
N	V	C4	C3	154.71(18)	.	.	.	.	no
N	V	C4	C5A	-81.7(6)	.	.	.	.	no
C1	V	C4	C3	-77.8(2)	.	.	.	.	no
C1	V	C4	C5A	45.8(6)	.	.	.	.	no
C2	V	C4	C3	-35.81(19)	.	.	.	.	no
C2	V	C4	C5A	87.8(6)	.	.	.	.	no
C3	V	C4	C5A	123.6(7)	.	.	.	.	no
C5A	V	C4	C3	-123.6(7)	.	.	.	.	no
P1	V	C5A	C1	102.7(5)	.	.	.	.	no
P1	V	C5A	C4	-10.8(9)	.	.	.	.	no
P2	V	C5A	C1	-32.0(6)	.	.	.	.	no
P2	V	C5A	C4	-145.5(4)	.	.	.	.	no
N	V	C5A	C1	-135.8(3)	.	.	.	.	no
N	V	C5A	C4	110.8(5)	.	.	.	.	no
C1	V	C5A	C4	-113.5(8)	.	.	.	.	no
C2	V	C5A	C1	39.1(3)	.	.	.	.	no
C2	V	C5A	C4	-74.4(5)	.	.	.	.	no
C3	V	C5A	C1	79.1(4)	.	.	.	.	no
C3	V	C5A	C4	-34.4(4)	.	.	.	.	no
C4	V	C5A	C1	113.5(8)	.	.	.	.	no
V	P1	C8	C9A	-5.2(4)	.	.	.	.	no
C6	P1	C8	C9A	-133.4(3)	.	.	.	.	no
C7	P1	C8	C9A	123.2(3)	.	.	.	.	no
V	P2	C9A	C8	-47.3(3)	.	.	.	.	no
C10A	P2	C9A	C8	-167.6(4)	.	.	.	.	no
C11	P2	C9A	C8	90.1(3)	.	.	.	.	no
V	C1	C2	C3	-63.8(2)	.	.	.	.	no
C5A	C1	C2	V	63.7(5)	.	.	.	.	no
C5A	C1	C2	C3	-0.1(5)	.	.	.	.	no

V	C1	C5A	C4	68.6(7)	.	.	.	.	no
C2	C1	C5A	V	-68.1(3)	.	.	.	.	no
C2	C1	C5A	C4	0.5(9)	.	.	.	.	no
V	C2	C3	C4	-61.9(2)	.	.	.	.	no
C1	C2	C3	V	61.6(2)	.	.	.	.	no
C1	C2	C3	C4	-0.4(4)	.	.	.	.	no
V	C3	C4	C5A	-61.4(7)	.	.	.	.	no
C2	C3	C4	V	62.2(2)	.	.	.	.	no
C2	C3	C4	C5A	0.8(8)	.	.	.	.	no
V	C4	C5A	C1	-63.1(6)	.	.	.	.	no
C3	C4	C5A	V	62.3(5)	.	.	.	.	no
C3	C4	C5A	C1	-0.8(10)	.	.	.	.	no
P1	C8	C9A	P2	33.8(4)	.	.	.	.	no
N	C12	C13	C14	178.1(2)	.	.	.	.	no
C17	C12	C13	C14	-1.8(3)	.	.	.	.	no
N	C12	C17	C16	-177.3(2)	.	.	.	.	no
C13	C12	C17	C16	2.6(3)	.	.	.	.	no
C12	C13	C14	C15	-0.7(4)	.	.	.	.	no
C13	C14	C15	C16	2.4(3)	.	.	.	.	no
C13	C14	C15	C18	-175.3(2)	.	.	.	.	no
C14	C15	C16	C17	-1.7(3)	.	.	.	.	no
C18	C15	C16	C17	176.1(2)	.	.	.	.	no
C15	C16	C17	C12	-0.9(3)	.	.	.	.	no

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P1	P2	3.0690(10)	.	.	no
P1	N	3.025(2)	.	.	no
P1	C2	3.466(3)	.	.	no
P1	C3	3.194(3)	.	.	no
P1	C9A	2.779(5)	.	.	no
P1	C9B	2.747(8)	.	.	no
P2	N	2.869(2)	.	.	no
P2	P1	3.0690(10)	.	.	no
P2	C8	2.756(4)	.	.	no
P2	C1	3.314(4)	.	.	no
P2	C2	3.428(3)	.	.	no
P1	H3	3.11	.	.	no
N	P1	3.025(2)	.	.	no
N	P2	2.869(2)	.	.	no
N	C4	3.414(4)	.	.	no
N	C5A	3.223(13)	.	.	no
N	C9A	3.312(5)	.	.	no
N	C10A	3.400(8)	.	.	no
N	C5B	3.325(15)	.	.	no
N	C10B	3.333(12)	.	.	no
C1	P2	3.314(4)	.	.	no
C1	C3	2.253(5)	.	.	no
C1	C4	2.275(6)	.	.	no
C2	C6	3.598(5)	.	.	no
C2	P2	3.428(3)	.	.	no
C2	C4	2.234(5)	.	.	no
C2	P1	3.466(3)	.	.	no
C2	C5B	2.194(16)	.	.	no
C2	C5A	2.338(13)	.	.	no
C3	P1	3.194(3)	.	.	no
C3	C6	3.331(5)	.	.	no
C3	C1	2.253(5)	.	.	no
C3	C5A	2.156(13)	.	.	no
C3	C5B	2.374(18)	.	.	no
C4	C1	2.275(6)	.	.	no

C4	N	3.414(4)	.	.	no
C4	C2	2.234(5)	.	.	no
C5A	C2	2.338(13)	.	.	no
C5A	C3	2.156(13)	.	.	no
C5A	N	3.223(13)	.	.	no
C5B	C3	2.374(18)	.	.	no
C5B	N	3.325(15)	.	.	no
C5B	C2	2.194(16)	.	.	no
C10B	C12	3.537(12)	.	.	no
C12	C10B	3.537(12)	.	.	no
C1	H51	2.33	.	.	no
C1	H52	1.91	.	.	no
C1	H2	2.10	.	.	no
C2	H1	2.14	.	.	no
C2	H3	2.07	.	.	no
C3	H11'	2.87	.	2_655	no
C3	H41	2.04	.	.	no
C3	H51	3.07	.	.	no
C3	H6	3.04	.	.	no
C3	H2	2.08	.	.	no
C4	H11'	3.00	.	2_655	no
C4	H51	1.92	.	.	no
C4	H52	2.39	.	.	no
C4	H3	2.06	.	.	no
C5A	H41	1.88	.	.	no
C5A	H3	3.04	.	.	no
C5A	H1	2.36	.	.	no
C5B	H41	2.46	.	.	no
C5B	H2	3.08	.	.	no
C5B	H1	1.78	.	.	no
C6	H3	2.84	.	.	no
C7	H16	3.06	.	4_555	no
C10B	H102'	3.03	.	3_555	no
C12	H7	3.00	.	2_555	no
C12	H101"	2.91	.	.	no
C12	H6"	2.99	.	2_555	no
C12	H102'	2.89	.	.	no
C13	H102"	3.06	.	3_555	no
C13	H6"	2.88	.	2_555	no
C14	H6"	2.79	.	2_555	no
C14	H102"	2.89	.	3_555	no
C15	H6"	2.78	.	2_555	no
C16	H6"	2.88	.	2_555	no
C17	H101"	2.89	.	.	no
C17	H6"	2.99	.	2_555	no
C17	H7	2.99	.	2_555	no
C17	H17	3.05	.	3_565	no
C18	H11	2.93	.	3_555	no
C18	H52	2.99	.	3_565	no
H101"	C12	2.91	.	.	no
H101"	C17	2.89	.	.	no
H3	H6	2.33	.	.	no
H3	C6	2.84	.	.	no
H102'	H102'	2.41	.	3_555	no
H102'	C10B	3.03	.	3_555	no
H102'	C12	2.89	.	.	no
H102"	H11	2.44	.	.	no
H102"	C14	2.89	.	3_555	no
H102"	H92	2.49	.	.	no
H102"	C13	3.06	.	3_555	no
H6	C3	3.04	.	.	no
H6	H3	2.33	.	.	no
H6"	H81	2.56	.	.	no
H6"	C12	2.99	.	2_545	no
H6"	C13	2.88	.	2_545	no
H6"	C14	2.79	.	2_545	no

H6"	C17	2.99	.	2_545	no
H6"	C15	2.78	.	2_545	no
H6"	C16	2.88	.	2_545	no
H7	C17	2.99	.	2_545	no
H7	H81'	2.51	.	.	no
H7	C12	3.00	.	2_545	no
H7'	H13	2.31	.	.	no
H11	C18	2.93	.	3_555	no
H11	H102"	2.44	.	.	no
H11	H92'	2.45	.	.	no
H11	H18	2.60	.	3_555	no
H11'	C4	3.00	.	2_645	no
H11'	H92'	2.13	.	.	no
H11'	C3	2.87	.	2_645	no
H11"	H14	2.30	.	1_655	no
H13	H7'	2.31	.	.	no
H13	H41	2.56	.	2_545	no
H14	H11"	2.30	.	1_455	no
H14	H18	2.38	.	.	no
H16	H51	2.32	.	3_565	no
H16	H52	2.32	.	3_565	no
H16	C7	3.06	.	4_554	no
H17	C17	3.05	.	3_565	no
H17	H17	2.52	.	3_565	no
H18	H14	2.38	.	.	no
H18	H11	2.60	.	3_555	no
H18"	H52	2.58	.	3_565	no
H41	H13	2.56	.	2_555	no
H51	H16	2.32	.	3_565	no
H52	H16	2.32	.	3_565	no
H52	H18"	2.58	.	3_565	no
H52	C18	2.99	.	3_565	no
H81	H6"	2.56	.	.	no
H81'	H7	2.51	.	.	no
H92	H102"	2.49	.	.	no
H92'	H11	2.45	.	.	no
H92'	H11'	2.13	.	.	no

#===END of Crystallographic Information File