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New mono- and di-nuclear complexes of PdII, PtII and NiII of PNNP ligands with a 2,2'-biaryl bridging unit

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# 3 CIF's belonging to 7/04170E      (From A.L.Spek - Utrecht University)

# ***** Complex 1 *****

# CIF-file generated for  (C26H22ClNPPd)2                CP339

#=====

data_cp339

#=====

# 5. CHEMICAL DATA

_chemical_name_systematic
;
?
;
_chemical_name_common          ?
_chemical_melting_point        ?
_chemical_formula_moiety       'C52 H44 Cl2 N2 P2 Pd2'
_chemical_formula_structural   ?
_chemical_formula_sum          'C52 H44 Cl2 N2 P2 Pd2'
_chemical_formula_weight       1042.63
_chemical_compound_source      ?

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
Pd Pd      -.9988      1.0072
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
P P        .1023      .0942
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N        .0061      .0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl Cl      .1484      .1585
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H        .0000      .0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C        .0033      .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_H-M 'C 2/c'

loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,y,1/2-z
-x,-y,-z
x,-y,1/2+z
1/2+x,1/2+y,z
1/2-x,1/2+y,1/2-z
1/2-x,1/2-y,-z
1/2+x,1/2-y,1/2+z

```

```

_cell_length_a          17.789(5)
_cell_length_b          14.170(4)
_cell_length_c          19.423(7)
_cell_angle_alpha       90
_cell_angle_beta        113.02(2)
_cell_angle_gamma       90
_cell_volume            4506(3)
_cell_formula_units_Z   4
_cell_measurement_temperature 130(2)
_cell_measurement_reflns_used 22
_cell_measurement_theta_min 18.00
_cell_measurement_theta_max 20.47
_cell_special_details
; ?
;

_exptl_crystal_description 'irregular fragment'
_exptl_crystal_colour      orange
_exptl_crystal_size_max    0.50
_exptl_crystal_size_mid    0.44
_exptl_crystal_size_min    0.19
_exptl_crystal_size_rad    ?
_exptl_crystal_density_meas 'Not Measured'
_exptl_crystal_density_diffrn 1.537
_exptl_crystal_density_method ?
_exptl_crystal_F_000       2104
_exptl_absorpt_coefficient_mu 1.03
_exptl_crystal_density_meas_temp ?
_exptl_absorpt_correction_type ?
_exptl_absorpt_correction_T_min ?
_exptl_absorpt_correction_T_max ?

#=====

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffn_ambient_temperature 130(2)
_diffn_radiation_wavelength 71073
_diffn_radiation_type      'Mo K\alpha'

_diffn_radiation_source    'fine-focus sealed tube'
_diffn_radiation_monochromator graphite

_diffn_measurement_device_type CAD4F
_diffn_measurement_method    '\w/2\q scan'

_diffn_special_details
;
  Crystal into the cold nitrogen stream of the low-temperature
unit
  (Bolhuis, 1971), on an Enraf-Nonius CAD4-4F diffractometer.
  Graphite-monochromated Mo K\alpha radiation,
  \w/2\q scan, \D\w = (1.00 + 0.34 tg \q)\%.
;

_diffn_standards_number    3
_diffn_standards_interval_count ?'
_diffn_standards_interval_time 10800
_diffn_standards_decay_%   .7?

loop_
_diffn_standard_refl_index_h

```

```

_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
  -1 -3 0
  -2 2 -2
  1 3 -4
# number of measured reflections (redundant set)
_diffrn_refl_number 9610
_diffrn_refl_av_R_equivalents ?
_diffrn_refl_av_sigmaI/netI 0.036
_diffrn_refl_limit_h_min -22
_diffrn_refl_limit_h_max 22
_diffrn_refl_limit_k_min -17
_diffrn_refl_limit_k_max 16
_diffrn_refl_limit_l_min -24
_diffrn_refl_limit_l_max 13
_diffrn_refl_theta_min 1.14
_diffrn_refl_theta_max 26.5
_diffrn_refl_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, scale
variation, but not for absorption and reduced to  $F_o \sim F_c^2$ 
;

# number of unique reflections
_reflns_number_total 4678
# number of observed reflections (> n sig(I))
_reflns_number_gt ?
_reflns_threshold_expression >0

_computing_data_collection ?
_computing_cell_refinement ?
_computing_data_reduction ?
_computing_structure_solution 'DIRDIF4 (Beurskens, 1994)'
_computing_structure_refinement 'SHELXL-93 (Sheldrick, 1993)'
_computing_molecular_graphics ?
_computing_publication_material 'PLATON (Spek, 1990)'

#=====

# 8. REFINEMENT DATA

_refine_special_details ?
_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme
'calc w=1/[\s^2^(Fo^2)+(0.06622P)^2+28.60P] where P=(Fo^2+2Fc^2)/3'
_refine_ls_hydrogen_treatment 'isotropic refinement '
_refine_ls_extinction_method ?
_refine_ls_extinction_coef ?
_refine_ls_extinction_expression ?
_refine_ls_abs_structure_details
;
?
;
_refine_ls_abs_structure_Flack ?
_refine_ls_number_refl 4269
_refine_ls_number_parameters 359
_refine_ls_number_restraints ?
_refine_ls_number_constraints ?
_refine_ls_R_factor_all ?
_refine_ls_R_factor_gt 0.0471
_refine_ls_wR_factor_obs .1298
_refine_ls_wR_factor_ref ?
_refine_ls_goodness_of_fit_ref 1.083
_refine_ls_restrained_S_all ?
_refine_ls_restrained_S_obs ?

```

```

_refine_ls_shift/su_max      ?
_refine_ls_shift/esd_mean    '< 0.001'
_refine_diff_density_max     1.22(13)
_refine_diff_density_min     -1.14

```

#=====

9. ATOMIC COORDINATES AND THERMAL PARAMETERS

```

loop_
_atom_site_label
_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
Pd      Uani      .05929(2)    .27636(2)    .09370(2)    1.000
.0279(1)
C1      Uani      -.07207(6)    .20936(7)    .03460(6)    1.000
.0306(3)
P      Uani      .18205(7)    .33582(9)    .15168(7)    1.000
.0326(4)
N      Uani      .0878(2)    .2244(3)    .2100(2)    1.000
.0267(11)
C1      Uani      .2635(3)    .2536(4)    .1610(3)    1.000
.0370(14)
C2      Uani      .2604(4)    .2023(5)    .0996(4)    1.000
.0489(19)
C3      Uani      .3215(5)    .1408(5)    .1045(5)    1.000
.062(3)
C4      Uani      .3866(4)    .1275(5)    .1717(5)    1.000
.062(2)
C5      Uani      .3899(4)    .1773(5)    .2341(5)    1.000
.060(2)
C6      Uani      .3284(3)    .2401(4)    .2271(4)    1.000
.0432(17)
C7      Uani      .2145(3)    .4466(4)    .1255(3)    1.000
.0369(16)
C8      Uani      .1686(4)    .5264(4)    .1215(4)    1.000
.0495(19)
C9      Uani      .1914(4)    .6115(4)    .0997(4)    1.000
.054(2)
C10     Uani      .2564(3)    .6158(4)    .0792(3)    1.000
.0462(17)
C11     Uani      .3006(3)    .5370(4)    .0806(3)    1.000
.0460(17)
C12     Uani      .2810(3)    .4511(4)    .1048(3)    1.000
.0383(16)
C13     Uani      .1842(3)    .3535(3)    .2443(3)    1.000
.0315(12)
C14     Uani      .2339(3)    .4164(4)    .2968(3)    1.000
.0403(17)
C15     Uani      .2282(3)    .4257(4)    .3651(3)    1.000
.0426(17)
C16     Uani      .1704(3)    .3748(4)    .3802(3)    1.000
.0407(17)
C17     Uani      .1217(3)    .3104(3)    .3299(3)    1.000
.0346(16)
C18     Uani      .1298(3)    .2965(3)    .2624(3)    1.000
.0281(12)
C19     Uani      .0768(3)    .1452(3)    .2372(3)    1.000
.0254(12)
C20     Uani      .0481(3)    .0599(3)    .1930(3)    1.000
.0267(12)
C21     Uani      .0678(3)    .0468(3)    .1306(3)    1.000
.0325(14)

```

C22	Uani	.0501(3)	-.0358(4)	.0904(3)	1.000
.0374(16)					
C23	Uani	.0099(3)	-.1065(4)	.1110(3)	1.000
.0420(16)					
C24	Uani	-.0098(3)	-.0952(3)	.1731(3)	1.000
.0362(16)					
C25	Uani	.0093(3)	-.0133(3)	.2159(2)	1.000
.0258(11)					
C26	Uani	.0444(4)	.3446(5)	-.0021(3)	1.000
.048(2)					
H2	Uiso	.217(4)	.205(4)	.062(4)	1.000
.043(17)					
H3	Uiso	.322(4)	.100(5)	.066(4)	1.000
.06(2)					
H4	Uiso	.428(4)	.088(5)	.178(4)	1.000
.060(19)					
H5	Uiso	.438(4)	.164(4)	.281(4)	1.000
.039(15)					
H6	Uiso	.335(4)	.260(4)	.264(4)	1.000
.034(16)					
H8	Uiso	.124(4)	.517(4)	.139(4)	1.000
.051(17)					
H9	Uiso	.161(3)	.655(4)	.096(3)	1.000
.028(14)					
H10	Uiso	.269(3)	.669(4)	.063(3)	1.000
.036(14)					
H11	Uiso	.344(4)	.543(5)	.067(4)	1.000
.058(19)					
H12	Uiso	.318(3)	.402(4)	.112(3)	1.000
.021(11)					
H14	Uiso	.272(4)	.453(5)	.287(4)	1.000
.07(2)					
H15	Uiso	.260(4)	.461(4)	.391(4)	1.000
.043(16)					
H16	Uiso	.163(3)	.389(4)	.426(3)	1.000
.041(15)					
H17	Uiso	.090(3)	.278(4)	.345(3)	1.000
.034(14)					
H19	Uiso	.087(3)	.141(3)	.279(3)	1.000
.015(11)					
H21	Uiso	.089(3)	.088(4)	.114(3)	1.000
.033(14)					
H22	Uiso	.061(3)	-.042(4)	.044(3)	1.000
.037(14)					
H23	Uiso	-.004(4)	-.156(5)	.084(4)	1.000
.049(17)					
H24	Uiso	-.035(3)	-.144(4)	.190(3)	1.000
.037(14)					
H26	Uiso	.036(6)	.398(8)	.008(6)	1.000
.11(4)					
H26'	Uiso	-.002(5)	.330(6)	-.040(5)	1.000
.07(2)					
H26''	Uiso	.083(5)	.321(6)	-.016(5)	1.000
.08(2)					

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

Pd	.0312(2)	.0289(2)	.0273(2)	-.0004(1)
----	----------	----------	----------	-----------

.0155(2)	-.0088(1)			
----------	-----------	--	--	--

Cl	.0307(5)	.0289(5)	.0358(6)	-.0049(4)
----	----------	----------	----------	-----------

.0170(4)	-.0060(4)			
----------	-----------	--	--	--

P	.0335(6)	.0333(6)	.0353(7)	-.0002(5)
.0182(5)	-.0109(5)			
N	.0304(18)	.0261(18)	.0274(19)	-.0017(15)
.0154(15)	-.0045(14)			
C1	.037(2)	.036(2)	.046(3)	.002(2)
.025(2)	-.010(2)			
C2	.052(3)	.051(3)	.051(4)	-.004(3)
.028(3)	-.009(3)			
C3	.071(4)	.051(4)	.090(5)	-.016(4)
.059(4)	-.012(3)			
C4	.043(3)	.049(3)	.108(6)	-.004(4)
.044(4)	-.002(3)			
C5	.043(3)	.053(4)	.089(5)	.005(4)
.030(4)	-.001(3)			
C6	.036(3)	.050(3)	.047(3)	.002(3)
.020(3)	.000(2)			
C7	.036(2)	.038(3)	.038(3)	.004(2)
.016(2)	-.013(2)			
C8	.047(3)	.042(3)	.065(4)	.007(3)
.028(3)	-.008(2)			
C9	.058(4)	.036(3)	.065(4)	.007(3)
.021(3)	-.008(3)			
C10	.048(3)	.045(3)	.036(3)	.009(2)
.006(2)	-.027(3)			
C11	.040(3)	.054(3)	.043(3)	.007(3)
.015(2)	-.025(3)			
C12	.034(2)	.044(3)	.037(3)	.007(2)
.014(2)	-.011(2)			
C13	.032(2)	.033(2)	.030(2)	-.0001(19)
.0128(19)	-.0066(18)			
C14	.039(3)	.038(3)	.043(3)	-.006(2)
.015(2)	-.013(2)			
C15	.045(3)	.038(3)	.039(3)	-.012(2)
.010(2)	-.011(2)			
C16	.055(3)	.038(3)	.032(3)	-.004(2)
.020(2)	-.003(2)			
C17	.046(3)	.031(2)	.033(3)	-.0008(19)
.022(2)	-.005(2)			
C18	.031(2)	.028(2)	.027(2)	-.0011(18)
.0133(18)	-.0068(18)			
C19	.026(2)	.030(2)	.024(2)	.0041(18)
.0140(17)	.0017(17)			
C20	.026(2)	.025(2)	.029(2)	.0045(17)
.0108(17)	.0070(16)			
C21	.034(2)	.031(2)	.034(3)	.005(2)
.015(2)	.0057(19)			
C22	.044(3)	.042(3)	.028(2)	-.003(2)
.016(2)	.013(2)			
C23	.055(3)	.029(2)	.042(3)	-.013(2)
.019(2)	.003(2)			
C24	.041(3)	.025(2)	.043(3)	-.004(2)
.017(2)	-.0007(19)			
C25	.028(2)	.0206(19)	.029(2)	.0009(17)
.0115(18)	.0029(16)			
C26	.055(4)	.057(4)	.031(3)	.008(3)
.016(3)	-.023(3)			

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

;

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
;

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

Pd C1 2.3625(15)

yes

. .

Pd P 2.1963(16)

yes

. .

Pd N 2.237(4)

yes

. .

Pd C26 2.020(6)

yes

. .

P C1 1.812(6)

yes

. .

P C7 1.813(6)

yes

. .

P C13 1.802(6)

yes

. .

N C18 1.429(6)

yes

. .

N C19 1.288(6)

yes

. .

C1 C2 1.379(9)

no

. .

C1 C6 1.363(9)

no

. .

C2 C3 1.367(11)

no

. .

C3 C4 1.378(13)

no

. .

C4 C5 1.384(12)

no

. .

C5 C6 1.375(10)

no

. .

C7 C8 1.379(9)

no

. .

C7 C12 1.392(8)

no

. .

C8 C9 1.390(9)

no

. .

C9 C10 1.364(10)

no

. .

C10 C11 1.360(8)

no

. .

C11 C12 1.397(8)

no

. .

C13 C14 1.382(7)

no

. .

C13 C18 1.407(8)

no

. .

C14 C15 1.376(8)

no

. .

C15 C16 1.378(8)

no

. .

C16 C17 1.370(7)

no

. .

C17 C18 1.388(8)

no

. .

C19 C20 1.455(7)

no

. .

C20 C21 1.399(8)

. .

C20	no C25	1.411(7)	.	.
C21	no C22	1.373(7)	.	.
C22	no C23	1.378(8)	.	.
C23	no C24	1.391(8)	.	.
C24	no C25	1.390(6)	.	.
C25	no C25	1.486(6)	.	2_555
C2	no H2	.83(7)	.	.
C3	no H3	.95(7)	.	.
C4	no H4	.89(8)	.	.
C5	no H5	.99(7)	.	.
C6	no H6	.74(7)	.	.
C8	no H8	.99(8)	.	.
C9	no H9	.80(6)	.	.
C10	no H10	.88(6)	.	.
C11	no H11	.91(8)	.	.
C12	no H12	.93(6)	.	.
C14	no H14	.93(8)	.	.
C15	no H15	.78(7)	.	.
C16	no H16	.97(6)	.	.
C17	no H17	.86(6)	.	.
C19	no H19	.76(5)	.	.
C21	no H21	.83(6)	.	.
C22	no H22	1.00(6)	.	.
C23	no H23	.85(7)	.	.
C24	no H24	.95(6)	.	.
C26	no H26	.81(11)	.	.
C26	no H26'	.89(9)	.	.
C26	no H26"	.90(9)	.	.
	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

C1	Pd	P	178.21(5)	.	.
.	yes				
C1	Pd	N	98.57(11)	.	.
.	yes				
C1	Pd	C26	89.8(2)	.	.
.	yes				
P	Pd	N	79.70(11)	.	.
.	yes				
P	Pd	C26	92.0(2)	.	.
.	yes				
N	Pd	C26	169.6(2)	.	.
.	yes				
Pd	P	C1	113.60(19)	.	.
.	yes				
Pd	P	C7	123.39(19)	.	.
.	yes				
Pd	P	C13	101.18(19)	.	.
.	yes				
C1	P	C7	104.8(3)	.	.
.	yes				
C1	P	C13	106.6(2)	.	.
.	yes				
C7	P	C13	106.0(2)	.	.
.	yes				
Pd	N	C18	109.4(3)	.	.
.	yes				
Pd	N	C19	133.7(3)	.	.
.	yes				
C18	N	C19	116.9(4)	.	.
.	yes				
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.	yes				
P	C1	C6	122.3(4)	.	.
.	yes				
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.	no				
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.	no				
P	C7	C8	118.6(5)	.	.
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C9	C10	C11	120.5(5)	.	.
.	no				
C10	C11	C12	120.2(5)	.	.
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C7	C12	C11	119.3(5)	.	.
.	no				
P	C13	C14	125.7(4)	.	.
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.	no				
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.	no				
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.	no				
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.	no				
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.	no				
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End of Crystallographic Information File

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_exptl_crystal_size_min          0.45
_exptl_crystal_density_meas      'Not Measured'
_exptl_crystal_density_diffn     1.519
_exptl_crystal_density_method    ?
_exptl_crystal_F_000             2436
_exptl_absorpt_coefficient_mu     0.91
_exptl_absorpt_correction_type    none

#=====

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffn_ambient_temperature        150
_diffn_radiation_wavelength       0.71073
_diffn_radiation_type             'Mo K\alpha'
_diffn_radiation_source           'Rotating Anode'
_diffn_radiation_monochromator     Graphite

_diffn_measurement_device_type     'CAD4T'
_diffn_measurement_method         '\w-scan'

# number of measured reflections (redundant set)
_diffn_reflns_number              ?
_diffn_reflns_av_R_equivalents    0.0794
_diffn_reflns_av_sigmaI/netI      0.1009
_diffn_reflns_limit_h_min         -18
_diffn_reflns_limit_h_max         16
_diffn_reflns_limit_k_min         0
_diffn_reflns_limit_k_max         23
_diffn_reflns_limit_l_min         -24
_diffn_reflns_limit_l_max         24
_diffn_reflns_theta_min           1.06
_diffn_reflns_theta_max           25.36

# number of unique reflections
_reflns_number_total              19488
# number of observed reflections (> n sig(I))
_reflns_number_gt                 11771
_reflns_threshold_expression       >2sigma(i)

_computing_structure_refinement    'SHELXL-97 (Sheldrick, 1997)'
_computing_publication_material    'PLATON (Spek, 1990)'

#=====

# 8. REFINEMENT DATA

_refine_ls_structure_factor_coef   Fsqd
_refine_ls_matrix_type             full
_refine_ls_weighting_scheme
'CALC W=1/[\S^2*(FO^2^)+(0.0675P)^2^+18.2225P] WHERE P=(FO^2^+2FC^2^)/3'
_refine_ls_hydrogen_treatment      'H-atom refinement: see text'
_refine_ls_number_reflns           18889
_refine_ls_number_parameters       1331
_refine_ls_number_restraints       1
_refine_ls_R_factor_all             0.1245
_refine_ls_R_factor_gt             0.0673
_refine_ls_wR_factor_ref           0.1735
_refine_ls_wR_factor_gt            0.1421
_refine_ls_goodness_of_fit_ref     1.008
_refine_ls_restrained_S_all        1.008
_refine_ls_shift/su_max            0.007
_refine_ls_shift/su_mean           0.000

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_refine_diff_density_max	1.168
_refine_diff_density_min	-1.082
_refine_diff_density_rms	0.142

#=====

9. ATOMIC COORDINATES AND THERMAL PARAMETERS

loop_					
_atom_site_label					
_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					
Pd1	Uani	0.15699(4)	0.23185(3)	0.68334(3)	1.000
0.0154(2)					
C11	Uani	0.11967(13)	0.17999(10)	0.79988(9)	1.000
0.0234(6)					
P1	Uani	-0.00609(13)	0.18941(10)	0.64312(9)	1.000
0.0159(5)					
P2	Uani	0.19177(13)	0.35886(10)	0.70101(9)	1.000
0.0166(6)					
N1	Uani	0.3071(4)	0.2615(3)	0.7181(3)	1.000
0.0168(17)					
N2	Uani	0.1337(4)	0.1147(3)	0.6358(3)	1.000
0.0158(17)					
C11	Uani	0.1072(5)	0.3885(4)	0.6511(4)	1.000
0.021(2)					
C21	Uani	0.0610(5)	0.4311(4)	0.6823(4)	1.000
0.026(2)					
C31	Uani	-0.0032(5)	0.4531(4)	0.6416(5)	1.000
0.030(3)					
C41	Uani	-0.0213(6)	0.4313(5)	0.5705(5)	1.000
0.040(3)					
C51	Uani	0.0221(6)	0.3881(5)	0.5389(5)	1.000
0.040(3)					
C61	Uani	0.0869(6)	0.3681(4)	0.5796(4)	1.000
0.028(3)					
C71	Uani	0.2201(5)	0.4127(4)	0.7914(3)	1.000
0.0158(19)					
C81	Uani	0.2048(6)	0.3738(4)	0.8421(4)	1.000
0.028(3)					
C91	Uani	0.2268(6)	0.4151(5)	0.9094(4)	1.000
0.037(3)					
C101	Uani	0.2647(6)	0.4947(5)	0.9285(4)	1.000
0.036(3)					
C111	Uani	0.2813(6)	0.5333(5)	0.8786(4)	1.000
0.029(3)					
C121	Uani	0.2593(5)	0.4926(4)	0.8095(4)	1.000
0.021(2)					
C131	Uani	0.3042(5)	0.4050(4)	0.6763(3)	1.000
0.017(2)					
C141	Uani	0.3189(5)	0.4709(4)	0.6517(4)	1.000
0.023(2)					
C151	Uani	0.4061(5)	0.5115(4)	0.6373(4)	1.000
0.026(3)					
C161	Uani	0.4815(5)	0.4868(4)	0.6462(4)	1.000
0.023(2)					
C171	Uani	0.4695(5)	0.4224(4)	0.6704(4)	1.000
0.023(2)					
C181	Uani	0.3816(5)	0.3810(4)	0.6853(4)	1.000
0.021(2)					
C191	Uani	0.3814(5)	0.3175(4)	0.7131(4)	1.000
0.019(2)					
C201	Uani	0.3339(5)	0.2093(4)	0.7523(4)	1.000

0.019(2)					
C211	Uani	0.3690(5)	0.2320(5)	0.8239(4)	1.000
0.027(3)					
C221	Uani	0.4042(6)	0.1858(5)	0.8556(4)	1.000
0.039(3)					
C231	Uani	0.4043(6)	0.1198(5)	0.8171(4)	1.000
0.035(3)					
C241	Uani	0.3686(5)	0.0982(4)	0.7464(4)	1.000
0.025(2)					
C251	Uani	0.3323(5)	0.1421(4)	0.7122(4)	1.000
0.018(2)					
C261	Uani	0.2998(5)	0.1188(4)	0.6359(4)	1.000
0.0183(19)					
C271	Uani	0.3603(6)	0.1040(4)	0.5968(4)	1.000
0.027(3)					
C281	Uani	0.3302(5)	0.0755(4)	0.5257(4)	1.000
0.026(3)					
C291	Uani	0.2361(5)	0.0626(4)	0.4908(4)	1.000
0.025(2)					
C301	Uani	0.1735(5)	0.0773(4)	0.5282(4)	1.000
0.022(2)					
C311	Uani	0.2045(5)	0.1047(4)	0.5993(4)	1.000
0.0173(19)					
C321	Uani	0.0621(5)	0.0514(4)	0.6330(3)	1.000
0.016(2)					
C331	Uani	-0.0260(5)	0.0428(4)	0.6565(4)	1.000
0.019(2)					
C341	Uani	-0.0733(5)	-0.0269(4)	0.6708(3)	1.000
0.018(2)					
C351	Uani	-0.1584(5)	-0.0419(4)	0.6934(4)	1.000
0.022(2)					
C361	Uani	-0.1962(6)	0.0135(4)	0.7012(4)	1.000
0.026(2)					
C371	Uani	-0.1496(5)	0.0824(4)	0.6857(4)	1.000
0.021(2)					
C381	Uani	-0.0638(5)	0.0991(4)	0.6638(3)	1.000
0.015(2)					
C391	Uani	-0.0639(5)	0.2475(4)	0.6809(4)	1.000
0.020(2)					
C401	Uani	-0.0434(5)	0.2686(4)	0.7527(4)	1.000
0.024(3)					
C411	Uani	-0.0915(6)	0.3083(4)	0.7852(5)	1.000
0.033(3)					
C421	Uani	-0.1579(6)	0.3274(5)	0.7462(5)	1.000
0.036(3)					
C431	Uani	-0.1782(5)	0.3068(4)	0.6747(4)	1.000
0.029(3)					
C441	Uani	-0.1317(5)	0.2671(4)	0.6411(4)	1.000
0.025(3)					
C451	Uani	-0.0461(5)	0.1657(4)	0.5494(4)	1.000
0.021(2)					
C461	Uani	-0.1451(6)	0.1284(4)	0.5143(4)	1.000
0.030(3)					
C471	Uani	-0.1746(7)	0.1128(5)	0.4434(4)	1.000
0.035(3)					
C481	Uani	-0.1049(7)	0.1331(5)	0.4068(4)	1.000
0.037(3)					
C491	Uani	-0.0064(7)	0.1683(5)	0.4401(4)	1.000
0.032(3)					
C501	Uani	0.0225(6)	0.1835(4)	0.5107(4)	1.000
0.029(3)					
Pd2	Uani	0.17064(4)	0.25634(3)	0.18083(3)	1.000
0.0157(2)					
P3	Uani	0.00681(13)	0.21212(10)	0.14163(9)	1.000
0.0169(6)					
P4	Uani	0.20516(13)	0.38369(10)	0.19723(10)	1.000
0.0173(6)					

N3	Uani	0.3221(4)	0.2872(3)	0.2146(3)	1.000
0.0159(17)					
N4	Uani	0.1452(4)	0.1375(3)	0.1381(3)	1.000
0.0184(17)					
C12	Uani	0.1179(5)	0.4108(4)	0.1473(4)	1.000
0.020(2)					
C22	Uani	0.0764(5)	0.4567(4)	0.1796(4)	1.000
0.025(3)					
C32	Uani	0.0092(6)	0.4757(4)	0.1396(4)	1.000
0.030(3)					
C42	Uani	-0.0148(6)	0.4508(5)	0.0682(5)	1.000
0.035(3)					
C52	Uani	0.0274(6)	0.4072(5)	0.0363(4)	1.000
0.033(3)					
C62	Uani	0.0938(6)	0.3870(4)	0.0752(4)	1.000
0.028(3)					
C72	Uani	0.2343(5)	0.4403(4)	0.2870(4)	1.000
0.018(2)					
C82	Uani	0.2100(6)	0.4063(4)	0.3388(4)	1.000
0.027(3)					
C92	Uani	0.2297(7)	0.4512(5)	0.4052(4)	1.000
0.042(3)					
C102	Uani	0.2768(6)	0.5303(5)	0.4213(4)	1.000
0.034(3)					
C112	Uani	0.3034(6)	0.5650(5)	0.3691(4)	1.000
0.030(3)					
C122	Uani	0.2818(5)	0.5209(4)	0.3027(4)	1.000
0.023(3)					
C132	Uani	0.3174(5)	0.4293(4)	0.1713(4)	1.000
0.019(2)					
C142	Uani	0.3283(6)	0.4926(4)	0.1445(4)	1.000
0.030(3)					
C152	Uani	0.4163(6)	0.5328(5)	0.1293(4)	1.000
0.031(3)					
C162	Uani	0.4930(6)	0.5111(5)	0.1412(4)	1.000
0.029(3)					
C172	Uani	0.4827(5)	0.4495(4)	0.1689(4)	1.000
0.021(2)					
C182	Uani	0.3952(5)	0.4078(4)	0.1832(4)	1.000
0.019(2)					
C192	Uani	0.3939(5)	0.3435(4)	0.2116(4)	1.000
0.019(2)					
C202	Uani	0.3497(5)	0.2369(4)	0.2509(3)	1.000
0.017(2)					
C212	Uani	0.3863(6)	0.2615(4)	0.3218(4)	1.000
0.027(3)					
C222	Uani	0.4221(6)	0.2193(5)	0.3577(4)	1.000
0.030(3)					
C232	Uani	0.4196(5)	0.1502(5)	0.3200(4)	1.000
0.032(3)					
C242	Uani	0.3826(5)	0.1252(4)	0.2489(4)	1.000
0.025(3)					
C252	Uani	0.3446(5)	0.1670(4)	0.2126(4)	1.000
0.018(2)					
C262	Uani	0.3089(5)	0.1403(4)	0.1362(4)	1.000
0.021(2)					
C272	Uani	0.3692(6)	0.1234(5)	0.0969(4)	1.000
0.031(3)					
C282	Uani	0.3379(6)	0.0938(5)	0.0261(4)	1.000
0.037(3)					
C292	Uani	0.2431(6)	0.0785(5)	-0.0075(4)	1.000
0.031(3)					
C302	Uani	0.1808(6)	0.0944(4)	0.0290(4)	1.000
0.026(3)					
C312	Uani	0.2148(5)	0.1256(4)	0.1000(4)	1.000
0.021(2)					
C322	Uani	0.0753(5)	0.0764(4)	0.1375(4)	1.000

0.019(2)					
C332	Uani	-0.0123(5)	0.0686(4)	0.1623(4)	1.000
0.019(2)					
C342	Uani	-0.0606(5)	0.0002(4)	0.1769(4)	1.000
0.021(2)					
C352	Uani	-0.1445(5)	-0.0118(4)	0.2008(4)	1.000
0.023(2)					
C362	Uani	-0.1793(6)	0.0436(4)	0.2093(4)	1.000
0.027(3)					
C372	Uani	-0.1325(5)	0.1126(4)	0.1933(4)	1.000
0.022(2)					
C382	Uani	-0.0489(5)	0.1266(4)	0.1703(3)	1.000
0.016(2)					
C392	Uani	-0.0555(5)	0.2700(4)	0.1711(4)	1.000
0.017(2)					
C402	Uani	-0.0370(5)	0.3000(4)	0.2418(4)	1.000
0.025(3)					
C412	Uani	-0.0850(6)	0.3418(4)	0.2680(5)	1.000
0.031(3)					
C422	Uani	-0.1543(6)	0.3532(5)	0.2230(5)	1.000
0.036(3)					
C432	Uani	-0.1733(6)	0.3250(4)	0.1536(5)	1.000
0.036(3)					
C442	Uani	-0.1244(5)	0.2832(4)	0.1252(4)	1.000
0.024(2)					
C452	Uani	-0.0368(5)	0.1760(4)	0.0474(4)	1.000
0.024(2)					
C462	Uani	-0.1345(6)	0.1277(4)	0.0154(4)	1.000
0.028(3)					
C472	Uani	-0.1650(7)	0.1007(5)	-0.0560(5)	1.000
0.042(3)					
C482	Uani	-0.0974(8)	0.1217(5)	-0.0951(5)	1.000
0.043(3)					
C492	Uani	-0.0022(7)	0.1685(5)	-0.0645(4)	1.000
0.037(3)					
C502	Uani	0.0297(6)	0.1962(4)	0.0071(4)	1.000
0.027(3)					
C119	Uani	0.2174(2)	0.61731(16)	0.08744(14)	1.000
0.0618(10)					
C120	Uiso	0.3363(7)	0.7527(10)	0.0411(7)	0.52(3)
0.078(4)					
C7	Uani	0.3216(10)	0.7045(6)	0.1053(6)	1.000
0.080(5)					
C122	Uiso	0.3472(17)	0.710(2)	0.0286(8)	0.32(3)
0.114(11)					
C121	Uiso	0.265(3)	0.7661(12)	0.0837(13)	0.158(10)
0.118(15)					
C115	Uiso	0.5375(5)	0.0239(3)	0.6745(4)	0.607(14)
0.073(2)					
C116	Uiso	0.6847(7)	0.1209(5)	0.7991(3)	0.607(14)
0.080(3)					
C6	Uani	0.6198(8)	0.1207(6)	0.7255(6)	1.000
0.064(4)					
C118	Uiso	0.5951(11)	0.0685(10)	0.6510(5)	0.393(14)
0.097(6)					
C117	Uiso	0.6228(17)	0.0824(13)	0.7981(9)	0.393(14)
0.139(7)					
C15	Uani	0.3221(3)	0.25552(16)	0.51623(16)	1.000
0.0908(16)					
C16	Uani	0.4414(2)	0.39167(15)	0.48132(13)	1.000
0.0719(10)					
C1	Uani	0.3236(8)	0.3298(5)	0.4810(5)	1.000
0.058(4)					
C17	Uani	0.4825(2)	0.37123(19)	-0.00543(14)	1.000
0.0870(11)					
C18	Uani	0.2955(2)	0.28631(18)	0.01782(16)	1.000
0.0765(11)					

C2	Uani	0.4161(8)	0.2974(6)	0.0286(5)	1.000
0.059(4)					
Cl9	Uani	0.7668(2)	0.38243(18)	0.39270(15)	1.000
0.0667(11)					
Cl10	Uani	0.7490(3)	0.2262(2)	0.3477(2)	1.000
0.108(2)					
C3	Uani	0.6908(8)	0.2884(7)	0.3396(6)	1.000
0.068(5)					
Cl11	Uani	0.6581(2)	0.26230(14)	0.50181(12)	1.000
0.0542(9)					
Cl12	Uani	0.5820(3)	0.10729(19)	0.5127(3)	1.000
0.144(3)					
C4	Uani	0.5816(8)	0.1974(5)	0.5376(5)	1.000
0.057(4)					
Cl13	Uani	0.6147(4)	0.1047(3)	0.0567(4)	1.000
0.181(4)					
Cl14	Uani	0.5783(3)	0.0731(3)	0.1846(4)	1.000
0.161(3)					
C5	Uani	0.6322(9)	0.1416(9)	0.1446(13)	1.000
0.155(11)					
Cl2	Uani	0.13642(13)	0.21416(10)	0.30874(9)	1.000
0.0246(6)					
Cl3	Uani	0.41078(14)	0.71306(11)	0.28358(11)	1.000
0.0338(7)					
Cl4	Uani	0.58694(15)	0.30788(13)	0.18176(13)	1.000
0.0445(8)					
H21	Uiso	0.0731(11)	0.4453(12)	0.732(4)	1.000
0.0310					
H31	Uiso	-0.035(3)	0.484(3)	0.6636(19)	1.000
0.0360					
H41	Uiso	-0.061(4)	0.4453(15)	0.545(3)	1.000
0.0480					
H51	Uiso	0.0099(14)	0.3746(16)	0.497(5)	1.000
0.0470					
H61	Uiso	0.120(3)	0.338(2)	0.5564(18)	1.000
0.0330					
H81	Uiso	0.178(2)	0.317(5)	0.8297(11)	1.000
0.0330					
H91	Uiso	0.2168(12)	0.391(3)	0.941(3)	1.000
0.0450					
H101	Uiso	0.27870	0.52180	0.97460	1.000
0.0420					
H111	Uiso	0.308(2)	0.588(5)	0.8912(11)	1.000
0.0340					
H121	Uiso	0.2690(10)	0.515(2)	0.781(3)	1.000
0.0260					
H141	Uiso	0.269(4)	0.4872(14)	0.6451(7)	1.000
0.0280					
H151	Uiso	0.4150(9)	0.559(4)	0.6206(13)	1.000
0.0310					
H161	Uiso	0.542(5)	0.515(2)	0.6356(9)	1.000
0.0280					
H171	Uiso	0.515(4)	0.4083(14)	0.6761(6)	1.000
0.0280					
H191	Uiso	0.438(5)	0.3173(4)	0.7282(13)	1.000
0.0230					
H211	Uiso	0.3691(5)	0.277(4)	0.850(2)	1.000
0.0320					
H221	Uiso	0.424(2)	0.1976(15)	0.895(5)	1.000
0.0470					
H231	Uiso	0.426(2)	0.093(3)	0.837(2)	1.000
0.0420					
H241	Uiso	0.3686(5)	0.050(4)	0.719(2)	1.000
0.0300					
H271	Uiso	0.417(6)	0.1125(9)	0.617(2)	1.000
0.0330					
H281	Uiso	0.373(4)	0.0650(10)	0.501(2)	1.000

0.0310					
H291	Uiso	0.2165(18)	0.0454(16)	0.446(4)	1.000
0.0300					
H301	Uiso	0.107(5)	0.0681(8)	0.5039(19)	1.000
0.0270					
H321	Uiso	0.0671(6)	0.006(4)	0.6139(15)	1.000
0.0200					
H341	Uiso	-0.047(2)	-0.065(3)	0.6650(6)	1.000
0.0220					
H351	Uiso	-0.190(3)	-0.089(4)	0.7033(9)	1.000
0.0270					
H361	Uiso	-0.253(5)	0.0045(9)	0.7166(14)	1.000
0.0310					
H371	Uiso	-0.175(2)	0.116(3)	0.6898(5)	1.000
0.0250					
H401	Uiso	0.005(4)	0.2558(11)	0.781(2)	1.000
0.0290					
H411	Uiso	-0.0787(13)	0.3218(13)	0.833(4)	1.000
0.0400					
H421	Uiso	-0.188(3)	0.354(3)	0.767(2)	1.000
0.0430					
H431	Uiso	-0.224(4)	0.3198(12)	0.649(2)	1.000
0.0350					
H441	Uiso	-0.1455(12)	0.2533(12)	0.591(4)	1.000
0.0300					
H461	Uiso	-0.193(4)	0.1136(13)	0.540(2)	1.000
0.0350					
H471	Uiso	-0.245(6)	0.087(2)	0.419(2)	1.000
0.0420					
H481	Uiso	-0.122(2)	0.1245(11)	0.366(5)	1.000
0.0450					
H491	Uiso	0.032(4)	0.1790(13)	0.420(2)	1.000
0.0390					
H501	Uiso	0.086(6)	0.205(2)	0.532(2)	1.000
0.0350					
H22	Uiso	0.0934(15)	0.4744(15)	0.228(4)	1.000
0.0290					
H32	Uiso	-0.020(3)	0.506(3)	0.1614(19)	1.000
0.0360					
H42	Uiso	-0.062(4)	0.4643(12)	0.040(2)	1.000
0.0420					
H52	Uiso	0.0129(16)	0.3926(15)	-0.007(4)	1.000
0.0400					
H62	Uiso	0.123(3)	0.357(3)	0.0528(19)	1.000
0.0340					
H82	Uiso	0.179(3)	0.351(5)	0.3287(9)	1.000
0.0330					
H92	Uiso	0.214(2)	0.432(2)	0.434(3)	1.000
0.0500					
H102	Uiso	0.2914(14)	0.562(3)	0.469(4)	1.000
0.0410					
H112	Uiso	0.337(3)	0.621(5)	0.3799(10)	1.000
0.0360					
H122	Uiso	0.2973(15)	0.543(2)	0.270(3)	1.000
0.0270					
H142	Uiso	0.280(5)	0.5070(14)	0.1372(8)	1.000
0.0360					
H152	Uiso	0.4229(8)	0.574(4)	0.1112(17)	1.000
0.0370					
H162	Uiso	0.550(5)	0.537(2)	0.1310(10)	1.000
0.0350					
H172	Uiso	0.538(4)	0.4349(12)	0.1786(8)	1.000
0.0250					
H192	Uiso	0.456(5)	0.3447(4)	0.2302(15)	1.000
0.0230					
H212	Uiso	0.3871(6)	0.307(4)	0.346(2)	1.000
0.0320					

H222	Uiso	0.449(2)	0.2373(16)	0.408(4)	1.000
0.0360					
H232	Uiso	0.440(2)	0.125(3)	0.340(2)	1.000
0.0390					
H242	Uiso	0.3829(5)	0.077(4)	0.223(2)	1.000
0.0300					
H272	Uiso	0.425(6)	0.1314(9)	0.117(2)	1.000
0.0370					
H282	Uiso	0.382(4)	0.0837(10)	0.000(2)	1.000
0.0440					
H292	Uiso	0.223(2)	0.0590(19)	-0.051(4)	1.000
0.0380					
H302	Uiso	0.120(5)	0.0848(10)	0.007(2)	1.000
0.0320					
H322	Uiso	0.0800(6)	0.031(4)	0.1191(15)	1.000
0.0230					
H342	Uiso	-0.0404(19)	-0.033(3)	0.1717(6)	1.000
0.0250					
H352	Uiso	-0.175(3)	-0.055(4)	0.2103(9)	1.000
0.0280					
H362	Uiso	-0.235(5)	0.0355(8)	0.2259(15)	1.000
0.0320					
H372	Uiso	-0.159(2)	0.152(3)	0.1985(5)	1.000
0.0270					
H402	Uiso	0.002(4)	0.2929(8)	0.268(3)	1.000
0.0300					
H412	Uiso	-0.0710(14)	0.3626(19)	0.316(4)	1.000
0.0370					
H422	Uiso	-0.189(3)	0.381(3)	0.2408(17)	1.000
0.0430					
H432	Uiso	-0.216(4)	0.3329(9)	0.127(3)	1.000
0.0430					
H442	Uiso	-0.1379(12)	0.2633(16)	0.074(4)	1.000
0.0290					
H462	Uiso	-0.179(4)	0.1137(13)	0.042(2)	1.000
0.0340					
H472	Uiso	-0.231(6)	0.069(3)	-0.078(2)	1.000
0.0500					
H482	Uiso	-0.120(2)	0.1019(19)	-0.147(5)	1.000
0.0520					
H492	Uiso	0.039(4)	0.1811(14)	-0.090(3)	1.000
0.0430					
H502	Uiso	0.093(6)	0.227(3)	0.0278(18)	1.000
0.0320					
H320	Uiso	0.37920	0.69410	0.11760	0.52(3)
0.1080					
H310	Uiso	0.32120	0.73960	0.14610	0.52(3)
0.1080					
H330	Uiso	0.36490	0.70000	0.07620	0.158(10)
0.1080					
H340	Uiso	0.35790	0.72210	0.15380	0.158(10)
0.1080					
H350	Uiso	0.30790	0.74790	0.12500	0.32(3)
0.1080					
H360	Uiso	0.37640	0.70450	0.13780	0.32(3)
0.1080					
H620	Uiso	0.58190	0.15050	0.73510	0.607(14)
0.0870					
H610	Uiso	0.66370	0.14500	0.69900	0.607(14)
0.0870					
H630	Uiso	0.57260	0.14360	0.72540	0.393(14)
0.0870					
H640	Uiso	0.68360	0.16250	0.73370	0.393(14)
0.0870					
H11	Uiso	0.29500	0.35940	0.50700	1.000
0.0780					
H201	Uiso	0.28300	0.30850	0.43350	1.000

0.0780					
H12	Uiso	0.44710	0.30950	0.07770	1.000
0.0790					
H202	Uiso	0.41740	0.24940	0.00550	1.000
0.0790					
H13	Uiso	0.62960	0.26950	0.35280	1.000
0.0910					
H203	Uiso	0.67570	0.28960	0.29150	1.000
0.0910					
H14	Uiso	0.60310	0.21640	0.58790	1.000
0.0770					
H204	Uiso	0.51520	0.19350	0.52290	1.000
0.0770					
H15	Uiso	0.70210	0.16690	0.16680	1.000
0.2090					
H205	Uiso	0.60570	0.18030	0.15100	1.000
0.2090					

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

Pd1	0.0145(3)	0.0131(3)	0.0217(3)	0.0063(2)
0.0057(2)	0.0079(2)			
C11	0.0297(10)	0.0212(9)	0.0259(10)	0.0121(8)
0.0112(8)	0.0131(8)			
P1	0.0153(9)	0.0153(9)	0.0222(10)	0.0081(8)
0.0069(8)	0.0094(8)			
P2	0.0177(9)	0.0164(10)	0.0209(10)	0.0072(8)
0.0077(8)	0.0105(8)			
N1	0.014(3)	0.014(3)	0.021(3)	0.001(2)
0.002(2)	0.007(3)			
N2	0.017(3)	0.021(3)	0.013(3)	0.009(2)
0.001(2)	0.011(3)			
C11	0.020(4)	0.020(4)	0.028(4)	0.010(3)
0.008(3)	0.010(3)			
C21	0.025(4)	0.024(4)	0.028(4)	0.006(3)
0.003(3)	0.012(3)			
C31	0.022(4)	0.021(4)	0.055(6)	0.014(4)
0.009(4)	0.015(3)			
C41	0.035(5)	0.037(5)	0.056(6)	0.028(5)
-0.001(4)	0.023(4)			
C51	0.039(5)	0.037(5)	0.040(5)	0.016(4)
-0.002(4)	0.015(4)			
C61	0.033(5)	0.032(5)	0.030(5)	0.018(4)
0.011(4)	0.021(4)			
C71	0.009(3)	0.011(3)	0.021(4)	0.001(3)
0.001(3)	0.000(3)			
C81	0.040(5)	0.016(4)	0.028(4)	0.009(3)
0.012(4)	0.010(4)			
C91	0.054(6)	0.030(5)	0.029(5)	0.018(4)
0.016(4)	0.011(4)			
C101	0.043(5)	0.034(5)	0.026(5)	-0.001(4)
0.009(4)	0.016(4)			
C111	0.026(4)	0.028(4)	0.028(5)	0.000(4)
0.004(3)	0.012(4)			
C121	0.016(4)	0.022(4)	0.034(4)	0.011(3)
0.009(3)	0.014(3)			
C131	0.016(4)	0.010(3)	0.020(4)	0.002(3)
0.005(3)	0.002(3)			
C141	0.027(4)	0.016(4)	0.032(4)	0.006(3)
0.008(3)	0.014(3)			
C151	0.027(4)	0.022(4)	0.035(5)	0.021(4)

0.012(4)	0.010(3)			
C161	0.020(4)	0.020(4)	0.021(4)	0.006(3)
0.007(3)	-0.002(3)			
C171	0.021(4)	0.028(4)	0.022(4)	0.010(3)
0.009(3)	0.009(3)			
C181	0.019(4)	0.013(4)	0.029(4)	0.005(3)
0.004(3)	0.007(3)			
C191	0.014(4)	0.023(4)	0.022(4)	0.004(3)
0.004(3)	0.011(3)			
C201	0.021(4)	0.012(4)	0.027(4)	0.009(3)
0.012(3)	0.005(3)			
C211	0.025(4)	0.032(5)	0.026(4)	0.010(4)
0.002(3)	0.016(4)			
C221	0.041(5)	0.053(6)	0.024(5)	0.015(4)
0.000(4)	0.022(5)			
C231	0.038(5)	0.035(5)	0.046(6)	0.023(4)
0.012(4)	0.023(4)			
C241	0.025(4)	0.027(4)	0.031(4)	0.013(3)
0.011(3)	0.017(3)			
C251	0.013(4)	0.020(4)	0.021(4)	0.008(3)
0.002(3)	0.007(3)			
C261	0.012(3)	0.011(3)	0.027(4)	0.008(3)
0.005(3)	-0.002(3)			
C271	0.020(4)	0.024(4)	0.040(5)	0.010(4)
0.010(4)	0.011(3)			
C281	0.021(4)	0.028(4)	0.031(5)	0.004(3)
0.013(4)	0.012(3)			
C291	0.024(4)	0.019(4)	0.026(4)	-0.001(3)
0.005(3)	0.006(3)			
C301	0.022(4)	0.015(4)	0.024(4)	0.000(3)
0.001(3)	0.007(3)			
C311	0.011(3)	0.012(3)	0.031(4)	0.005(3)
0.009(3)	0.006(3)			
C321	0.017(4)	0.017(4)	0.022(4)	0.007(3)
0.006(3)	0.013(3)			
C331	0.019(4)	0.021(4)	0.020(4)	0.009(3)
0.004(3)	0.010(3)			
C341	0.022(4)	0.012(4)	0.022(4)	0.006(3)
0.006(3)	0.007(3)			
C351	0.019(4)	0.016(4)	0.030(4)	0.011(3)
0.005(3)	0.003(3)			
C361	0.028(4)	0.025(4)	0.028(4)	0.009(3)
0.011(4)	0.011(4)			
C371	0.020(4)	0.014(4)	0.033(4)	0.009(3)
0.011(3)	0.008(3)			
C381	0.018(4)	0.008(3)	0.022(4)	0.001(3)
0.008(3)	0.008(3)			
C391	0.015(4)	0.017(4)	0.033(4)	0.011(3)
0.009(3)	0.010(3)			
C401	0.022(4)	0.017(4)	0.036(5)	0.007(3)
0.012(3)	0.010(3)			
C411	0.035(5)	0.029(5)	0.034(5)	0.000(4)
0.014(4)	0.013(4)			
C421	0.024(4)	0.032(5)	0.052(6)	-0.002(4)
0.008(4)	0.018(4)			
C431	0.013(4)	0.024(4)	0.049(5)	0.003(4)
0.002(4)	0.013(3)			
C441	0.017(4)	0.023(4)	0.035(5)	0.008(3)
0.004(3)	0.008(3)			
C451	0.022(4)	0.019(4)	0.026(4)	0.010(3)
0.008(3)	0.011(3)			
C461	0.026(4)	0.019(4)	0.041(5)	0.007(4)
0.004(4)	0.009(3)			
C471	0.044(5)	0.031(5)	0.027(5)	0.006(4)
0.000(4)	0.018(4)			
C481	0.065(7)	0.028(5)	0.022(4)	0.006(4)
0.003(4)	0.026(5)			

C491	0.054(6)	0.039(5)	0.023(4)	0.020(4)
0.025(4)	0.030(5)			
C501	0.035(5)	0.019(4)	0.035(5)	0.006(3)
0.012(4)	0.012(4)			
Pd2	0.0144(3)	0.0149(3)	0.0219(3)	0.0080(2)
0.0053(2)	0.0087(2)			
P3	0.0156(9)	0.0191(10)	0.0219(10)	0.0086(8)
0.0074(8)	0.0111(8)			
P4	0.0166(9)	0.0164(10)	0.0253(10)	0.0109(8)
0.0085(8)	0.0100(8)			
N3	0.016(3)	0.010(3)	0.017(3)	0.003(2)
-0.001(2)	0.003(3)			
N4	0.014(3)	0.018(3)	0.024(3)	0.004(3)
0.003(3)	0.009(3)			
C12	0.019(4)	0.014(4)	0.029(4)	0.011(3)
0.006(3)	0.007(3)			
C22	0.022(4)	0.024(4)	0.034(5)	0.014(3)
0.013(3)	0.011(3)			
C32	0.027(4)	0.027(4)	0.042(5)	0.010(4)
0.002(4)	0.019(4)			
C42	0.036(5)	0.035(5)	0.046(6)	0.021(4)
0.007(4)	0.025(4)			
C52	0.042(5)	0.035(5)	0.027(5)	0.018(4)
0.008(4)	0.016(4)			
C62	0.033(5)	0.021(4)	0.032(5)	0.011(3)
0.008(4)	0.012(4)			
C72	0.014(4)	0.015(4)	0.026(4)	0.004(3)
0.002(3)	0.008(3)			
C82	0.037(5)	0.015(4)	0.031(5)	0.011(3)
0.006(4)	0.011(3)			
C92	0.069(7)	0.036(5)	0.027(5)	0.013(4)
0.023(5)	0.022(5)			
C102	0.039(5)	0.028(5)	0.027(5)	0.001(4)
-0.002(4)	0.013(4)			
C112	0.023(4)	0.023(4)	0.040(5)	-0.001(4)
0.001(4)	0.013(3)			
C122	0.016(4)	0.023(4)	0.034(5)	0.012(4)
0.008(3)	0.011(3)			
C132	0.015(4)	0.019(4)	0.028(4)	0.009(3)
0.010(3)	0.009(3)			
C142	0.029(4)	0.031(5)	0.045(5)	0.022(4)
0.018(4)	0.019(4)			
C152	0.029(5)	0.030(5)	0.043(5)	0.026(4)
0.018(4)	0.012(4)			
C162	0.026(4)	0.033(5)	0.037(5)	0.018(4)
0.019(4)	0.014(4)			
C172	0.021(4)	0.019(4)	0.021(4)	0.005(3)
0.003(3)	0.006(3)			
C182	0.021(4)	0.019(4)	0.019(4)	0.005(3)
0.004(3)	0.010(3)			
C192	0.019(4)	0.019(4)	0.024(4)	0.008(3)
0.006(3)	0.012(3)			
C202	0.013(3)	0.022(4)	0.016(4)	0.010(3)
0.003(3)	0.005(3)			
C212	0.033(5)	0.023(4)	0.030(4)	0.012(3)
0.009(4)	0.015(4)			
C222	0.030(5)	0.040(5)	0.027(4)	0.020(4)
0.005(4)	0.018(4)			
C232	0.024(4)	0.043(5)	0.049(6)	0.036(5)
0.012(4)	0.023(4)			
C242	0.015(4)	0.025(4)	0.039(5)	0.010(4)
0.005(3)	0.013(3)			
C252	0.009(3)	0.013(4)	0.031(4)	0.009(3)
0.006(3)	0.001(3)			
C262	0.020(4)	0.013(4)	0.031(4)	0.009(3)
0.009(3)	0.007(3)			
C272	0.020(4)	0.040(5)	0.037(5)	0.006(4)

0.009(4)	0.019(4)			
C282	0.028(5)	0.047(6)	0.038(5)	0.002(4)
0.015(4)	0.020(4)			
C292	0.038(5)	0.033(5)	0.021(4)	0.002(4)
0.010(4)	0.015(4)			
C302	0.018(4)	0.031(4)	0.031(5)	0.006(4)
0.005(3)	0.013(3)			
C312	0.021(4)	0.023(4)	0.027(4)	0.009(3)
0.008(3)	0.015(3)			
C322	0.019(4)	0.014(4)	0.025(4)	0.005(3)
0.005(3)	0.007(3)			
C332	0.016(4)	0.020(4)	0.024(4)	0.009(3)
0.005(3)	0.010(3)			
C342	0.019(4)	0.026(4)	0.024(4)	0.012(3)
0.002(3)	0.014(3)			
C352	0.022(4)	0.016(4)	0.023(4)	0.011(3)
0.001(3)	-0.001(3)			
C362	0.026(4)	0.033(5)	0.034(5)	0.019(4)
0.014(4)	0.018(4)			
C372	0.018(4)	0.025(4)	0.033(4)	0.015(3)
0.012(3)	0.014(3)			
C382	0.014(4)	0.009(3)	0.022(4)	0.003(3)
0.001(3)	0.004(3)			
C392	0.008(3)	0.012(4)	0.027(4)	0.004(3)
0.002(3)	0.000(3)			
C402	0.024(4)	0.019(4)	0.034(5)	0.007(3)
0.010(3)	0.009(3)			
C412	0.031(5)	0.022(4)	0.045(5)	0.008(4)
0.019(4)	0.012(4)			
C422	0.035(5)	0.025(4)	0.064(7)	0.014(4)
0.032(5)	0.021(4)			
C432	0.025(4)	0.028(5)	0.063(6)	0.019(4)
0.011(4)	0.018(4)			
C442	0.022(4)	0.023(4)	0.031(4)	0.011(3)
0.006(3)	0.011(3)			
C452	0.022(4)	0.024(4)	0.032(4)	0.013(3)
0.006(3)	0.015(3)			
C462	0.031(4)	0.016(4)	0.032(5)	0.005(3)
0.000(4)	0.007(3)			
C472	0.040(5)	0.030(5)	0.043(6)	0.005(4)
-0.010(4)	0.012(4)			
C482	0.069(7)	0.039(5)	0.027(5)	0.007(4)
0.008(5)	0.031(5)			
C492	0.055(6)	0.036(5)	0.027(5)	0.008(4)
0.017(4)	0.025(5)			
C502	0.033(5)	0.026(4)	0.034(5)	0.012(4)
0.020(4)	0.020(4)			
C119	0.0733(19)	0.0611(17)	0.0494(16)	0.0057(13)
-0.0007(14)	0.0378(15)			
C7	0.107(11)	0.053(7)	0.072(9)	0.022(6)
0.007(8)	0.030(7)			
C6	0.066(7)	0.065(7)	0.094(9)	0.047(7)
0.029(7)	0.046(6)			
C15	0.161(4)	0.0423(16)	0.068(2)	0.0292(15)
0.048(2)	0.0259(19)			
C16	0.085(2)	0.0506(16)	0.0397(15)	-0.0048(12)
0.0251(14)	-0.0122(15)			
C1	0.069(7)	0.037(6)	0.055(7)	0.016(5)
0.021(6)	0.004(5)			
C17	0.078(2)	0.085(2)	0.0441(16)	-0.0025(15)
0.0239(15)	-0.0194(17)			
C18	0.0652(19)	0.0669(19)	0.075(2)	0.0245(16)
0.0132(16)	0.0022(15)			
C2	0.070(7)	0.057(7)	0.040(6)	-0.003(5)
0.021(5)	0.020(6)			
C19	0.089(2)	0.081(2)	0.0662(18)	0.0394(16)
0.0358(16)	0.0584(18)			

C110	0.163(4)	0.097(3)	0.155(4)	0.091(3)
0.109(3)	0.096(3)			
C3	0.070(8)	0.088(9)	0.081(8)	0.058(7)
0.037(7)	0.048(7)			
C111	0.0676(17)	0.0501(15)	0.0372(13)	0.0151(11)
0.0161(12)	0.0132(13)			
C112	0.062(2)	0.052(2)	0.346(7)	0.071(3)
0.084(3)	0.0324(17)			
C4	0.056(7)	0.047(6)	0.059(7)	0.010(5)
0.023(5)	0.009(5)			
C113	0.100(4)	0.135(5)	0.328(9)	0.046(5)
0.105(5)	0.056(3)			
C114	0.086(3)	0.101(3)	0.342(8)	0.097(4)
0.066(4)	0.068(3)			
C5	0.043(8)	0.085(11)	0.37(3)	0.075(16)
0.060(14)	0.053(8)			
C12	0.0294(10)	0.0211(9)	0.0262(10)	0.0107(8)
0.0075(8)	0.0113(8)			
C13	0.0260(10)	0.0349(11)	0.0519(13)	0.0213(10)
0.0150(9)	0.0183(9)			
C14	0.0329(12)	0.0418(13)	0.0783(17)	0.0331(12)
0.0239(12)	0.0246(10)			

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

;

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

;

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

Pd1	C11	2.8025(19)	.	.
-----	-----	------------	---	---

yes

Pd1	P1	2.243(2)	.	.
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yes

Pd1	P2	2.262(2)	.	.
-----	----	----------	---	---

yes

Pd1	N1	2.086(6)	.	.
-----	----	----------	---	---

yes

Pd1	N2	2.164(6)	.	.
-----	----	----------	---	---

yes

P1	C381	1.811(8)	.	.
----	------	----------	---	---

yes

P1	C391	1.803(8)	.	.
----	------	----------	---	---

yes

P1	C451	1.810(8)	.	.
----	------	----------	---	---

yes

P2	C11	1.820(8)	.	.
----	-----	----------	---	---

yes

P2	C71	1.824(6)	.	.
----	-----	----------	---	---

yes

P2	C131	1.817(8)	.	.
----	------	----------	---	---

yes

N1	C191	1.281(10)	.	.
----	------	-----------	---	---

yes

N1	C201	1.461(10)	.	.
	yes			
N2	C311	1.452(10)	.	.
	yes			
N2	C321	1.290(10)	.	.
	yes			
C11	C21	1.397(11)	.	.
	no			
C11	C61	1.379(11)	.	.
	no			
C21	C31	1.405(12)	.	.
	no			
C31	C41	1.375(14)	.	.
	no			
C41	C51	1.375(14)	.	.
	no			
C51	C61	1.385(13)	.	.
	no			
C71	C81	1.387(10)	.	.
	no			
C71	C121	1.387(11)	.	.
	no			
C81	C91	1.363(11)	.	.
	no			
C91	C101	1.382(13)	.	.
	no			
C101	C111	1.371(12)	.	.
	no			
C111	C121	1.391(11)	.	.
	no			
C131	C141	1.413(10)	.	.
	no			
C131	C181	1.409(11)	.	.
	no			
C141	C151	1.382(11)	.	.
	no			
C151	C161	1.390(11)	.	.
	no			
C161	C171	1.387(11)	.	.
	no			
C171	C181	1.399(11)	.	.
	no			
C181	C191	1.445(11)	.	.
	no			
C201	C211	1.384(11)	.	.
	no			
C201	C251	1.390(11)	.	.
	no			
C211	C221	1.395(13)	.	.
	no			
C221	C231	1.369(13)	.	.
	no			
C231	C241	1.369(11)	.	.
	no			
C241	C251	1.393(11)	.	.
	no			
C251	C261	1.470(11)	.	.
	no			
C261	C271	1.382(12)	.	.
	no			
C261	C311	1.409(11)	.	.
	no			
C271	C281	1.375(11)	.	.
	no			
C281	C291	1.389(11)	.	.
	no			
C291	C301	1.386(11)	.	.

C301	no C311	1.373(11)	.	.
C321	no C331	1.458(11)	.	.
C331	no C341	1.389(11)	.	.
C331	no C381	1.402(11)	.	.
C341	no C351	1.392(11)	.	.
C351	no C361	1.387(12)	.	.
C361	no C371	1.386(11)	.	.
C371	no C381	1.392(11)	.	.
C391	no C401	1.385(11)	.	.
C391	no C441	1.404(11)	.	.
C401	no C411	1.394(12)	.	.
C411	no C421	1.374(14)	.	.
C421	no C431	1.379(12)	.	.
C431	no C441	1.385(11)	.	.
C451	no C461	1.390(12)	.	.
C451	no C501	1.391(12)	.	.
C461	no C471	1.372(11)	.	.
C471	no C481	1.377(14)	.	.
C481	no C491	1.375(15)	.	.
C491	no C501	1.366(11)	.	.
C21	no H21	0.96(8)	.	.
C31	no H31	0.99(5)	.	.
C41	no H41	0.88(6)	.	.
C51	no H51	0.81(10)	.	.
C61	no H61	1.00(4)	.	.
C81	no H81	0.99(9)	.	.
C91	no H91	0.86(6)	.	.
C101	no H101	0.9293	.	.
C111	no H111	0.95(9)	.	.
C121	no H121	0.79(5)	.	.
C141	no H141	0.92(6)	.	.
C151	no H151	1.01(7)	.	.
C161	no H161	0.96(6)	.	.

C171	H171 no	0.83(6)	.	.
C191	H191 no	0.86(7)	.	.
C211	H211 no	0.93(6)	.	.
C221	H221 no	0.76(10)	.	.
C231	H231 no	0.84(5)	.	.
C241	H241 no	0.99(6)	.	.
C271	H271 no	0.83(8)	.	.
C281	H281 no	0.94(6)	.	.
C291	H291 no	0.87(8)	.	.
C301	H301 no	0.98(7)	.	.
C321	H321 no	0.93(6)	.	.
C341	H341 no	0.96(5)	.	.
C351	H351 no	0.94(7)	.	.
C361	H361 no	0.93(7)	.	.
C371	H371 no	0.87(5)	.	.
C401	H401 no	0.99(5)	.	.
C411	H411 no	0.92(8)	.	.
C421	H421 no	0.90(5)	.	.
C431	H431 no	0.93(5)	.	.
C441	H441 no	0.97(8)	.	.
C461	H461 no	0.96(5)	.	.
C471	H471 no	0.99(8)	.	.
C481	H481 no	0.79(10)	.	.
C491	H491 no	0.76(5)	.	.
C501	H501 no	0.89(8)	.	.
Pd2	P3 yes	2.248(2)	.	.
Pd2	P4 yes	2.271(2)	.	.
Pd2	N3 yes	2.099(6)	.	.
Pd2	N4 yes	2.166(6)	.	.
P3	C382 yes	1.816(8)	.	.
P3	C392 yes	1.796(8)	.	.
P3	C452 yes	1.821(8)	.	.
P4	C12 yes	1.818(8)	.	.
P4	C72	1.828(8)	.	.

P4	yes C132	1.826(8)	.	.
N3	yes C192	1.248(10)	.	.
N3	yes C202	1.459(9)	.	.
N4	yes C312	1.468(10)	.	.
N4	yes C322	1.263(10)	.	.
C12	yes C22	1.396(11)	.	.
C12	no C62	1.389(11)	.	.
C22	no C32	1.392(12)	.	.
C32	no C42	1.377(12)	.	.
C42	no C52	1.369(14)	.	.
C52	no C62	1.387(13)	.	.
C72	no C82	1.374(11)	.	.
C72	no C122	1.404(11)	.	.
C82	no C92	1.377(11)	.	.
C92	no C102	1.377(13)	.	.
C102	no C112	1.397(12)	.	.
C112	no C122	1.367(11)	.	.
C132	no C142	1.399(11)	.	.
C132	no C182	1.387(11)	.	.
C142	no C152	1.397(13)	.	.
C152	no C162	1.374(14)	.	.
C162	no C172	1.381(12)	.	.
C172	no C182	1.390(11)	.	.
C182	no C192	1.462(11)	.	.
C202	no C212	1.373(10)	.	.
C202	no C252	1.398(10)	.	.
C212	no C222	1.381(12)	.	.
C222	no C232	1.396(13)	.	.
C232	no C242	1.377(11)	.	.
C242	no C252	1.396(11)	.	.
C252	no C262	1.475(11)	.	.
C262	no C272	1.397(12)	.	.
C262	no C312	1.387(11)	.	.

C272	C282 no	1.371(11)	.	.
C282	C292 no	1.378(13)	.	.
C292	C302 no	1.380(13)	.	.
C302	C312 no	1.379(11)	.	.
C322	C332 no	1.467(12)	.	.
C332	C342 no	1.375(11)	.	.
C332	C382 no	1.420(11)	.	.
C342	C352 no	1.395(11)	.	.
C352	C362 no	1.355(12)	.	.
C362	C372 no	1.393(11)	.	.
C372	C382 no	1.377(11)	.	.
C392	C402 no	1.381(11)	.	.
C392	C442 no	1.406(11)	.	.
C402	C412 no	1.368(12)	.	.
C412	C422 no	1.380(14)	.	.
C422	C432 no	1.351(14)	.	.
C432	C442 no	1.396(12)	.	.
C452	C462 no	1.387(12)	.	.
C452	C502 no	1.397(12)	.	.
C462	C472 no	1.378(12)	.	.
C472	C482 no	1.393(15)	.	.
C482	C492 no	1.348(15)	.	.
C492	C502 no	1.383(11)	.	.
C22	H22 no	0.93(8)	.	.
C32	H32 no	0.95(5)	.	.
C42	H42 no	0.98(5)	.	.
C52	H52 no	0.83(8)	.	.
C62	H62 no	0.95(5)	.	.
C82	H82 no	0.96(9)	.	.
C92	H92 no	0.78(5)	.	.
C102	H102 no	0.98(7)	.	.
C112	H112 no	0.98(9)	.	.
C122	H122 no	0.87(5)	.	.
C142	H142	0.87(7)	.	.

C152	no H152	0.92(7)	.	.
C162	no H162	0.91(7)	.	.
C172	no H172	0.98(6)	.	.
C192	no H192	0.94(7)	.	.
C212	no H212	0.92(6)	.	.
C222	no H222	0.98(8)	.	.
C232	no H232	0.80(5)	.	.
C242	no H242	0.98(6)	.	.
C272	no H272	0.82(8)	.	.
C282	no H282	0.97(6)	.	.
C292	no H292	0.85(8)	.	.
C302	no H302	0.89(7)	.	.
C322	no H322	0.92(6)	.	.
C342	no H342	0.81(5)	.	.
C352	no H352	0.87(7)	.	.
C362	no H362	0.93(7)	.	.
C372	no H372	0.98(5)	.	.
C402	no H402	0.79(6)	.	.
C412	no H412	0.94(8)	.	.
C422	no H422	0.95(5)	.	.
C432	no H432	0.85(6)	.	.
C442	no H442	1.00(8)	.	.
C462	no H462	0.93(5)	.	.
C472	no H472	0.93(8)	.	.
C482	no H482	1.00(10)	.	.
C492	no H492	0.87(6)	.	.
C502	no H502	0.90(8)	.	.
C119	no C7	1.762(13)	.	.
C120	yes C7	1.74(2)	.	.
C121	yes C7	1.78(4)	.	.
C122	yes C7	1.68(2)	.	.
C7	yes H310	0.9710	.	.
C7	no H320	0.9691	.	.
	no			

C7	H330	0.9710	.	.
	no			
C7	H340	0.9700	.	.
	no			
C7	H350	0.9698	.	.
	no			
C7	H360	0.9689	.	.
	no			
C115	C6	1.807(13)	.	.
	yes			
C116	C6	1.641(14)	.	.
	yes			
C117	C6	1.77(2)	.	.
	yes			
C118	C6	1.552(16)	.	.
	yes			
C6	H610	0.9703	.	.
	no			
C6	H620	0.9698	.	.
	no			
C6	H630	0.9702	.	.
	no			
C6	H640	0.9699	.	.
	no			
C15	C1	1.717(10)	.	.
	yes			
C16	C1	1.747(12)	.	.
	yes			
C1	H11	0.9709	.	.
	no			
C1	H201	0.9706	.	.
	no			
C17	C2	1.757(12)	.	.
	yes			
C18	C2	1.731(13)	.	.
	yes			
C2	H12	0.9704	.	.
	no			
C2	H202	0.9688	.	.
	no			
C19	C3	1.765(13)	.	.
	yes			
C110	C3	1.749(14)	.	.
	yes			
C3	H13	0.9695	.	.
	no			
C3	H203	0.9708	.	.
	no			
C111	C4	1.736(11)	.	.
	yes			
C112	C4	1.727(11)	.	.
	yes			
C4	H14	0.9709	.	.
	no			
C4	H204	0.9706	.	.
	no			
C113	C5	1.73(3)	.	.
	yes			
C114	C5	1.71(2)	.	.
	yes			
C5	H15	0.9701	.	.
	no			
C5	H205	0.9707	.	.
	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

C11	Pd1	P1	86.86(7)	.	.
.	yes				
C11	Pd1	P2	112.39(6)	.	.
.	yes				
C11	Pd1	N1	92.08(17)	.	.
.	yes				
C11	Pd1	N2	85.59(16)	.	.
.	yes				
P1	Pd1	P2	96.56(8)	.	.
.	yes				
P1	Pd1	N1	175.08(17)	.	.
.	yes				
P1	Pd1	N2	85.08(18)	.	.
.	yes				
P2	Pd1	N1	88.29(17)	.	.
.	yes				
P2	Pd1	N2	161.98(16)	.	.
.	yes				
N1	Pd1	N2	90.0(2)	.	.
.	yes				
Pd1	P1	C381	108.2(3)	.	.
.	yes				
Pd1	P1	C391	117.4(3)	.	.
.	yes				
Pd1	P1	C451	113.0(3)	.	.
.	yes				
C381	P1	C391	103.1(4)	.	.
.	yes				
C381	P1	C451	104.6(3)	.	.
.	yes				
C391	P1	C451	109.4(4)	.	.
.	yes				
Pd1	P2	C11	119.3(3)	.	.
.	yes				
Pd1	P2	C71	115.2(2)	.	.
.	yes				
Pd1	P2	C131	108.8(3)	.	.
.	yes				
C11	P2	C71	106.4(4)	.	.
.	yes				
C11	P2	C131	102.2(3)	.	.
.	yes				
C71	P2	C131	103.1(3)	.	.
.	yes				
Pd1	N1	C191	130.8(5)	.	.
.	yes				
Pd1	N1	C201	115.9(5)	.	.
.	yes				
C191	N1	C201	113.3(7)	.	.
.	yes				
Pd1	N2	C311	117.0(4)	.	.
.	yes				
Pd1	N2	C321	128.4(5)	.	.
.	yes				
C311	N2	C321	114.6(6)	.	.
.	yes				
P2	C11	C21	122.6(6)	.	.
.	yes				
P2	C11	C61	119.3(6)	.	.
.	yes				

C21	C11	C61	118.1(7)	.	.
.	no				
C11	C21	C31	120.5(7)	.	.
.	no				
C21	C31	C41	119.2(8)	.	.
.	no				
C31	C41	C51	121.0(9)	.	.
.	no				
C41	C51	C61	119.3(9)	.	.
.	no				
C11	C61	C51	121.8(8)	.	.
.	no				
P2	C71	C81	120.0(6)	.	.
.	yes				
P2	C71	C121	119.8(5)	.	.
.	yes				
C81	C71	C121	120.1(6)	.	.
.	no				
C71	C81	C91	119.1(7)	.	.
.	no				
C81	C91	C101	121.7(8)	.	.
.	no				
C91	C101	C111	119.2(7)	.	.
.	no				
C101	C111	C121	120.2(8)	.	.
.	no				
C71	C121	C111	119.5(7)	.	.
.	no				
P2	C131	C141	119.6(6)	.	.
.	yes				
P2	C131	C181	122.5(6)	.	.
.	yes				
C141	C131	C181	117.8(7)	.	.
.	no				
C131	C141	C151	121.8(7)	.	.
.	no				
C141	C151	C161	119.6(7)	.	.
.	no				
C151	C161	C171	120.0(7)	.	.
.	no				
C161	C171	C181	120.8(7)	.	.
.	no				
C131	C181	C171	120.0(7)	.	.
.	no				
C131	C181	C191	125.3(7)	.	.
.	no				
C171	C181	C191	114.6(7)	.	.
.	no				
N1	C191	C181	127.7(7)	.	.
.	yes				
N1	C201	C211	118.5(7)	.	.
.	yes				
N1	C201	C251	119.5(7)	.	.
.	yes				
C211	C201	C251	121.7(7)	.	.
.	no				
C201	C211	C221	118.2(8)	.	.
.	no				
C211	C221	C231	121.1(7)	.	.
.	no				
C221	C231	C241	119.7(8)	.	.
.	no				
C231	C241	C251	121.5(8)	.	.
.	no				
C201	C251	C241	117.8(7)	.	.
.	no				
C201	C251	C261	122.6(7)	.	.

.	no				
C241	C251	C261	119.5(7)	.	.
.	no				
C251	C261	C271	120.5(7)	.	.
.	no				
C251	C261	C311	122.5(7)	.	.
.	no				
C271	C261	C311	116.8(7)	.	.
.	no				
C261	C271	C281	122.7(8)	.	.
.	no				
C271	C281	C291	119.3(8)	.	.
.	no				
C281	C291	C301	119.6(7)	.	.
.	no				
C291	C301	C311	120.2(8)	.	.
.	no				
N2	C311	C261	121.0(7)	.	.
.	yes				
N2	C311	C301	117.5(7)	.	.
.	yes				
C261	C311	C301	121.3(7)	.	.
.	no				
N2	C321	C331	127.5(7)	.	.
.	yes				
C321	C331	C341	115.5(7)	.	.
.	no				
C321	C331	C381	123.9(7)	.	.
.	no				
C341	C331	C381	120.6(7)	.	.
.	no				
C331	C341	C351	120.7(7)	.	.
.	no				
C341	C351	C361	119.2(7)	.	.
.	no				
C351	C361	C371	119.7(8)	.	.
.	no				
C361	C371	C381	122.1(8)	.	.
.	no				
P1	C381	C331	121.7(6)	.	.
.	yes				
P1	C381	C371	120.6(6)	.	.
.	yes				
C331	C381	C371	117.6(7)	.	.
.	no				
P1	C391	C401	116.7(6)	.	.
.	yes				
P1	C391	C441	123.1(6)	.	.
.	yes				
C401	C391	C441	120.1(7)	.	.
.	no				
C391	C401	C411	119.7(8)	.	.
.	no				
C401	C411	C421	120.1(9)	.	.
.	no				
C411	C421	C431	120.3(9)	.	.
.	no				
C421	C431	C441	120.7(8)	.	.
.	no				
C391	C441	C431	119.0(7)	.	.
.	no				
P1	C451	C461	121.3(6)	.	.
.	yes				
P1	C451	C501	120.2(6)	.	.
.	yes				
C461	C451	C501	118.5(7)	.	.
.	no				

C451	C461	C471	120.7(8)	.	.
.	no				
C461	C471	C481	119.3(9)	.	.
.	no				
C471	C481	C491	121.1(8)	.	.
.	no				
C481	C491	C501	119.3(9)	.	.
.	no				
C451	C501	C491	121.1(9)	.	.
.	no				
C11	C21	H21	119.7(17)	.	.
.	no				
C31	C21	H21	119.8(17)	.	.
.	no				
C21	C31	H31	121(2)	.	.
.	no				
C41	C31	H31	120(2)	.	.
.	no				
C31	C41	H41	119(4)	.	.
.	no				
C51	C41	H41	120(4)	.	.
.	no				
C41	C51	H51	120(3)	.	.
.	no				
C61	C51	H51	120(3)	.	.
.	no				
C11	C61	H61	119(2)	.	.
.	no				
C51	C61	H61	119(2)	.	.
.	no				
C71	C81	H81	120.6(19)	.	.
.	no				
C91	C81	H81	120.3(19)	.	.
.	no				
C81	C91	H91	119(4)	.	.
.	no				
C101	C91	H91	119(4)	.	.
.	no				
C91	C101	H101	120.45	.	.
.	no				
C111	C101	H101	120.32	.	.
.	no				
C101	C111	H111	120(2)	.	.
.	no				
C121	C111	H111	120(2)	.	.
.	no				
C71	C121	H121	121(4)	.	.
.	no				
C111	C121	H121	120(4)	.	.
.	no				
C131	C141	H141	119(2)	.	.
.	no				
C151	C141	H141	119(2)	.	.
.	no				
C141	C151	H151	120(2)	.	.
.	no				
C161	C151	H151	120(2)	.	.
.	no				
C151	C161	H161	119(3)	.	.
.	no				
C171	C161	H161	121(3)	.	.
.	no				
C161	C171	H171	120(2)	.	.
.	no				
C181	C171	H171	120(2)	.	.
.	no				
N1	C191	H191	116.1(14)	.	.

.	no				
C181	C191	H191	116.2(14)	.	.
.	no				
C201	C211	H211	121(3)	.	.
.	no				
C221	C211	H211	121(3)	.	.
.	no				
C211	C221	H221	120(3)	.	.
.	no				
C231	C221	H221	119(3)	.	.
.	no				
C221	C231	H231	120(3)	.	.
.	no				
C241	C231	H231	121(3)	.	.
.	no				
C231	C241	H241	119(3)	.	.
.	no				
C251	C241	H241	119(3)	.	.
.	no				
C261	C271	H271	119(4)	.	.
.	no				
C281	C271	H271	119(4)	.	.
.	no				
C271	C281	H281	120(3)	.	.
.	no				
C291	C281	H281	120(3)	.	.
.	no				
C281	C291	H291	120(2)	.	.
.	no				
C301	C291	H291	120(2)	.	.
.	no				
C291	C301	H301	120(3)	.	.
.	no				
C311	C301	H301	120(3)	.	.
.	no				
N2	C321	H321	116(3)	.	.
.	no				
C331	C321	H321	116(3)	.	.
.	no				
C331	C341	H341	120(3)	.	.
.	no				
C351	C341	H341	120(3)	.	.
.	no				
C341	C351	H351	121(3)	.	.
.	no				
C361	C351	H351	120(3)	.	.
.	no				
C351	C361	H361	120.3(19)	.	.
.	no				
C371	C361	H361	119.9(19)	.	.
.	no				
C361	C371	H371	119(3)	.	.
.	no				
C381	C371	H371	119(3)	.	.
.	no				
C391	C401	H401	120(3)	.	.
.	no				
C411	C401	H401	120(3)	.	.
.	no				
C401	C411	H411	120.0(19)	.	.
.	no				
C421	C411	H411	120(2)	.	.
.	no				
C411	C421	H421	120(3)	.	.
.	no				
C431	C421	H421	119(3)	.	.
.	no				

C421	C431	H431	119(3)	.	.
.	no				
C441	C431	H431	120(3)	.	.
.	no				
C391	C441	H441	120.5(17)	.	.
.	no				
C431	C441	H441	120.5(17)	.	.
.	no				
C451	C461	H461	119(3)	.	.
.	no				
C471	C461	H461	120(3)	.	.
.	no				
C461	C471	H471	120(3)	.	.
.	no				
C481	C471	H471	121(3)	.	.
.	no				
C471	C481	H481	119(3)	.	.
.	no				
C491	C481	H481	120(3)	.	.
.	no				
C481	C491	H491	121(4)	.	.
.	no				
C501	C491	H491	120(4)	.	.
.	no				
C451	C501	H501	120(3)	.	.
.	no				
C491	C501	H501	119(3)	.	.
.	no				
P3	Pd2	P4	97.19(8)	.	.
.	yes				
P3	Pd2	N3	174.79(16)	.	.
.	yes				
P3	Pd2	N4	84.04(18)	.	.
.	yes				
P4	Pd2	N3	87.93(17)	.	.
.	yes				
P4	Pd2	N4	164.41(16)	.	.
.	yes				
N3	Pd2	N4	90.8(2)	.	.
.	yes				
Pd2	P3	C382	108.0(3)	.	.
.	yes				
Pd2	P3	C392	120.1(3)	.	.
.	yes				
Pd2	P3	C452	113.2(3)	.	.
.	yes				
C382	P3	C392	102.3(4)	.	.
.	yes				
C382	P3	C452	102.9(3)	.	.
.	yes				
C392	P3	C452	108.5(4)	.	.
.	yes				
Pd2	P4	C12	118.3(3)	.	.
.	yes				
Pd2	P4	C72	116.3(3)	.	.
.	yes				
Pd2	P4	C132	108.7(3)	.	.
.	yes				
C12	P4	C72	105.6(4)	.	.
.	yes				
C12	P4	C132	103.2(4)	.	.
.	yes				
C72	P4	C132	102.9(4)	.	.
.	yes				
Pd2	N3	C192	131.0(5)	.	.
.	yes				
Pd2	N3	C202	115.5(5)	.	.

.		yes				
C192	N3		C202	113.4(7)	.	.
.		yes				
Pd2	N4		C312	115.9(4)	.	.
.		yes				
Pd2	N4		C322	129.2(5)	.	.
.		yes				
C312	N4		C322	114.8(6)	.	.
.		yes				
P4	C12		C22	121.6(6)	.	.
.		yes				
P4	C12		C62	119.3(6)	.	.
.		yes				
C22	C12		C62	119.1(7)	.	.
.		no				
C12	C22		C32	119.9(7)	.	.
.		no				
C22	C32		C42	120.2(8)	.	.
.		no				
C32	C42		C52	120.1(9)	.	.
.		no				
C42	C52		C62	120.7(8)	.	.
.		no				
C12	C62		C52	120.0(8)	.	.
.		no				
P4	C72		C82	122.0(6)	.	.
.		yes				
P4	C72		C122	118.5(6)	.	.
.		yes				
C82	C72		C122	119.5(7)	.	.
.		no				
C72	C82		C92	120.1(7)	.	.
.		no				
C82	C92		C102	120.8(8)	.	.
.		no				
C92	C102		C112	119.2(7)	.	.
.		no				
C102	C112		C122	120.3(8)	.	.
.		no				
C72	C122		C112	120.0(7)	.	.
.		no				
P4	C132		C142	118.4(6)	.	.
.		yes				
P4	C132		C182	122.1(6)	.	.
.		yes				
C142	C132		C182	119.2(8)	.	.
.		no				
C132	C142		C152	120.1(8)	.	.
.		no				
C142	C152		C162	120.4(8)	.	.
.		no				
C152	C162		C172	119.4(9)	.	.
.		no				
C162	C172		C182	121.1(8)	.	.
.		no				
C132	C182		C172	119.8(7)	.	.
.		no				
C132	C182		C192	124.7(7)	.	.
.		no				
C172	C182		C192	115.5(7)	.	.
.		no				
N3	C192		C182	129.1(8)	.	.
.		yes				
N3	C202		C212	119.2(6)	.	.
.		yes				
N3	C202		C252	119.5(6)	.	.
.		yes				

C212	C202	C252	121.2(7)	.	.
.	no				
C202	C212	C222	121.3(7)	.	.
.	no				
C212	C222	C232	118.2(7)	.	.
.	no				
C222	C232	C242	120.6(8)	.	.
.	no				
C232	C242	C252	121.3(7)	.	.
.	no				
C202	C252	C242	117.3(7)	.	.
.	no				
C202	C252	C262	122.4(7)	.	.
.	no				
C242	C252	C262	120.0(7)	.	.
.	no				
C252	C262	C272	119.6(7)	.	.
.	no				
C252	C262	C312	123.7(7)	.	.
.	no				
C272	C262	C312	116.6(7)	.	.
.	no				
C262	C272	C282	122.2(9)	.	.
.	no				
C272	C282	C292	119.1(9)	.	.
.	no				
C282	C292	C302	120.8(7)	.	.
.	no				
C292	C302	C312	118.9(8)	.	.
.	no				
N4	C312	C262	119.8(7)	.	.
.	yes				
N4	C312	C302	117.7(7)	.	.
.	yes				
C262	C312	C302	122.3(8)	.	.
.	no				
N4	C322	C332	128.2(7)	.	.
.	yes				
C322	C332	C342	116.5(7)	.	.
.	no				
C322	C332	C382	123.5(7)	.	.
.	no				
C342	C332	C382	120.0(7)	.	.
.	no				
C332	C342	C352	120.1(7)	.	.
.	no				
C342	C352	C362	120.3(7)	.	.
.	no				
C352	C362	C372	120.4(8)	.	.
.	no				
C362	C372	C382	120.8(8)	.	.
.	no				
P3	C382	C332	119.8(6)	.	.
.	yes				
P3	C382	C372	121.5(6)	.	.
.	yes				
C332	C382	C372	118.4(7)	.	.
.	no				
P3	C392	C402	118.1(6)	.	.
.	yes				
P3	C392	C442	122.5(6)	.	.
.	yes				
C402	C392	C442	119.4(7)	.	.
.	no				
C392	C402	C412	121.2(8)	.	.
.	no				
C402	C412	C422	119.4(9)	.	.

.	no				
C412	C422	C432	120.6(9)	.	.
.	no				
C422	C432	C442	121.4(9)	.	.
.	no				
C392	C442	C432	118.0(7)	.	.
.	no				
P3	C452	C462	120.9(6)	.	.
.	yes				
P3	C452	C502	119.4(6)	.	.
.	yes				
C462	C452	C502	119.8(7)	.	.
.	no				
C452	C462	C472	119.5(8)	.	.
.	no				
C462	C472	C482	119.7(9)	.	.
.	no				
C472	C482	C492	121.3(9)	.	.
.	no				
C482	C492	C502	119.8(9)	.	.
.	no				
C452	C502	C492	120.0(8)	.	.
.	no				
C12	C22	H22	120(2)	.	.
.	no				
C32	C22	H22	120(2)	.	.
.	no				
C22	C32	H32	120(3)	.	.
.	no				
C42	C32	H32	120(3)	.	.
.	no				
C32	C42	H42	120(3)	.	.
.	no				
C52	C42	H42	120(3)	.	.
.	no				
C42	C52	H52	120(2)	.	.
.	no				
C62	C52	H52	120(2)	.	.
.	no				
C12	C62	H62	120(3)	.	.
.	no				
C52	C62	H62	120(3)	.	.
.	no				
C72	C82	H82	120.0(18)	.	.
.	no				
C92	C82	H82	119.9(18)	.	.
.	no				
C82	C92	H92	120(4)	.	.
.	no				
C102	C92	H92	119(4)	.	.
.	no				
C92	C102	H102	120(4)	.	.
.	no				
C112	C102	H102	120(4)	.	.
.	no				
C102	C112	H112	120.0(18)	.	.
.	no				
C122	C112	H112	119.8(18)	.	.
.	no				
C72	C122	H122	120(3)	.	.
.	no				
C112	C122	H122	120(3)	.	.
.	no				
C132	C142	H142	120(3)	.	.
.	no				
C152	C142	H142	120(3)	.	.
.	no				

C142	C152	H152	120(2)	.	.
.	no				
C162	C152	H152	120(2)	.	.
.	no				
C152	C162	H162	120(4)	.	.
.	no				
C172	C162	H162	120(4)	.	.
.	no				
C162	C172	H172	119.5(19)	.	.
.	no				
C182	C172	H172	119.4(19)	.	.
.	no				
N3	C192	H192	115.5(14)	.	.
.	no				
C182	C192	H192	115.5(13)	.	.
.	no				
C202	C212	H212	120(3)	.	.
.	no				
C222	C212	H212	119(3)	.	.
.	no				
C212	C222	H222	121(2)	.	.
.	no				
C232	C222	H222	121(2)	.	.
.	no				
C222	C232	H232	120(3)	.	.
.	no				
C242	C232	H232	120(3)	.	.
.	no				
C232	C242	H242	120(3)	.	.
.	no				
C252	C242	H242	119(3)	.	.
.	no				
C262	C272	H272	119(4)	.	.
.	no				
C282	C272	H272	119(4)	.	.
.	no				
C272	C282	H282	120(3)	.	.
.	no				
C292	C282	H282	120(3)	.	.
.	no				
C282	C292	H292	119(3)	.	.
.	no				
C302	C292	H292	120(3)	.	.
.	no				
C292	C302	H302	120(3)	.	.
.	no				
C312	C302	H302	121(3)	.	.
.	no				
N4	C322	H322	116(3)	.	.
.	no				
C332	C322	H322	116(3)	.	.
.	no				
C332	C342	H342	120(3)	.	.
.	no				
C352	C342	H342	120(3)	.	.
.	no				
C342	C352	H352	120(4)	.	.
.	no				
C362	C352	H352	119(4)	.	.
.	no				
C352	C362	H362	119.9(18)	.	.
.	no				
C372	C362	H362	119.8(19)	.	.
.	no				
C362	C372	H372	120(3)	.	.
.	no				
C382	C372	H372	119(3)	.	.

.	no				
C392	C402	H402	120(4)	.	.
.	no				
C412	C402	H402	119(4)	.	.
.	no				
C402	C412	H412	120(2)	.	.
.	no				
C422	C412	H412	120(2)	.	.
.	no				
C412	C422	H422	120(2)	.	.
.	no				
C432	C422	H422	120(2)	.	.
.	no				
C422	C432	H432	119(4)	.	.
.	no				
C442	C432	H432	120(4)	.	.
.	no				
C392	C442	H442	121.0(19)	.	.
.	no				
C432	C442	H442	121.0(19)	.	.
.	no				
C452	C462	H462	120(3)	.	.
.	no				
C472	C462	H462	120(3)	.	.
.	no				
C462	C472	H472	120(3)	.	.
.	no				
C482	C472	H472	120(3)	.	.
.	no				
C472	C482	H482	119(3)	.	.
.	no				
C492	C482	H482	119(2)	.	.
.	no				
C482	C492	H492	120(4)	.	.
.	no				
C502	C492	H492	120(4)	.	.
.	no				
C452	C502	H502	120(3)	.	.
.	no				
C492	C502	H502	120(3)	.	.
.	no				
C119	C7	C120	118.6(9)	.	.
.	yes				
C119	C7	C121	100.5(14)	.	.
.	yes				
C119	C7	C122	105.8(13)	.	.
.	yes				
C119	C7	H310	107.68	.	.
.	no				
C119	C7	H320	107.76	.	.
.	no				
C119	C7	H330	111.67	.	.
.	no				
C119	C7	H340	111.71	.	.
.	no				
C119	C7	H350	110.58	.	.
.	no				
C119	C7	H360	110.63	.	.
.	no				
C120	C7	H310	107.64	.	.
.	no				
C120	C7	H320	107.57	.	.
.	no				
H310	C7	H320	107.12	.	.
.	no				
C121	C7	H330	111.58	.	.
.	no				

C121	C7	H340	111.64	.	.
.	no				
C122	C7	H350	110.49	.	.
.	no				
C122	C7	H360	110.60	.	.
.	no				
H330	C7	H340	109.57	.	.
.	no				
H350	C7	H360	108.71	.	.
.	no				
C115	C6	C116	111.6(7)	.	.
.	yes				
C117	C6	C118	120.8(12)	.	.
.	yes				
C115	C6	H610	109.27	.	.
.	no				
C115	C6	H620	109.24	.	.
.	no				
C116	C6	H610	109.34	.	.
.	no				
C116	C6	H620	109.32	.	.
.	no				
H610	C6	H620	108.05	.	.
.	no				
C117	C6	H630	107.22	.	.
.	no				
C117	C6	H640	107.15	.	.
.	no				
C118	C6	H630	107.05	.	.
.	no				
C118	C6	H640	107.13	.	.
.	no				
H630	C6	H640	106.77	.	.
.	no				
C15	C1	C16	113.3(7)	.	.
.	yes				
C15	C1	H11	108.94	.	.
.	no				
C15	C1	H201	108.99	.	.
.	no				
C16	C1	H11	108.85	.	.
.	no				
C16	C1	H201	108.92	.	.
.	no				
H11	C1	H201	107.72	.	.
.	no				
C17	C2	C18	111.4(6)	.	.
.	yes				
C17	C2	H12	109.32	.	.
.	no				
C17	C2	H202	109.39	.	.
.	no				
C18	C2	H12	109.33	.	.
.	no				
C18	C2	H202	109.40	.	.
.	no				
H12	C2	H202	107.97	.	.
.	no				
C19	C3	C110	110.6(7)	.	.
.	yes				
C19	C3	H13	109.60	.	.
.	no				
C19	C3	H203	109.43	.	.
.	no				
C110	C3	H13	109.56	.	.
.	no				
C110	C3	H203	109.46	.	.

.		no				
H13	C3		H203	108.10	.	.
.		no				
Cl11	C4		Cl12	111.5(7)	.	.
.		yes				
Cl11	C4		H14	109.35	.	.
.		no				
Cl11	C4		H204	109.30	.	.
.		no				
Cl12	C4		H14	109.32	.	.
.		no				
Cl12	C4		H204	109.43	.	.
.		no				
H14	C4		H204	107.87	.	.
.		no				
Cl13	C5		Cl14	113.4(11)	.	.
.		yes				
Cl13	C5		H15	108.94	.	.
.		no				
Cl13	C5		H205	108.87	.	.
.		no				
Cl14	C5		H15	108.86	.	.
.		no				
Cl14	C5		H205	108.95	.	.
.		no				
H15	C5		H205	107.71	.	.
.		no				

loop_

_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

_geom_torsion_atom_site_label_4

_geom_torsion

_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion_publ_flag

Cl1	Pd1	P1	C381	-39.4(2)	.	.
.	.	no				
Cl1	Pd1	P1	C391	76.6(3)	.	.
.	.	no				
Cl1	Pd1	P1	C451	-154.7(3)	.	.
.	.	no				
P2	Pd1	P1	C381	-151.6(2)	.	.
.	.	no				
P2	Pd1	P1	C391	-35.6(3)	.	.
.	.	no				
P2	Pd1	P1	C451	93.1(3)	.	.
.	.	no				
N2	Pd1	P1	C381	46.4(3)	.	.
.	.	no				
N2	Pd1	P1	C391	162.4(3)	.	.
.	.	no				
N2	Pd1	P1	C451	-68.9(3)	.	.
.	.	no				
Cl1	Pd1	P2	Cl1	-114.0(3)	.	.
.	.	no				
Cl1	Pd1	P2	C71	14.4(3)	.	.
.	.	no				
Cl1	Pd1	P2	Cl131	129.6(2)	.	.
.	.	no				
P1	Pd1	P2	Cl1	-24.7(3)	.	.
.	.	no				
P1	Pd1	P2	C71	103.7(3)	.	.
.	.	no				

P1	Pd1	P2	C131	-141.1(2)	.	.
.	no					
N1	Pd1	P2	C11	154.5(3)	.	.
.	no					
N1	Pd1	P2	C71	-77.1(3)	.	.
.	no					
N1	Pd1	P2	C131	38.0(3)	.	.
.	no					
C11	Pd1	N1	C191	-144.3(7)	.	.
.	no					
C11	Pd1	N1	C201	37.7(5)	.	.
.	no					
P2	Pd1	N1	C191	-32.0(7)	.	.
.	no					
P2	Pd1	N1	C201	150.1(5)	.	.
.	no					
N2	Pd1	N1	C191	130.1(7)	.	.
.	no					
N2	Pd1	N1	C201	-47.9(5)	.	.
.	no					
C11	Pd1	N2	C311	-134.0(5)	.	.
.	no					
C11	Pd1	N2	C321	49.1(6)	.	.
.	no					
P1	Pd1	N2	C311	138.8(5)	.	.
.	no					
P1	Pd1	N2	C321	-38.1(6)	.	.
.	no					
N1	Pd1	N2	C311	-41.9(5)	.	.
.	no					
N1	Pd1	N2	C321	141.2(6)	.	.
.	no					
C451	P1	C391	C441	2.1(8)	.	.
.	no					
C391	P1	C381	C371	15.3(6)	.	.
.	no					
C451	P1	C381	C371	-99.0(6)	.	.
.	no					
Pd1	P1	C391	C401	-51.6(7)	.	.
.	no					
Pd1	P1	C381	C331	-41.6(6)	.	.
.	no					
C391	P1	C381	C331	-166.6(6)	.	.
.	no					
C451	P1	C381	C331	79.1(6)	.	.
.	no					
Pd1	P1	C381	C371	140.4(5)	.	.
.	no					
C391	P1	C451	C501	124.7(7)	.	.
.	no					
C451	P1	C391	C401	178.0(6)	.	.
.	no					
Pd1	P1	C451	C461	170.8(6)	.	.
.	no					
C381	P1	C391	C401	67.1(7)	.	.
.	no					
C381	P1	C451	C461	53.4(7)	.	.
.	no					
Pd1	P1	C391	C441	132.5(6)	.	.
.	no					
C381	P1	C391	C441	-108.7(7)	.	.
.	no					
C381	P1	C451	C501	-125.5(7)	.	.
.	no					
C391	P1	C451	C461	-56.4(7)	.	.
.	no					
Pd1	P1	C451	C501	-8.1(7)	.	.

.	C131	P2	no	C11	C21	-120.0(7)	.	.
.	C131	P2	no	C71	C81	-128.2(7)	.	.
.	Pd1	P2	no	C11	C61	-59.5(7)	.	.
.	C71	P2	no	C11	C21	-12.2(8)	.	.
.	Pd1	P2	no	C11	C21	120.1(6)	.	.
.	C71	P2	no	C131	C141	-86.3(6)	.	.
.	Pd1	P2	no	C71	C121	168.5(6)	.	.
.	C11	P2	no	C71	C121	-57.0(8)	.	.
.	C131	P2	no	C71	C121	50.1(7)	.	.
.	C71	P2	no	C11	C61	168.2(6)	.	.
.	C131	P2	no	C11	C61	60.4(7)	.	.
.	C11	P2	no	C131	C181	-160.7(6)	.	.
.	Pd1	P2	no	C131	C141	150.9(5)	.	.
.	Pd1	P2	no	C131	C181	-33.7(6)	.	.
.	Pd1	P2	no	C71	C81	-9.9(8)	.	.
.	C71	P2	no	C131	C181	89.0(6)	.	.
.	C11	P2	no	C131	C141	24.0(6)	.	.
.	C11	P2	no	C71	C81	124.7(7)	.	.
.	C191	N1	no	C201	C251	-96.8(9)	.	.
.	Pd1	N1	no	C201	C211	-104.4(7)	.	.
.	Pd1	N1	no	C201	C251	81.6(8)	.	.
.	C191	N1	no	C201	C211	77.3(9)	.	.
.	Pd1	N1	no	C191	C181	5.1(12)	.	.
.	C201	N1	no	C191	C181	-176.9(7)	.	.
.	Pd1	N2	no	C311	C261	73.1(8)	.	.
.	C321	N2	no	C311	C301	67.2(9)	.	.
.	Pd1	N2	no	C321	C331	5.4(10)	.	.
.	Pd1	N2	no	C311	C301	-110.2(7)	.	.
.	C311	N2	no	C321	C331	-171.6(7)	.	.
.	C321	N2	no	C311	C261	-109.6(8)	.	.
.	C21	C11	no	C61	C51	-0.6(12)	.	.
.	P2	C11	no	C21	C31	179.6(6)	.	.
.	P2	C11	no	C61	C51	179.1(7)	.	.
.	.	.	no	.	.	.	.	.

C61	C11	C21	C31	-0.8(11)	.	.
.	no					
C11	C21	C31	C41	0.9(12)	.	.
.	no					
C21	C31	C41	C51	0.3(13)	.	.
.	no					
C31	C41	C51	C61	-1.7(14)	.	.
.	no					
C41	C51	C61	C11	1.8(13)	.	.
.	no					
P2	C71	C81	C91	179.7(8)	.	.
.	no					
C121	C71	C81	C91	1.4(13)	.	.
.	no					
P2	C71	C121	C111	-179.6(7)	.	.
.	no					
C81	C71	C121	C111	-1.3(13)	.	.
.	no					
C71	C81	C91	C101	-0.6(15)	.	.
.	no					
C81	C91	C101	C111	-0.5(15)	.	.
.	no					
C91	C101	C111	C121	0.6(14)	.	.
.	no					
C101	C111	C121	C71	0.3(15)	.	.
.	no					
P2	C131	C181	C191	1.4(10)	.	.
.	no					
P2	C131	C181	C171	-175.0(6)	.	.
.	no					
C141	C131	C181	C171	0.4(11)	.	.
.	no					
P2	C131	C141	C151	175.0(6)	.	.
.	no					
C181	C131	C141	C151	-0.6(11)	.	.
.	no					
C141	C131	C181	C191	176.8(7)	.	.
.	no					
C131	C141	C151	C161	0.9(11)	.	.
.	no					
C141	C151	C161	C171	-1.0(12)	.	.
.	no					
C151	C161	C171	C181	0.8(12)	.	.
.	no					
C161	C171	C181	C191	-177.3(7)	.	.
.	no					
C161	C171	C181	C131	-0.5(11)	.	.
.	no					
C131	C181	C191	N1	18.8(13)	.	.
.	no					
C171	C181	C191	N1	-164.7(8)	.	.
.	no					
N1	C201	C211	C221	-173.3(8)	.	.
.	no					
N1	C201	C251	C261	-3.1(12)	.	.
.	no					
C251	C201	C211	C221	0.6(13)	.	.
.	no					
N1	C201	C251	C241	173.0(7)	.	.
.	no					
C211	C201	C251	C261	-177.0(8)	.	.
.	no					
C211	C201	C251	C241	-0.8(12)	.	.
.	no					
C201	C211	C221	C231	0.1(17)	.	.
.	no					
C211	C221	C231	C241	-0.6(14)	.	.

.	no					
C221	C231	C241	C251	0.3(14)	.	.
.	no					
C231	C241	C251	C201	0.3(12)	.	.
.	no					
C231	C241	C251	C261	176.6(8)	.	.
.	no					
C201	C251	C261	C271	124.7(9)	.	.
.	no					
C241	C251	C261	C311	123.6(9)	.	.
.	no					
C201	C251	C261	C311	-60.3(11)	.	.
.	no					
C241	C251	C261	C271	-51.4(11)	.	.
.	no					
C251	C261	C311	N2	1.7(11)	.	.
.	no					
C271	C261	C311	N2	176.9(7)	.	.
.	no					
C271	C261	C311	C301	0.2(11)	.	.
.	no					
C311	C261	C271	C281	-1.2(11)	.	.
.	no					
C251	C261	C271	C281	174.0(7)	.	.
.	no					
C251	C261	C311	C301	-174.9(7)	.	.
.	no					
C261	C271	C281	C291	1.7(12)	.	.
.	no					
C271	C281	C291	C301	-1.2(11)	.	.
.	no					
C281	C291	C301	C311	0.2(10)	.	.
.	no					
C291	C301	C311	C261	0.2(12)	.	.
.	no					
C291	C301	C311	N2	-176.5(7)	.	.
.	no					
N2	C321	C331	C381	23.1(11)	.	.
.	no					
N2	C321	C331	C341	-157.9(7)	.	.
.	no					
C341	C331	C381	C371	0.0(10)	.	.
.	no					
C381	C331	C341	C351	-0.7(11)	.	.
.	no					
C321	C331	C341	C351	-179.8(6)	.	.
.	no					
C321	C331	C381	C371	179.0(7)	.	.
.	no					
C341	C331	C381	P1	-178.1(5)	.	.
.	no					
C321	C331	C381	P1	0.8(10)	.	.
.	no					
C331	C341	C351	C361	0.4(11)	.	.
.	no					
C341	C351	C361	C371	0.7(11)	.	.
.	no					
C351	C361	C371	C381	-1.5(12)	.	.
.	no					
C361	C371	C381	C331	1.1(11)	.	.
.	no					
C361	C371	C381	P1	179.3(5)	.	.
.	no					
P1	C391	C401	C411	-175.0(6)	.	.
.	no					
C401	C391	C441	C431	-0.8(11)	.	.
.	no					

C441	C391	C401	C411	1.0(12)	.	.
.	no					
P1	C391	C441	C431	174.9(6)	.	.
.	no					
C391	C401	C411	C421	-0.9(12)	.	.
.	no					
C401	C411	C421	C431	0.7(13)	.	.
.	no					
C411	C421	C431	C441	-0.4(13)	.	.
.	no					
C421	C431	C441	C391	0.5(12)	.	.
.	no					
P1	C451	C461	C471	178.1(7)	.	.
.	no					
C501	C451	C461	C471	-3.0(12)	.	.
.	no					
P1	C451	C501	C491	-177.9(7)	.	.
.	no					
C461	C451	C501	C491	3.2(12)	.	.
.	no					
C451	C461	C471	C481	1.3(13)	.	.
.	no					
C461	C471	C481	C491	0.4(14)	.	.
.	no					
C471	C481	C491	C501	-0.2(15)	.	.
.	no					
C481	C491	C501	C451	-1.6(13)	.	.
.	no					
P4	Pd2	P3	C382	-147.0(2)	.	.
.	no					
P4	Pd2	P3	C392	-30.5(3)	.	.
.	no					
P4	Pd2	P3	C452	99.8(3)	.	.
.	no					
N4	Pd2	P3	C382	48.7(3)	.	.
.	no					
N4	Pd2	P3	C392	165.2(3)	.	.
.	no					
N4	Pd2	P3	C452	-64.6(3)	.	.
.	no					
P3	Pd2	P4	C12	-24.1(3)	.	.
.	no					
P3	Pd2	P4	C72	103.2(3)	.	.
.	no					
P3	Pd2	P4	C132	-141.3(3)	.	.
.	no					
N3	Pd2	P4	C12	154.9(3)	.	.
.	no					
N3	Pd2	P4	C72	-77.7(3)	.	.
.	no					
N3	Pd2	P4	C132	37.7(3)	.	.
.	no					
P4	Pd2	N3	C192	-28.1(7)	.	.
.	no					
P4	Pd2	N3	C202	148.5(4)	.	.
.	no					
N4	Pd2	N3	C192	136.4(7)	.	.
.	no					
N4	Pd2	N3	C202	-47.0(5)	.	.
.	no					
P3	Pd2	N4	C312	137.6(5)	.	.
.	no					
P3	Pd2	N4	C322	-37.6(7)	.	.
.	no					
N3	Pd2	N4	C312	-42.9(5)	.	.
.	no					
N3	Pd2	N4	C322	142.0(7)	.	.

.	C452	P3	no	C392	C442	-0.9(8)	.	.
.	C392	P3	no	C382	C372	12.6(7)	.	.
.	C452	P3	no	C382	C372	-99.9(6)	.	.
.	Pd2	P3	no	C392	C402	-51.0(7)	.	.
.	Pd2	P3	no	C382	C332	-46.6(6)	.	.
.	C392	P3	no	C382	C332	-174.1(6)	.	.
.	C452	P3	no	C382	C332	73.4(6)	.	.
.	Pd2	P3	no	C382	C372	140.1(5)	.	.
.	C392	P3	no	C452	C502	118.8(7)	.	.
.	C452	P3	no	C392	C402	176.7(6)	.	.
.	Pd2	P3	no	C452	C462	161.7(6)	.	.
.	C382	P3	no	C392	C402	68.4(7)	.	.
.	C382	P3	no	C452	C462	45.4(7)	.	.
.	Pd2	P3	no	C392	C442	131.4(6)	.	.
.	C382	P3	no	C392	C442	-109.2(7)	.	.
.	C382	P3	no	C452	C502	-133.3(7)	.	.
.	C392	P3	no	C452	C462	-62.4(7)	.	.
.	Pd2	P3	no	C452	C502	-17.0(7)	.	.
.	C132	P4	no	C12	C22	-116.5(7)	.	.
.	C132	P4	no	C72	C82	-136.8(7)	.	.
.	Pd2	P4	no	C12	C62	-58.2(7)	.	.
.	C72	P4	no	C12	C22	-8.8(8)	.	.
.	Pd2	P4	no	C12	C22	123.5(6)	.	.
.	C72	P4	no	C132	C142	-86.9(7)	.	.
.	Pd2	P4	no	C72	C122	162.7(6)	.	.
.	C12	P4	no	C72	C122	-63.9(7)	.	.
.	C132	P4	no	C72	C122	44.0(7)	.	.
.	C72	P4	no	C12	C62	169.5(6)	.	.
.	C132	P4	no	C12	C62	61.8(7)	.	.
.	C12	P4	no	C132	C182	-163.2(7)	.	.
.	Pd2	P4	no	C132	C142	149.2(6)	.	.
.	Pd2	P4	no	C132	C182	-36.8(7)	.	.
.	Pd2	P4	no	C72	C82	-18.2(8)	.	.
.	.	.	no	.	.	.	.	.

C72	P4	C132	C182	87.1(7)	.	.
.	no					
C12	P4	C132	C142	22.8(7)	.	.
.	no					
C12	P4	C72	C82	115.2(8)	.	.
.	no					
C192	N3	C202	C252	-103.1(8)	.	.
.	no					
Pd2	N3	C202	C212	-104.5(7)	.	.
.	no					
Pd2	N3	C202	C252	79.7(8)	.	.
.	no					
C192	N3	C202	C212	72.7(10)	.	.
.	no					
Pd2	N3	C192	C182	0.4(13)	.	.
.	no					
C202	N3	C192	C182	-176.2(7)	.	.
.	no					
Pd2	N4	C312	C262	74.4(8)	.	.
.	no					
C322	N4	C312	C302	65.5(9)	.	.
.	no					
Pd2	N4	C322	C332	3.9(12)	.	.
.	no					
Pd2	N4	C312	C302	-110.3(7)	.	.
.	no					
C312	N4	C322	C332	-171.2(7)	.	.
.	no					
C322	N4	C312	C262	-109.7(8)	.	.
.	no					
C22	C12	C62	C52	-1.6(12)	.	.
.	no					
P4	C12	C22	C32	-179.5(6)	.	.
.	no					
P4	C12	C62	C52	-180.0(7)	.	.
.	no					
C62	C12	C22	C32	2.3(12)	.	.
.	no					
C12	C22	C32	C42	-1.5(12)	.	.
.	no					
C22	C32	C42	C52	0.0(13)	.	.
.	no					
C32	C42	C52	C62	0.6(14)	.	.
.	no					
C42	C52	C62	C12	0.2(15)	.	.
.	no					
P4	C72	C82	C92	-177.4(8)	.	.
.	no					
C122	C72	C82	C92	1.8(14)	.	.
.	no					
P4	C72	C122	C112	179.1(7)	.	.
.	no					
C82	C72	C122	C112	-0.1(13)	.	.
.	no					
C72	C82	C92	C102	-2.2(16)	.	.
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C82	C92	C102	C112	0.9(15)	.	.
.	no					
C92	C102	C112	C122	0.8(15)	.	.
.	no					
C102	C112	C122	C72	-1.2(14)	.	.
.	no					
P4	C132	C182	C192	5.4(11)	.	.
.	no					
P4	C132	C182	C172	-173.5(6)	.	.
.	no					
C142	C132	C182	C172	0.5(11)	.	.

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P4	C132	C142	C152	174.9(6)	.	.
.	no					
C182	C132	C142	C152	0.7(12)	.	.
.	no					
C142	C132	C182	C192	179.4(7)	.	.
.	no					
C132	C142	C152	C162	-0.7(12)	.	.
.	no					
C142	C152	C162	C172	-0.5(12)	.	.
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C152	C162	C172	C182	1.7(12)	.	.
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C162	C172	C182	C192	179.3(7)	.	.
.	no					
C162	C172	C182	C132	-1.7(12)	.	.
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C132	C182	C192	N3	18.8(13)	.	.
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C172	C182	C192	N3	-162.2(8)	.	.
.	no					
N3	C202	C212	C222	-173.8(8)	.	.
.	no					
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C252	C202	C212	C222	1.9(13)	.	.
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N3	C202	C252	C242	172.6(7)	.	.
.	no					
C212	C202	C252	C262	-177.8(8)	.	.
.	no					
C212	C202	C252	C242	-3.1(12)	.	.
.	no					
C202	C212	C222	C232	-0.4(14)	.	.
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C212	C222	C232	C242	0.2(14)	.	.
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C222	C232	C242	C252	-1.4(13)	.	.
.	no					
C232	C242	C252	C202	2.8(12)	.	.
.	no					
C232	C242	C252	C262	177.7(8)	.	.
.	no					
C202	C252	C262	C272	123.1(9)	.	.
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C242	C252	C262	C312	123.9(9)	.	.
.	no					
C202	C252	C262	C312	-61.5(11)	.	.
.	no					
C242	C252	C262	C272	-51.5(11)	.	.
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C272	C262	C312	N4	176.3(7)	.	.
.	no					
C272	C262	C312	C302	1.3(12)	.	.
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C312	C262	C272	C282	0.0(13)	.	.
.	no					
C252	C262	C272	C282	175.8(8)	.	.
.	no					
C252	C262	C312	C302	-174.3(7)	.	.
.	no					
C262	C272	C282	C292	-1.5(14)	.	.
.	no					
C272	C282	C292	C302	1.6(14)	.	.
.	no					

C282	C292	C302	C312	-0.3(13)	.	.
.	no					
C292	C302	C312	C262	-1.2(12)	.	.
.	no					
C292	C302	C312	N4	-176.3(7)	.	.
.	no					
N4	C322	C332	C382	21.6(13)	.	.
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N4	C322	C332	C342	-159.5(8)	.	.
.	no					
C342	C332	C382	C372	0.5(11)	.	.
.	no					
C382	C332	C342	C352	-1.2(11)	.	.
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C322	C332	C342	C352	179.9(9)	.	.
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C322	C332	C382	C372	179.3(7)	.	.
.	no					
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C322	C332	C382	P3	5.8(10)	.	.
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C332	C342	C352	C362	0.5(12)	.	.
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C352	C362	C372	C382	-1.6(12)	.	.
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C362	C372	C382	C332	0.9(11)	.	.
.	no					
C362	C372	C382	P3	174.3(6)	.	.
.	no					
P3	C392	C402	C412	-177.2(6)	.	.
.	no					
C402	C392	C442	C432	-1.5(11)	.	.
.	no					
C442	C392	C402	C412	0.5(12)	.	.
.	no					
P3	C392	C442	C432	176.0(6)	.	.
.	no					
C392	C402	C412	C422	1.0(12)	.	.
.	no					
C402	C412	C422	C432	-1.5(13)	.	.
.	no					
C412	C422	C432	C442	0.5(13)	.	.
.	no					
C422	C432	C442	C392	1.1(12)	.	.
.	no					
P3	C452	C462	C472	-179.3(7)	.	.
.	no					
C502	C452	C462	C472	-0.6(12)	.	.
.	no					
P3	C452	C502	C492	179.3(7)	.	.
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C462	C452	C502	C492	0.5(11)	.	.
.	no					
C452	C462	C472	C482	0.5(13)	.	.
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C462	C472	C482	C492	-0.3(15)	.	.
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C472	C482	C492	C502	0.3(14)	.	.
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C482	C492	C502	C452	-0.4(14)	.	.
.	no					

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	no			
C11	C81	3.371(8)	.	.
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C11	C492	3.565(10)	.	1_556
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C11	C342	3.417(8)	.	2_556
	no			
C11	C401	3.590(8)	.	.
	no			
C11	C352	3.411(8)	.	2_556
	no			
C12	C212	3.506(10)	.	.
	no			
C12	C332	3.435(8)	.	.
	no			
C12	Pd2	2.9361(19)	.	.
	no			
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	no			
C12	C351	3.466(8)	.	2_556
	no			
C12	C382	3.272(7)	.	.
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	no			
C12	C202	3.533(8)	.	.
	no			
C12	P3	3.604(3)	.	.
	no			
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	no			
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	no			
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	no			
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	no			

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C16	C161 no	3.339(8)	.	.
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C17	C172 no	3.580(8)	.	.
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C18	C132 no	3.639(8)	.	.
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C111	C3 no	3.513(12)	.	.
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C114	C117 no	3.54(3)	.	.
C116	C7 no	3.614(15)	.	.
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C11	no C391	3.244(11)	.	.
C12	no C442	3.491(11)	.	.
C12	no C392	3.203(11)	.	.
C21	no C431	3.501(11)	.	.
C21	no C121	3.272(11)	.	.
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C21	no C441	3.272(11)	.	.
C22	no C442	3.430(11)	.	.
C22	no C392	3.386(11)	.	.
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C22	no C402	3.481(11)	.	.
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C32	no C442	3.457(11)	.	.
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C81	C401 no	3.505(12)	.	.
C82	C402 no	3.531(12)	.	.
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C112	C111 no	3.630(9)	.	2_666
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C121	C172 no	3.575(12)	.	2_666
C121	C21 no	3.272(11)	.	.
C122	C13 no	3.647(8)	.	.
C122	C142 no	3.393(11)	.	.
C122	C22 no	3.293(11)	.	.
C122	C171 no	3.431(12)	.	2_666
C132	C18 no	3.639(8)	.	.
C141	C61 no	3.242(12)	.	.
C141	C121 no	3.467(11)	.	.
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C152	C17 no	3.620(9)	.	2_665
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C182	no C2	3.585(13)	.	.
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C232	no C361	3.584(12)	.	2_556
C241	no C362	3.553(11)	.	2_556
C242	no C361	3.559(11)	.	2_556
C261	no C191	3.521(11)	.	.
C262	no C192	3.586(11)	.	.
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C421	C13	3.538(10)	.	2_566
	no			
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C502	no C62	3.394(11)	.	.
C502	no C302	3.553(13)	.	.
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Pd1	no H401	3.38(6)	.	.
Pd1	no H61	3.68(4)	.	.
Pd1	no H501	2.96(4)	.	.
Pd2	no H62	3.66(5)	.	.
Pd2	no H82	3.17(4)	.	.
Pd2	no H502	2.99(4)	.	.
Pd2	no H402	3.55(6)	.	.
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C12	H82	2.42(9)	.	.
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C12	H201	2.8412	.	.
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C12	H341	2.90(5)	.	2_556
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C12	H491	3.01(5)	.	.
	no			
C12	H351	2.81(7)	.	2_556
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C12	H402	3.06(5)	.	.
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C13	H340	2.6774	.	.
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C13	H310	3.1066	.	.
	no			
C13	H122	3.04(4)	.	.
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	no			
C14	H192	2.62(7)	.	.
	no			
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C16	H222	3.13(5)	.	.
	no			
C17	H152	2.93(5)	.	.
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	no			
C18	H502	2.92(9)	.	.
	no			
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	no			
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C114	no H231	3.14(5)	.	.
C115	no H232	2.99(5)	.	.
C115	no H241	3.03(3)	.	.
C116	no H361	3.08(5)	.	.
C116	no H472	3.11(6)	.	.
C117	no H242	3.00(7)	.	.
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C122	no H111	3.11(5)	.	.
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C2	no H221	3.07(8)	.	.
C5	no H372	3.09(4)	.	.
C5	no H272	3.02(9)	.	.
C11	no H141	2.54(5)	.	.
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C62	no H142	2.80(5)	.	.
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C122	H22	2.72(5)	.	.
	no			
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	no			
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	no			
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	no			
C132	H122	2.83(5)	.	.
	no			
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	no			
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	no			
C182	H12	2.9970	.	.
	no			
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H12	C182 no	2.9970	.	.
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H14	C13 no	2.7903	.	2_666
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H21	C121 no	2.71(5)	.	.
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H142	no C62	2.80(5)	.	.
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H171	no Cl22	2.79(6)	.	2_666
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H212	C192 no	2.95(5)	.	.
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H231	C114 no	3.14(5)	.	2_656
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128(4)	2_556				
C352	H352	C11	0.87(7)	2.82(7)	3.411(8)
126(4)	2_556				
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161(4)	.				
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End of Crystallographic Information File

Complex # 4

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Refinement on F^2^ for ALL reflections except for 186 with very
negative F^2^
or flagged by the user for potential systematic errors.
Weighted R-factors
wR and all goodnesses 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
observed criterion
of F^2^ > 2sigma(F^2^) is used only for calculating
_R_factor_obs etc. and is
not relevant to the choice of reflections for refinement.

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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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_atom_sites_solution_secondary    difmap
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'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack    -0.13(6)
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Pd1 Pd 0.36067(6) 0.18223(6) 0.21680(2) 0.0350(2) Uani 1 d . .
P1 P 0.5001(2) 0.3676(2) 0.18973(7) 0.0376(6) Uani 1 d . .
Cl1 Cl 0.0382(4) 0.1372(4) 0.30919(10) 0.0922(12) Uani 1 d . .
Cl2 Cl 0.0745(3) 0.2275(3) 0.21816(9) 0.0725(9) Uani 1 d . .
Cl4 Cl 0.1744(5) 0.6864(5) 0.03177(15) 0.132(2) Uani 1 d . .
Cl3 Cl 0.0651(5) 0.4351(5) 0.05016(11) 0.120(2) Uani 1 d . .
Cl6 C 0.3011(10) 0.3500(8) 0.0596(3) 0.041(2) Uani 1 d . .
H161 H 0.2595(10) 0.3445(8) 0.0334(3) 0.049 Uiso 1 calc R .
C20 C 0.1445(8) -0.0197(8) 0.1893(2) 0.030(2) Uani 1 d . .
C6 C 0.7267(10) 0.4765(9) 0.1476(3) 0.052(3) Uani 1 d . .
H61 H 0.7124(10) 0.5356(9) 0.1372(3) 0.062 Uiso 1 calc R .
Cl5 C 0.4072(10) 0.4530(9) 0.0683(3) 0.046(3) Uani 1 d . .
H151 H 0.4368(10) 0.5162(9) 0.0482(3) 0.055 Uiso 1 calc R .
Cl8 C 0.3183(8) 0.2626(8) 0.1274(2) 0.034(2) Uani 1 d . .
C7 C 0.5274(10) 0.5019(8) 0.2182(3) 0.043(2) Uani 1 d . .
C25 C 0.0393(8) -0.1276(8) 0.1872(3) 0.032(2) Uani 1 d . .
C22 C 0.1820(9) -0.0544(8) 0.2638(3) 0.039(2) Uani 1 d . .
H221 H 0.2273(9) -0.0316(8) 0.2900(3) 0.047 Uiso 1 calc R .
Cl9 C 0.1818(8) 0.0685(8) 0.1531(3) 0.035(2) Uani 1 d . .
H191 H 0.1366(8) 0.0521(8) 0.1267(3) 0.048 Uiso 1 calc R .
C26 C 0.4463(9) 0.2375(11) 0.3060(3) 0.049(3) Uani 1 d . .
Cl4 C 0.4685(9) 0.4606(8) 0.1072(3) 0.045(2) Uani 1 d . .
```

H141 H 0.5398(9) 0.5295(8) 0.1132(3) 0.054 Uiso 1 calc R .
 C12 C 0.6378(10) 0.5805(9) 0.2364(3) 0.058(3) Uani 1 d . .
 H121 H 0.7027(10) 0.5695(9) 0.2327(3) 0.070 Uiso 1 calc R .
 C23 C 0.0800(9) -0.1600(9) 0.2632(3) 0.045(3) Uani 1 d . .
 H231 H 0.0587(9) -0.2076(9) 0.2887(3) 0.054 Uiso 1 calc R .
 C17 C 0.2568(9) 0.2576(9) 0.0884(2) 0.043(3) Uani 1 d . .
 H171 H 0.1845(9) 0.1900(9) 0.0822(2) 0.052 Uiso 1 calc R .
 C2 C 0.6704(10) 0.3024(9) 0.1907(3) 0.055(3) Uani 1 d . .
 H21 H 0.6180(10) 0.2433(9) 0.2101(3) 0.066 Uiso 1 calc R .
 C3 C 0.7766(10) 0.3047(12) 0.1778(3) 0.059(3) Uani 1 d . .
 H31 H 0.7943(10) 0.2485(12) 0.1888(3) 0.071 Uiso 1 calc R .
 C9 C 0.4436(14) 0.6143(11) 0.2482(3) 0.072(4) Uani 1 d . .
 H91 H 0.3792(14) 0.6259(11) 0.2521(3) 0.087 Uiso 1 calc R .
 C5 C 0.8305(11) 0.4787(11) 0.1356(3) 0.057(3) Uani 1 d . .
 H51 H 0.8869(11) 0.5407(11) 0.1182(3) 0.069 Uiso 1 calc R .
 C1 C 0.6431(8) 0.3862(9) 0.1751(3) 0.039(2) Uani 1 d . .
 C8 C 0.4318(12) 0.5196(10) 0.2246(3) 0.059(3) Uani 1 d . .
 H81 H 0.3583(12) 0.4657(10) 0.2125(3) 0.071 Uiso 1 calc R .
 C4 C 0.8505(11) 0.3894(12) 0.1495(4) 0.060(3) Uani 1 d . .
 H41 H 0.9169(11) 0.3878(12) 0.1389(4) 0.072 Uiso 1 calc R .
 C21 C 0.2223(8) 0.0222(9) 0.2266(3) 0.036(2) Uani 1 d . .
 C27 C 0.5262(10) 0.2463(12) 0.3451(3) 0.069(4) Uani 1 d . .
 H271 H 0.6076(11) 0.2885(68) 0.3355(9) 0.103 Uiso 1 calc R .
 H272 H 0.5060(52) 0.1680(12) 0.3548(19) 0.103 Uiso 1 calc R .
 H273 H 0.5154(59) 0.2880(69) 0.3696(11) 0.103 Uiso 1 calc R .
 C10 C 0.5537(15) 0.6933(12) 0.2662(3) 0.073(4) Uani 1 d . .
 H101 H 0.5623(15) 0.7584(12) 0.2824(3) 0.088 Uiso 1 calc R .
 C11 C 0.6472(11) 0.6791(11) 0.2612(4) 0.063(3) Uani 1 d . .
 H111 H 0.7195(11) 0.7338(11) 0.2740(4) 0.075 Uiso 1 calc R .
 C13 C 0.4258(8) 0.3675(8) 0.1373(2) 0.034(2) Uani 1 d . .
 C24 C 0.0052(9) -0.2007(9) 0.2257(3) 0.042(2) Uani 1 d . .
 H241 H -0.0648(9) -0.2735(9) 0.2261(3) 0.051 Uiso 1 calc R .
 C29 C 0.0447(15) 0.5426(13) 0.0267(4) 0.094(5) Uani 1 d . .
 H291 H -0.0216(15) 0.5434(13) 0.0414(4) 0.127 Uiso 1 calc R .
 H292 H 0.0249(15) 0.5246(13) -0.0049(4) 0.127 Uiso 1 calc R .
 C28 C 0.1336(12) 0.2470(12) 0.2718(4) 0.075(4) Uani 1 d . .
 H281 H 0.1507(12) 0.3239(12) 0.2832(4) 0.101 Uiso 1 calc R .
 H282 H 0.2078(12) 0.2465(12) 0.2703(4) 0.101 Uiso 1 calc R .
 N1 N 0.2762(7) 0.1683(6) 0.1589(2) 0.032(2) Uani 1 d . .
 O2 O 0.3903(7) 0.2902(7) 0.3074(2) 0.056(2) Uani 1 d . .
 O1 O 0.4449(6) 0.1759(6) 0.2742(2) 0.049(2) Uani 1 d . .

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 P1 0.041(2) 0.0285(14) 0.0391(10) -0.0016(10) -0.0037(10)
 0.0147(13)
 Cl1 0.088(3) 0.097(3) 0.076(2) 0.003(2) -0.017(2) 0.034(2)
 Cl2 0.076(2) 0.079(2) 0.070(2) 0.000(2) 0.005(2) 0.045(2)
 Cl4 0.147(5) 0.112(4) 0.136(3) -0.029(3) -0.021(3) 0.065(4)
 Cl3 0.173(5) 0.134(4) 0.079(2) 0.011(2) -0.003(3) 0.095(4)
 Cl6 0.054(7) 0.031(6) 0.043(4) 0.003(4) 0.003(4) 0.025(5)
 C20 0.027(5) 0.025(5) 0.036(4) -0.003(4) 0.002(4) 0.012(5)
 C6 0.053(8) 0.030(6) 0.066(6) 0.011(5) 0.000(5) 0.015(6)
 Cl5 0.064(7) 0.044(7) 0.043(4) 0.016(4) 0.012(4) 0.037(6)
 Cl8 0.042(6) 0.032(6) 0.031(3) 0.005(4) 0.004(4) 0.020(5)
 C7 0.056(7) 0.016(5) 0.045(4) 0.000(4) 0.006(4) 0.009(5)
 C25 0.026(5) 0.022(5) 0.048(4) 0.000(4) 0.004(4) 0.012(4)
 C22 0.045(6) 0.026(5) 0.032(4) 0.004(3) -0.003(4) 0.007(5)
 Cl9 0.037(6) 0.036(6) 0.037(4) -0.006(4) 0.001(4) 0.021(5)
 C26 0.045(6) 0.070(9) 0.040(4) 0.003(5) 0.005(4) 0.035(6)

```

C14 0.051(6) 0.023(5) 0.052(4) -0.002(4) 0.000(4) 0.012(5)
C12 0.057(7) 0.022(6) 0.059(5) -0.011(5) 0.010(5) -0.007(6)
C23 0.039(6) 0.045(6) 0.052(5) 0.012(4) 0.009(4) 0.021(5)
C17 0.044(7) 0.050(7) 0.038(4) 0.002(4) 0.002(4) 0.026(6)
C2 0.058(8) 0.041(6) 0.056(5) 0.013(5) -0.006(5) 0.018(6)
C3 0.046(7) 0.070(9) 0.070(6) -0.003(6) -0.005(6) 0.036(7)
C9 0.113(13) 0.058(9) 0.057(6) -0.012(6) -0.010(7) 0.051(9)
C5 0.048(8) 0.041(7) 0.068(6) 0.007(5) 0.006(6) 0.011(6)
C1 0.027(5) 0.033(6) 0.047(4) 0.004(4) -0.005(4) 0.007(5)
C8 0.082(9) 0.051(8) 0.050(5) -0.015(5) -0.014(5) 0.038(8)
C4 0.046(7) 0.067(9) 0.067(6) -0.005(6) 0.004(5) 0.028(7)
C21 0.035(6) 0.043(6) 0.039(4) -0.002(4) -0.009(4) 0.025(5)
C27 0.053(7) 0.101(11) 0.047(5) 0.000(6) -0.001(5) 0.035(8)
C10 0.121(14) 0.048(8) 0.046(5) 0.000(5) 0.013(7) 0.039(9)
C11 0.055(8) 0.042(7) 0.062(6) 0.005(5) -0.003(6) 0.002(6)
C13 0.037(6) 0.027(5) 0.042(4) -0.002(3) -0.001(4) 0.018(5)
C24 0.027(5) 0.044(7) 0.051(5) 0.012(4) 0.006(4) 0.015(5)
C29 0.145(15) 0.098(12) 0.076(7) 0.018(7) 0.022(9) 0.088(12)
C28 0.054(9) 0.078(9) 0.089(7) -0.017(7) -0.016(7) 0.031(8)
N1 0.030(4) 0.027(4) 0.039(3) -0.002(3) 0.002(3) 0.013(3)
O2 0.074(6) 0.078(6) 0.040(3) -0.010(3) -0.005(3) 0.055(5)
O1 0.045(4) 0.054(5) 0.058(4) -0.005(3) -0.011(3) 0.033(4)

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_geom_special_details

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All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

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P1 C1 1.805(10) . ?

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C11 C28 1.743(13) . ?

C12 C28 1.733(11) . ?

C14 C29 1.79(2) . ?

C13 C29 1.697(13) . ?

C16 C17 1.347(13) . ?

C16 C15 1.385(14) . ?

C20 C25 1.389(12) . ?

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C20 C19 1.467(12) . ?

C6 C5 1.38(2) . ?

C6 C1 1.397(13) . ?

C15 C14 1.379(12) . ?

C18 C17 1.391(11) . ?

C18 C13 1.412(13) . ?

C18 N1 1.418(10) . ?

C7 C8 1.387(15) . ?
 C7 C12 1.390(14) . ?
 C25 C24 1.409(11) . ?
 C25 C25 1.51(2) 5 ?
 C22 C23 1.351(13) . ?
 C22 C21 1.403(12) . ?
 C19 N1 1.277(11) . ?
 C26 O2 1.226(13) . ?
 C26 O1 1.234(11) . ?
 C26 C27 1.524(13) . ?
 C14 C13 1.379(11) . ?
 C12 C11 1.43(2) . ?
 C23 C24 1.397(13) . ?
 C2 C1 1.384(14) . ?
 C2 C3 1.419(15) . ?
 C3 C4 1.34(2) . ?
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 N1 Pd1 P1 84.5(2) . . ?
 O1 Pd1 P1 100.0(2) . . ?
 C1 P1 C7 106.9(5) . . ?
 C1 P1 C13 107.6(4) . . ?
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 C7 P1 Pd1 121.0(3) . . ?
 C13 P1 Pd1 99.0(3) . . ?
 C17 C16 C15 121.4(9) . . ?
 C25 C20 C21 125.3(8) . . ?
 C25 C20 C19 122.1(8) . . ?
 C21 C20 C19 112.4(8) . . ?
 C5 C6 C1 120.7(10) . . ?
 C14 C15 C16 119.0(8) . . ?
 C17 C18 C13 119.2(8) . . ?
 C17 C18 N1 123.0(9) . . ?
 C13 C18 N1 117.8(7) . . ?
 C8 C7 C12 120.5(10) . . ?
 C8 C7 P1 117.7(8) . . ?
 C12 C7 P1 121.6(9) . . ?
 C20 C25 C24 117.7(8) . . ?
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 C23 C22 C21 122.6(9) . . ?
 N1 C19 C20 117.9(7) . . ?
 O2 C26 O1 124.7(9) . . ?
 O2 C26 C27 120.4(9) . . ?
 O1 C26 C27 114.8(10) . . ?
 C13 C14 C15 121.1(9) . . ?
 C7 C12 C11 116.9(12) . . ?
 C22 C23 C24 122.7(9) . . ?
 C16 C17 C18 120.5(10) . . ?
 C1 C2 C3 121.5(10) . . ?
 C4 C3 C2 118.6(12) . . ?

C8 C9 C10 118.6(14) . . ?
 C4 C5 C6 120.0(11) . . ?
 C2 C1 C6 117.4(10) . . ?
 C2 C1 P1 117.8(8) . . ?
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 C3 C4 C5 121.6(12) . . ?
 C22 C21 C20 113.8(8) . . ?
 C22 C21 Pd1 133.1(6) . . ?
 C20 C21 Pd1 112.9(6) . . ?
 C11 C10 C9 122.1(13) . . ?
 C10 C11 C12 120.7(12) . . ?
 C14 C13 C18 118.9(8) . . ?
 C14 C13 P1 124.7(7) . . ?
 C18 C13 P1 116.4(6) . . ?
 C23 C24 C25 117.8(9) . . ?
 C13 C29 C14 111.8(9) . . ?
 C12 C28 C11 112.6(7) . . ?
 C19 N1 C18 123.3(7) . . ?
 C19 N1 Pd1 114.5(6) . . ?
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#=====

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