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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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```
# Copyright The Royal Society of Chemistry, 1998.

# 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_diffn 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_reflns_number          9610
_diffrn_reflns_av_R_equivalents ?
_diffrn_reflns_av_sigmaI/netI  0.036
_diffrn_reflns_limit_h_min     -22
_diffrn_reflns_limit_h_max      22
_diffrn_reflns_limit_k_min     -17
_diffrn_reflns_limit_k_max      16
_diffrn_reflns_limit_l_min     -24
_diffrn_reflns_limit_l_max      13
_diffrn_reflns_theta_min       1.14
_diffrn_reflns_theta_max       26.5
_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, scale
variation, but not for absorption and reduced to  $F_o \sim F_o^2$ 
;

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

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_geom_angle
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_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				
P	C1	C2	119.5(5)	.	.
.	yes				
P	C1	C6	122.3(4)	.	.
.	yes				
C2	C1	C6	118.2(6)	.	.
.	no				
C1	C2	C3	120.9(7)	.	.
.	no				
C2	C3	C4	120.3(8)	.	.
.	no				
C3	C4	C5	119.5(7)	.	.
.	no				
C4	C5	C6	118.9(8)	.	.
.	no				
C1	C6	C5	122.1(7)	.	.
.	no				
P	C7	C8	118.6(5)	.	.
.	yes				
P	C7	C12	121.4(4)	.	.
.	yes				
C8	C7	C12	119.8(6)	.	.
.	no				
C7	C8	C9	119.4(7)	.	.
.	no				
C8	C9	C10	120.6(6)	.	.
.	no				
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.	no				
C10	C11	C12	120.2(5)	.	.
.	no				
C7	C12	C11	119.3(5)	.	.
.	no				
P	C13	C14	125.7(4)	.	.
.	yes				
P	C13	C18	114.9(4)	.	.
.	yes				
C14	C13	C18	119.3(5)	.	.

.		no				
C13	C14		C15	120.4(5)	.	.
.		no				
C14	C15		C16	119.8(5)	.	.
.		no				
C15	C16		C17	120.9(5)	.	.
.		no				
C16	C17		C18	119.9(5)	.	.
.		no				
N	C18		C13	116.8(5)	.	.
.		yes				
N	C18		C17	123.8(5)	.	.
.		yes				
C13	C18		C17	119.4(5)	.	.
.		no				
N	C19		C20	123.8(5)	.	.
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C19	C20		C21	118.2(5)	.	.
.		no				
C19	C20		C25	121.8(5)	.	.
.		no				
C21	C20		C25	119.6(4)	.	.
.		no				
C20	C21		C22	121.7(5)	.	.
.		no				
C21	C22		C23	119.0(5)	.	.
.		no				
C22	C23		C24	120.2(5)	.	.
.		no				
C23	C24		C25	122.0(5)	.	.
.		no				
C20	C25		C24	117.4(4)	.	.
.		no				
C20	C25		C25	126.0(4)	.	.
2_555		no				
C24	C25		C25	116.5(4)	.	.
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C1	C2		H2	116(5)	.	.
.		no				
C3	C2		H2	122(5)	.	.
.		no				
C2	C3		H3	126(5)	.	.
.		no				
C4	C3		H3	114(5)	.	.
.		no				
C3	C4		H4	124(5)	.	.
.		no				
C5	C4		H4	117(5)	.	.
.		no				
C4	C5		H5	116(4)	.	.
.		no				
C6	C5		H5	125(4)	.	.
.		no				
C1	C6		H6	128(6)	.	.
.		no				
C5	C6		H6	110(6)	.	.
.		no				
C7	C8		H8	114(3)	.	.
.		no				
C9	C8		H8	126(3)	.	.
.		no				
C8	C9		H9	115(4)	.	.
.		no				
C10	C9		H9	124(4)	.	.
.		no				
C9	C10		H10	120(4)	.	.
.		no				

C11	C10	H10	119(4)	.	.
.	no				
C10	C11	H11	118(5)	.	.
.	no				
C12	C11	H11	122(5)	.	.
.	no				
C7	C12	H12	124(4)	.	.
.	no				
C11	C12	H12	117(4)	.	.
.	no				
C13	C14	H14	121(4)	.	.
.	no				
C15	C14	H14	119(4)	.	.
.	no				
C14	C15	H15	112(6)	.	.
.	no				
C16	C15	H15	128(6)	.	.
.	no				
C15	C16	H16	118(3)	.	.
.	no				
C17	C16	H16	121(3)	.	.
.	no				
C16	C17	H17	115(4)	.	.
.	no				
C18	C17	H17	125(4)	.	.
.	no				
N	C19	H19	120(3)	.	.
.	no				
C20	C19	H19	117(3)	.	.
.	no				
C20	C21	H21	123(4)	.	.
.	no				
C22	C21	H21	115(4)	.	.
.	no				
C21	C22	H22	120(3)	.	.
.	no				
C23	C22	H22	120(3)	.	.
.	no				
C22	C23	H23	119(5)	.	.
.	no				
C24	C23	H23	121(5)	.	.
.	no				
C23	C24	H24	122(3)	.	.
.	no				
C25	C24	H24	116(3)	.	.
.	no				
Pd	C26	H26	101(8)	.	.
.	no				
Pd	C26	H26'	113(6)	.	.
.	no				
Pd	C26	H26"	105(6)	.	.
.	no				
H26	C26	H26'	103(10)	.	.
.	no				
H26	C26	H26"	131(10)	.	.
.	no				
H26'	C26	H26"	104(8)	.	.
.	no				

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_geom_torsion_publ_flag

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N	Pd	P	C7	-147.8(3)	.	.
.	.	no				
N	Pd	P	C13	-30.05(19)	.	.
.	.	no				
C26	Pd	P	C1	-102.5(3)	.	.
.	.	no				
C26	Pd	P	C7	25.9(3)	.	.
.	.	no				
C26	Pd	P	C13	143.7(3)	.	.
.	.	no				
C1	Pd	N	C18	-141.1(3)	.	.
.	.	no				
C1	Pd	N	C19	41.7(5)	.	.
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P	Pd	N	C18	39.3(3)	.	.
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P	Pd	N	C19	-137.8(5)	.	.
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Pd	P	C1	C2	47.6(6)	.	.
.	.	no				
Pd	P	C1	C6	-132.3(5)	.	.
.	.	no				
C7	P	C1	C2	-89.9(5)	.	.
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C7	P	C1	C6	90.3(5)	.	.
.	.	no				
C13	P	C1	C2	158.1(5)	.	.
.	.	no				
C13	P	C1	C6	-21.7(6)	.	.
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Pd	P	C7	C8	54.4(5)	.	.
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Pd	P	C7	C12	-121.3(4)	.	.
.	.	no				
C1	P	C7	C8	-173.5(5)	.	.
.	.	no				
C1	P	C7	C12	10.8(5)	.	.
.	.	no				
C13	P	C7	C8	-61.0(5)	.	.
.	.	no				
C13	P	C7	C12	123.3(5)	.	.
.	.	no				
Pd	P	C13	C14	-157.0(5)	.	.
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Pd	P	C13	C18	23.3(4)	.	.
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C1	P	C13	C14	84.0(5)	.	.
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C1	P	C13	C18	-95.7(4)	.	.
.	.	no				
C7	P	C13	C14	-27.2(6)	.	.
.	.	no				
C7	P	C13	C18	153.1(4)	.	.
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Pd	N	C18	C13	-35.5(5)	.	.
.	.	no				
Pd	N	C18	C17	146.8(4)	.	.
.	.	no				
C19	N	C18	C13	142.2(5)	.	.
.	.	no				
C19	N	C18	C17	-35.5(7)	.	.
.	.	no				

C15	C4 no	3.423(9)	.	6_555
C16	C10 no	3.560(8)	.	4_565
C17	C10 no	3.525(8)	.	6_545
C17	Cl no	3.402(6)	.	2_555
C17	Pd no	4.067(6)	.	2_555
C19	C20 no	3.254(8)	.	2_555
C19	C19 no	2.962(8)	.	2_555
C20	C19 no	3.254(8)	.	2_555
C21	Pd no	3.322(4)	.	.
C21	Cl no	3.368(5)	.	.
C22	Cl no	3.583(6)	.	3_555
C22	C22 no	3.412(8)	.	3_555
C24	C12 no	3.490(8)	.	5_445
Pd	H17 no	3.31(6)	.	2_555
Pd	H8 no	3.60(6)	.	.
Pd	H23 no	3.62(7)	.	3_555
Pd	H2 no	3.26(8)	.	.
Pd	H21 no	2.72(6)	.	.
Cl	H22 no	2.87(6)	.	3_555
Cl	H11 no	2.99(7)	.	5_445
Cl	H10 no	3.14(6)	.	5_445
Cl	H9 no	3.08(6)	.	3_565
Cl	H17 no	2.66(6)	.	2_555
N	H21 no	2.69(6)	.	.
C1	H12 no	2.64(6)	.	.
C2	H12 no	2.99(6)	.	.
C3	H26 " no	2.90(9)	.	7_555
C3	H15 no	2.95(6)	.	6_545
C4	H5 no	2.93(8)	.	2_655
C7	H14 no	2.90(7)	.	.
C10	H16 no	2.78(5)	.	4_564
C10	H19 no	3.08(6)	.	6_555
C11	H19 no	3.06(5)	.	6_555
C13	H8	3.00(6)	.	.

C13	no H6	2.88(7)	.	.
C14	no H6	3.07(7)	.	.
C17	no H10	2.99(6)	.	6_545
C17	no H19	2.58(4)	.	.
C19	no H17	2.76(6)	.	.
C19	no H19	2.81(6)	.	2_555
C20	no H19	2.90(6)	.	2_555
C21	no H14	2.98(7)	.	6_545
C22	no H22	2.81(5)	.	3_555
C24	no H24	2.55(5)	.	2_555
C24	no H12	2.82(6)	.	5_445
C25	no H19	2.80(5)	.	2_555
C26	no H23	3.05(7)	.	3_555
H2	no Pd	3.26(8)	.	.
H3	no H26"	2.52(12)	.	7_555
H4	no H5	2.45(11)	.	2_655
H5	no C4	2.93(8)	.	2_655
H5	no H4	2.45(11)	.	2_655
H6	no C13	2.88(7)	.	.
H6	no C14	3.07(7)	.	.
H8	no Pd	3.60(6)	.	.
H8	no C13	3.00(6)	.	.
H9	no C1	3.08(6)	.	3_565
H10	no C1	3.14(6)	.	5_555
H10	no C17	2.99(6)	.	6_555
H11	no C1	2.99(7)	.	5_555
H12	no C1	2.64(6)	.	.
H12	no C2	2.99(6)	.	.
H12	no C24	2.82(6)	.	5_555
H12	no H24	2.54(8)	.	5_555
H14	no C7	2.90(7)	.	.
H14	no C21	2.98(8)	.	6_555
H15	no C3	2.95(6)	.	6_555

H16	C10	2.78(5)	.	4_565
	no			
H17	C19	2.76(6)	.	.
	no			
H17	H19	2.32(7)	.	.
	no			
H17	Pd	3.31(6)	.	2_555
	no			
H17	Cl	2.66(5)	.	2_555
	no			
H19	C17	2.58(4)	.	.
	no			
H19	H17	2.32(7)	.	.
	no			
H19	C19	2.81(6)	.	2_555
	no			
H19	C20	2.90(6)	.	2_555
	no			
H19	C25	2.80(5)	.	2_555
	no			
H19	C10	3.08(6)	.	6_545
	no			
H19	C11	3.06(5)	.	6_545
	no			
H21	Pd	2.72(6)	.	.
	no			
H21	N	2.69(6)	.	.
	no			
H22	Cl	2.87(6)	.	3_555
	no			
H22	C22	2.81(5)	.	3_555
	no			
H22	H22	2.48(8)	.	3_555
	no			
H23	Pd	3.62(7)	.	3_555
	no			
H23	C26	3.05(7)	.	3_555
	no			
H24	C24	2.56(5)	.	2_555
	no			
H24	H24	2.17(8)	.	2_555
	no			
H24	H12	2.54(8)	.	5_445
	no			
H26 "	C3	2.90(9)	.	7_555
	no			
H26 "	H3	2.52(12)	.	7_555
	no			

loop_

_geom_bond_atom_site_label_D

_geom_bond_atom_site_label_H

_geom_contact_atom_site_label_A

_geom_bond_distance_DH

_geom_contact_distance_HA

_geom_contact_distance_DA

_geom_angle_DHA

_geom_contact_site_symmetry_A

#

#D H A D - H H...A D...A D - H...A symm(A)

#

C17 H17 Cl .86(6) 2.66(5) 3.402(6)

144(5) 2_555

End of Crystallographic Information File

#=== COMPLEX 6

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data_s1420c

#=====

5. CHEMICAL DATA

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;

?

;

_chemical_name_common

?

_chemical_melting_point

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_chemical_formula_structural

?

Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2O)'

_chemical_formula_sum

'?'

_chemical_formula_weight

1203.38

_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 -0.9988 1.0072

'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'

Cl Cl 0.1484 0.1585

'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

Triclinic

_symmetry_space_group_name_H-M

'P -1'

loop_

_symmetry_equiv_pos_as_xyz

x,y,z

-x,-y,-z

_cell_length_a 15.1653(18)

_cell_length_b 19.369(2)

_cell_length_c 20.3003(17)

_cell_angle_alpha 100.755(9)

_cell_angle_beta 99.828(8)

_cell_angle_gamma 111.470(10)

_cell_volume 5262.1(11)

_cell_formula_units_Z 2

_cell_measurement_temperature 150

_exptl_crystal_description block

_exptl_crystal_colour orange

_exptl_crystal_size_max 0.70

_exptl_crystal_size_mid 0.70

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_exptl_crystal_size_min          0.45
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_exptl_crystal_density_method    ?
_exptl_crystal_F_000             2436
_exptl_absorpt_coefficient_mu    0.91
_exptl_absorpt_correction_type    none

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7. EXPERIMENTAL DATA

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_diffn_radiation_source          'Rotating Anode'
_diffn_radiation_monochromator    Graphite

_diffn_measurement_device_type    'CAD4T'
_diffn_measurement_method        '\w-scan'

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number of measured reflections (redundant set)

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_diffn_reflms_number            ?
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_diffn_reflms_limit_h_min       -18
_diffn_reflms_limit_h_max       16
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_diffn_reflms_limit_k_max       23
_diffn_reflms_limit_l_min       -24
_diffn_reflms_limit_l_max       24
_diffn_reflms_theta_min         1.06
_diffn_reflms_theta_max         25.36

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number of unique reflections

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_reflms_number_total            19488
# number of observed reflections (> n sig(I))
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_reflms_threshold_expression     >2sigma(i)

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

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8. REFINEMENT DATA

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_refine_ls_hydrogen_treatment    'H-atom refinement: see text'
_refine_ls_number_reflms         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
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_refine_ls_wR_factor_gt         0.1421
_refine_ls_goodness_of_fit_ref   1.008
_refine_ls_restrained_S_all     1.008
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_refine_ls_shift/su_mean         0.000

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_refine_diff_density_rms 0.142

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9. ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
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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)					
C19	Uani	0.7668(2)	0.38243(18)	0.39270(15)	1.000
0.0667(11)					
C110	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)					
C111	Uani	0.6581(2)	0.26230(14)	0.50181(12)	1.000
0.0542(9)					
C112	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)					
C113	Uani	0.6147(4)	0.1047(3)	0.0567(4)	1.000
0.181(4)					
C114	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)					
C12	Uani	0.13642(13)	0.21416(10)	0.30874(9)	1.000
0.0246(6)					
C13	Uani	0.41078(14)	0.71306(11)	0.28358(11)	1.000
0.0338(7)					
C14	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)			

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10. MOLECULAR GEOMETRY

_geom_special_details

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

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loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Pd1 C11 2.8025(19) . .

yes

Pd1 P1 2.243(2) . .

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	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 yes	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)	.	.
	no		.	.

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			

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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	.	.

.	H13	C3	no	H203	108.10	.	.
.	Cl111	C4	no	Cl112	111.5(7)	.	.
.	Cl111	C4	yes	H14	109.35	.	.
.	Cl111	C4	no	H204	109.30	.	.
.	Cl112	C4	no	H14	109.32	.	.
.	Cl112	C4	no	H204	109.43	.	.
.	H14	C4	no	H204	107.87	.	.
.	Cl113	C5	no	Cl114	113.4(11)	.	.
.	Cl113	C5	yes	H15	108.94	.	.
.	Cl113	C5	no	H205	108.87	.	.
.	Cl114	C5	no	H15	108.86	.	.
.	Cl114	C5	no	H205	108.95	.	.
.	H15	C5	no	H205	107.71	.	.
.	.	.	no

loop_

_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

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_geom_torsion_publ_flag

.	Cl11	Pd1	P1	C381	-39.4(2)	.	.
.	Cl11	Pd1	P1	C391	76.6(3)	.	.
.	Cl11	Pd1	P1	C451	-154.7(3)	.	.
.	P2	Pd1	P1	C381	-151.6(2)	.	.
.	P2	Pd1	P1	C391	-35.6(3)	.	.
.	P2	Pd1	P1	C451	93.1(3)	.	.
.	N2	Pd1	P1	C381	46.4(3)	.	.
.	N2	Pd1	P1	C391	162.4(3)	.	.
.	N2	Pd1	P1	C451	-68.9(3)	.	.
.	Cl11	Pd1	P2	C11	-114.0(3)	.	.
.	Cl11	Pd1	P2	C71	14.4(3)	.	.
.	Cl11	Pd1	P2	C131	129.6(2)	.	.
.	P1	Pd1	P2	C11	-24.7(3)	.	.
.	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)	.	.

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

.	.	no				
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)	.	.
.	.	no				
C152	C162	C172	C182	1.7(12)	.	.
.	.	no				
C162	C172	C182	C192	179.3(7)	.	.
.	.	no				
C162	C172	C182	C132	-1.7(12)	.	.
.	.	no				
C132	C182	C192	N3	18.8(13)	.	.
.	.	no				
C172	C182	C192	N3	-162.2(8)	.	.
.	.	no				
N3	C202	C212	C222	-173.8(8)	.	.
.	.	no				
N3	C202	C252	C262	-2.1(12)	.	.
.	.	no				
C252	C202	C212	C222	1.9(13)	.	.
.	.	no				
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)	.	.
.	.	no				
C212	C222	C232	C242	0.2(14)	.	.
.	.	no				
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)	.	.
.	.	no				
C242	C252	C262	C312	123.9(9)	.	.
.	.	no				
C202	C252	C262	C312	-61.5(11)	.	.
.	.	no				
C242	C252	C262	C272	-51.5(11)	.	.
.	.	no				
C252	C262	C312	N4	0.7(11)	.	.
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C272	C282	C292	C302	1.6(14)	.	.
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C412	C422	C432	C442	0.5(13)	.	.
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C422	C432	C442	C392	1.1(12)	.	.
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P3	C452	C462	C472	-179.3(7)	.	.
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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			
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C11	C401	3.590(8)	.	.
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C12	C212	3.506(10)	.	.
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	no			
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	no			
C12	P3	3.604(3)	.	.
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C81	C401 no	3.505(12)	.	.
C82	C402 no	3.531(12)	.	.
C82	C12 no	3.369(8)	.	.
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C111	C14 no	3.564(10)	.	2_666
C111	C17 no	3.620(9)	.	2_666
C112	C13 no	3.646(9)	.	.
C112	C111 no	3.630(9)	.	2_666
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C121	C172 no	3.575(12)	.	2_666
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C122	C171 no	3.431(12)	.	2_666
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C232	no C361	3.584(12)	.	2_556
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Pd2	no H62	3.66(5)	.	.
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Pd2	no H502	2.99(4)	.	.
Pd2	no H402	3.55(6)	.	.
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C12	H341	2.90(5)	.	2_556
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C12	H491	3.01(5)	.	.
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C14	H192	2.62(7)	.	.
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C16	H222	3.13(5)	.	.
	no			
C17	H152	2.93(5)	.	.
	no			
C17	H211	2.98(4)	.	.
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C122	no H111	3.11(5)	.	.
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C112	no H431	2.95(5)	.	2_566
C112	no H171	2.95(6)	.	2_666

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C122	H22	2.72(5)	.	.
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C122	H171	2.79(6)	.	2_666
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C132	H122	2.83(5)	.	.
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C141	H121	2.92(5)	.	.
	no			
C142	H122	2.74(5)	.	.
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C172	H12	2.7903	.	.
	no			
C182	H12	2.9970	.	.
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C192	H212	2.95(5)	.	.
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C192	H12	2.9904	.	.
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C211	H191	2.87(3)	.	.
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C232	H361	2.98(4)	.	2_556
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C241	H620	3.0796	.	.
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C241	H271	2.88(5)	.	.
	no			
C241	H362	2.87(4)	.	2_556
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C241	H352	3.07(6)	.	2_556
	no			
C242	H272	2.87(5)	.	.
	no			
C242	H361	2.86(4)	.	2_556
	no			
C271	H241	2.87(5)	.	.
	no			
C272	H242	2.87(5)	.	.
	no			
C281	H204	2.9167	.	.
	no			
C282	H202	2.9486	.	.
	no			
C301	H321	2.79(5)	.	.
	no			
C302	H322	2.76(5)	.	.

C321	no H301	2.86(4)	.	.
C322	no H302	2.86(5)	.	.
C331	no H291	2.93(6)	.	2_556
C341	no H291	2.80(7)	.	2_556
C342	no H292	2.93(7)	.	2_555
C351	no H291	2.80(8)	.	2_556
C352	no H292	2.90(8)	.	2_555
C361	no H482	3.02(9)	.	1_556
C361	no H291	2.91(8)	.	2_556
C362	no H481	3.09(9)	.	.
C371	no H291	3.01(7)	.	2_556
C372	no H462	3.04(4)	.	.
C372	no H15	3.0609	.	1_455
C381	no H291	3.05(6)	.	2_556
C381	no H461	3.04(5)	.	.
C382	no H462	2.89(5)	.	.
C391	no H371	2.55(5)	.	.
C392	no H372	2.48(5)	.	.
C401	no H371	2.78(5)	.	.
C402	no H372	2.65(5)	.	.
C412	no H31	3.09(5)	.	2_566
C432	no H15	3.0435	.	1_455
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C451	no H441	2.76(3)	.	.
C452	no H442	2.71(3)	.	.
C461	no H441	2.62(5)	.	.
C462	no H442	2.70(5)	.	.
C481	no H321	2.92(6)	.	2_556
C482	no H322	3.02(7)	.	2_555
C491	no H321	3.07(7)	.	2_556
C491	no H341	3.06(3)	.	2_556
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C501	no H301	2.95(6)	.	.

C502	H302 no	2.95(6)	.	.
C502	H62 no	2.79(5)	.	.
H12	C14 no	2.7395	.	.
H12	H172 no	2.5930	.	.
H12	C192 no	2.9904	.	.
H12	C172 no	2.7903	.	.
H12	C182 no	2.9970	.	.
H13	C111 no	3.0186	.	.
H13	C232 no	3.0397	.	.
H13	C222 no	2.9599	.	.
H14	H431 no	2.5580	.	.
H14	C13 no	2.7903	.	2_666
H15	C372 no	3.0609	.	.
H15	H372 no	2.2330	.	.
H15	C432 no	3.0435	.	.
H21	H32 no	2.57(8)	.	2_566
H21	C121 no	2.71(5)	.	.
H21	C71 no	2.69(4)	.	.
H22	C122 no	2.72(5)	.	.
H22	C72 no	2.63(4)	.	.
H31	C412 no	3.09(5)	.	2_566
H32	H21 no	2.57(8)	.	2_566
H42	C119 no	2.90(4)	.	.
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H61	C131 no	3.04(4)	.	.
H61	H501 no	2.37(6)	.	.
H61	C501 no	2.69(4)	.	.
H62	Pd2 no	3.66(5)	.	.
H62	C502 no	2.79(5)	.	.
H62	H502 no	2.33(8)	.	.
H81	H401 no	2.38(8)	.	.
H81	Pd1 no	3.02(3)	.	.
H81	C11 no	2.39(9)	.	.
H82	H402	2.48(8)	.	.

H82	no Cl2	2.42(9)	.	.
H82	no Pd2	3.17(4)	.	.
H102	no Cl11	3.12(6)	.	2_666
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H111	no Cl4	2.89(7)	.	2_666
H111	no Cl22	3.11(5)	.	1_556
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H112	no Cl3	2.97(7)	.	.
H121	no Cl41	2.92(5)	.	.
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H121	no Cl31	2.98(5)	.	.
H122	no Cl3	3.04(4)	.	.
H122	no Cl42	2.74(5)	.	.
H122	no H142	2.60(6)	.	.
H122	no Cl32	2.83(5)	.	.
H141	no Cl9	2.97(4)	.	2_666
H141	no Cl1	2.54(5)	.	.
H141	no C61	2.77(4)	.	.
H142	no Cl19	2.91(5)	.	.
H142	no H122	2.60(6)	.	.
H142	no C62	2.80(5)	.	.
H142	no Cl2	2.55(6)	.	.
H152	no Cl7	2.93(5)	.	2_665
H171	no H191	2.28(4)	.	.
H171	no Cl22	2.79(6)	.	2_666
H171	no Cl12	2.95(6)	.	2_666
H171	no Cl3	3.13(4)	.	2_666
H172	no Cl11	3.06(6)	.	2_666
H172	no H12	2.5930	.	.
H172	no H192	2.29(4)	.	.
H172	no Cl4	2.83(4)	.	.
H172	no Cl21	2.82(6)	.	2_666
	no			

H191	C13 no	2.60(7)	.	2_666
H191	H171 no	2.28(4)	.	.
H191	C211 no	2.87(3)	.	.
H192	C212 no	2.78(3)	.	.
H192	H172 no	2.29(4)	.	.
H192	C14 no	2.62(7)	.	.
H201	H212 no	2.5729	.	.
H201	C12 no	2.8412	.	.
H202	H221 no	2.3149	.	.
H202	C221 no	3.0050	.	.
H202	C282 no	2.9486	.	.
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H205	C14 no	2.5645	.	.
H205	H272 no	2.4685	.	.
H211	C191 no	3.04(5)	.	.
H211	C17 no	2.98(4)	.	1_556
H212	C1 no	3.06(4)	.	.
H212	H201 no	2.5729	.	.
H212	C16 no	2.73(4)	.	.
H212	C192 no	2.95(5)	.	.
H221	H202 no	2.3149	.	1_556
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H222	C16 no	3.13(5)	.	.
H231	C114 no	3.14(5)	.	2_656
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H241	C115 no	3.03(3)	.	.
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H271	C118 no	3.13(9)	.	.
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H272	no C5	3.02(9)	.	.
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H281	no H204	2.5246	.	.
H291	no C341	2.80(7)	.	2_556
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H291	no C331	2.93(6)	.	2_556
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H301	no C321	2.86(4)	.	.
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H362	C241 no	2.87(4)	.	2_556
H362	C231 no	3.00(4)	.	2_556
H371	C391 no	2.55(5)	.	.
H371	C401 no	2.78(5)	.	.
H372	C392 no	2.48(5)	.	.
H372	C5 no	3.09(4)	.	1_455
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H402	Pd2 no	3.55(6)	.	.
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H402	C12 no	3.06(5)	.	.
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H422	C14 no	3.07(5)	.	1_455
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H431	C112 no	2.95(5)	.	2_566
H432	H111 no	2.46(8)	.	2_566
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H441	C451 no	2.76(3)	.	.
H441	C461 no	2.62(5)	.	.
H442	C462 no	2.70(5)	.	.
H442	C452 no	2.71(3)	.	.
H461	H441	2.49(5)	.	.

H461	no C381	3.04(5)	.	.
H461	no C441	2.99(3)	.	.
H462	no C372	3.04(4)	.	.
H462	no C382	2.89(5)	.	.
H462	no Cl13	3.14(6)	.	1_455
H472	no Cl16	3.11(6)	.	1_454
H481	no C362	3.09(9)	.	.
H482	no C361	3.02(9)	.	.
H491	no Cl2	3.01(5)	.	.
H492	no Cl1	2.73(6)	.	.
H501	no H61	2.37(6)	.	.
H501	no Pd1	2.96(4)	.	.
H502	no Cl8	2.92(9)	.	.
H502	no C62	3.06(6)	.	.
H502	no Pd2	2.99(4)	.	.
H502	no H62	2.33(8)	.	.
H620	no Cl3	2.7044	.	2_666
H620	no C241	3.0796	.	.
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	C4		H14		Cl3	0.9709	2.7903	3.682(10)
	153.08		2_666					
	C81		H81		Cl1	0.99(9)	2.39(9)	3.371(8)
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	C82		H82		Cl2	0.96(9)	2.42(9)	3.369(8)
	168(5)		.					
	C172		H172		Cl4	0.98(6)	2.83(4)	3.660(8)
	143(3)		.					
	C191		H191		Cl3	0.86(7)	2.60(7)	3.405(9)
	155(3)		2_666					
	C192		H192		Cl4	0.94(7)	2.62(7)	3.368(9)

137(3)	.				
C3	H203	C14	0.9708	2.5534	3.472(12)
157.83	.				
C5	H205	C14	0.9707	2.5645	3.507(18)
163.86	.				
C212	H212	C16	0.92(6)	2.73(4)	3.468(8)
138(4)	.				
C351	H351	C12	0.94(7)	2.81(7)	3.466(8)
128(4)	2_556				
C352	H352	C11	0.87(7)	2.82(7)	3.411(8)
126(4)	2_556				
C401	H401	C11	0.99(5)	2.68(5)	3.590(8)
154(3)	.				
C492	H492	C11	0.87(6)	2.73(6)	3.565(10)
161(4)	.				
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End of Crystallographic Information File

Complex # 4

data_S1421A

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Refinement on F2 for ALL reflections except for 186 with very
negative F2
or flagged by the user for potential systematic errors.
Weighted R-factors
wR and all goodnesses of fit S are based on F2, conventional
R-factors R
are based on F, with F set to zero for negative F2. The
observed criterion
of F2 > 2sigma(F2) 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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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 .
C15 C 0.4072(10) 0.4530(9) 0.0683(3) 0.046(3) Uani 1 d . .
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C18 C 0.3183(8) 0.2626(8) 0.1274(2) 0.034(2) Uani 1 d . .
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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 . .
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P1 0.041(2) 0.0285(14) 0.0391(10) -0.0016(10) -0.0037(10)
0.0147(13)
C11 0.088(3) 0.097(3) 0.076(2) 0.003(2) -0.017(2) 0.034(2)
C12 0.076(2) 0.079(2) 0.070(2) 0.000(2) 0.005(2) 0.045(2)
C14 0.147(5) 0.112(4) 0.136(3) -0.029(3) -0.021(3) 0.065(4)
C13 0.173(5) 0.134(4) 0.079(2) 0.011(2) -0.003(3) 0.095(4)
C16 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)
C15 0.064(7) 0.044(7) 0.043(4) 0.016(4) 0.012(4) 0.037(6)
C18 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)
C19 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)
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 C8 0.082(9) 0.051(8) 0.050(5) -0.015(5) -0.014(5) 0.038(8)
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 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)
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 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)
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 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)

_geom_special_details

;
 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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 Pd1 N1 1.999(6) . ?
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C19 N1 1.277(11) . ?
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C26 O1 1.234(11) . ?
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C12 C11 1.43(2) . ?
C23 C24 1.397(13) . ?
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C2 C3 1.419(15) . ?
C3 C4 1.34(2) . ?
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C5 C4 1.37(2) . ?
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loop_

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C21 Pd1 O1 93.4(3) . . ?
N1 Pd1 O1 172.7(3) . . ?
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N1 Pd1 P1 84.5(2) . . ?
O1 Pd1 P1 100.0(2) . . ?
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C7 P1 C13 104.3(4) . . ?
C1 P1 Pd1 116.2(3) . . ?
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C17 C16 C15 121.4(9) . . ?
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C12 C28 C11 112.6(7) . . ?
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