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Reactions of cationic palladium alpha-diimine complexes with nitrogen-containing olefins

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Published in:
 Organometallics

DOI:
[10.1021/om701059t](https://doi.org/10.1021/om701059t)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
 Publisher's PDF, also known as Version of record

Publication date:
 2008

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Li, W., Zhang, X., Meetsma, A., & Hessen, B. (2008). Reactions of cationic palladium alpha-diimine complexes with nitrogen-containing olefins: Branched polyethylene with carbazole functionalities. *Organometallics*, 27(9), 2052-2057. <https://doi.org/10.1021/om701059t>

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?
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# 1. SUBMISSION DETAILS

_publ_contact_author_name # Name of author for correspondence
;
  Drs. A. Meetsma
;
_publ_contact_author_address # Address of author for correspondence
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email A.Meetsma@rug.nl
_publ_contact_author_fax '+31 50 3634441'
_publ_contact_author_phone '+31 50 3634368'

_publ_requested_journal 'Organometallics'
# Publication chose FI FM FO CI CM CO
_publ_requested_category ?
_publ_requested_coeditor_name ?

_publ_contact_letter # Include date of submission
;
  Date of submission : 2007-09-20 09:14:03

  Consider this CIF submission for deposition of the first
  X-ray structure of a manuscript to be submitted to : Organometallics
  (Our Compound_Identification_Code : CP826B)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_from_coeditor ?

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_journal_date_accepted ?

_journal_date_printers_first ?

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_journal_issue ?

_journal_page_first ?

_journal_page_last ?

_journal_suppl_publ_number ?

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3. TITLE AND AUTHOR LIST

_publ_section_title

;

?

;

_publ_section_title_footnote

;

?

;

The loop structure below should contain the names and addresses of all

authors, in the required order of publication. Repeat as necessary.

loop_

_publ_author_name

_publ_author_footnote

_publ_author_address

'Meetsma, Auke'

;

? # author related footnote

;

;

Crystal Structure Center, Chemical Physics,
Zernike Institute for Advanced Materials,
University of Groningen,

```

Nijenborgh 4,
NL-9747 AG Groningen, The Netherlands.
;

#=====

# 4. TEXT

_publ_section_synopsis
;
?
;
_publ_section_abstract
;
The asymmetric unit consists of two moieties: a cationic Pd-complex and
a heavy disordered fluorinated-tetraphenylborate.
;

# Insert blank lines between paragraphs

_publ_section_comment
; ?
;
_publ_section_exptl_prep
;
?
;
_publ_section_exptl_refinement
;
The structure was solved by Patterson methods and extension of the model
was accomplished by direct methods applied to difference structure factors
using the program DIRDIF. The positional and anisotropic displacement
parameters for the non-hydrogen atoms were refined. Some atoms showed
unrealistic displacement parameters when allowed to vary anisotropically,
suggesting again disorder. The disorder ?revealed itself? more at the -CF3
fragments of the anion; meaning rotational disorder. Some F-positions of
the heavily disordered --CF3 fragments were refined using two alternative
positions.
The hydrogen atoms were included in the final refinement riding on their
carrier atoms with their positions calculated by using sp2 or sp3 hybridization
at the C-atom as appropriate with Uiso = c x Uequiv of their parent atom,
where c = 1.2 for the aromatic / non-methyl hydrogen atoms and c = 1.5 for
the methyl hydrogen atoms and where values Uequiv are related to the atoms
to which the hydrogen atoms are bonded. The methyl-groups were refined as
rigid groups, which were allowed to rotate freely.
;

# Insert blank lines between references

_publ_section_references
;
Beurskens, P.T., Beurskens, G., Gelder, R. de Garc\'ia-Granda, S.
Gould, R.O. Isra\'el, & Smits, J.M.M. (1999).
The DIRDIF99 program system, Technical Report of the Crystallography
Laboratory, University of Nijmegen, The Netherlands.

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Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

```

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Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel.
(Present distributor Kluwer Academic Publishers, Dordrecht).

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Edited by A.J.C Wilson, Kluwer Academic Publishers,
Dordrecht, The Netherlands.

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Refinement. University of G\ottingen, Germany, 1997.

Sheldrick, G.M. SADABS. Version 2. Multi-Scan Absorption Correction Program.
University of G\ottingen, Germany, 2001

Spek, A.L. (1988). J. Appl. Cryst. 21, 578-579.

Spek, A.L. (1990). Acta Cryst. A46, C-34.

Spek, A.L. (1994). Am. Crystallogr. Assoc.-Abstracts, 22, 66.

;

_publ_section_figure_captions

;

Fig. 1. Perspective PLUTO drawing of the molecule illustrating the
configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective ORTEP drawing of the title compound.
Displacement ellipsoids for non-H are represented at the 50%
probability level.
The H-atoms have been omitted to improve clarity.

;

#=====

5. CHEMICAL DATA

_chemical_name_systematic

; ?

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety

'C34 H54 N3 Pd, C32 H12 B F24'

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

_chemical_formula_structural ?

_chemical_formula_sum

'C66 H66 B F24.00 N3 Pd'

_chemical_formula_iupac ?

_chemical_formula_weight 1474.46

_chemical_compound_source 'see text'

```

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
Pd Pd -0.9988 1.0072
'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'
F F 0.0171 0.0103
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
B B 0.0013 0.0007
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0.0000 0.0000
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C C 0.0033 0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#=====

# 6. CRYSTAL DATA

_symmetry_cell_setting Monoclinic
_symmetry_space_group_name_Hall '-C 2yc'
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15

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 41.414(2)
_cell_length_b 12.7965(5)
_cell_length_c 26.010(1)
_cell_angle_alpha 90
_cell_angle_beta 103.000(1)
_cell_angle_gamma 90
_cell_volume 13430.8(10)
_cell_formula_units_Z 8

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 5327
_cell_measurement_theta_min 2.20
_cell_measurement_theta_max 20.53
_cell_special_details
;
The final unit cell was obtained from the xyz centroids of
5327 reflections after integration using the SAINT software
package (Bruker, 2000).
;

_exptl_crystal_description 'block'
_exptl_crystal_colour 'orange'

```

```

_exptl_crystal_size_max 0.35
_exptl_crystal_size_mid 0.31
_exptl_crystal_size_min 0.23
_exptl_crystal_size_rad ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 1.458
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000 6000
_exptl_absorpt_coefficient_mu 0.385
_exptl_absorpt_correction_type 'Multi-Scan'
_exptl_absorpt_process_details '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min 0.7829
_exptl_absorpt_correction_T_max 0.9167

```

```

#=====

```

``` # 7. EXPERIMENTAL DATA ```

```

_exptl_special_details
; ?
;
_diffn_ambient_temperature 100(1)
_diffn_radiation_wavelength 0.71073
_diffn_radiation_type 'MoK\alpha'
_diffn_radiation_source 'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator 'parallel mounted graphite'
_diffn_radiation_detector
;
    CCD area-detector
;
_diffn_measurement_device_type
;
    Bruker Smart Apex
;
_diffn_measurement_method 'phi and omega scans'
_diffn_special_details
;
    Crystal into the cold nitrogen stream of the low-temperature unit
    (KRYOFLEX, (Bruker, 2000)).
;
_diffn_detector_area_resol_mean 66.06

_diffn_standards_number ?
_diffn_standards_interval_count ?
_diffn_standards_interval_time ?

loop_
_diffn_standard_refl_index_h
_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffn_reflns_number 47500
_diffn_reflns_av_R_equivalents 0.0734
_diffn_reflns_av_sigmaI/netI 0.0781
_diffn_reflns_limit_h_min -49
_diffn_reflns_limit_h_max 49
_diffn_reflns_limit_k_min -13
_diffn_reflns_limit_k_max 15
_diffn_reflns_limit_l_min -30

```

```

_diffn_reflms_limit_l_max 30
_diffn_reflms_theta_min 2.20
_diffn_reflms_theta_max 25.03
_diffn_measured_fraction_theta_max 0.999
_diffn_reflms_theta_full 25.00
_diffn_measured_fraction_theta_full 0.999

_diffn_reflms_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflms_number_total 11866
_reflms_number_gt 7997
_reflms_threshold_expression  $I > 2\sigma(I)$ 

_computing_data_collection 'SMART, Bruker Version 5.624, 2001'
_computing_cell_refinement 'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction 'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2003)
PLATON (Spek, 1994)
;
_computing_publication_material 'PLATON (Spek, 1990)'

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on  $F^2$ , conventional R-factors R are based
on F, with F set to zero for negative  $F^2$ . The threshold expression of
 $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on  $F^2$  are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
'calc w=1/[\sigma^2(Fo^2)+(0.0644P)^2+65.10P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary heavy
_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment constr
_refine_ls_extinction_method none

```


_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration ?

_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns 11866
_refine_ls_number_parameters 907
_refine_ls_number_restraints 0
_refine_ls_number_constraints ?
_refine_ls_R_factor_all 0.0989
_refine_ls_R_factor_gt 0.0618
_refine_ls_wR_factor_ref 0.1664
_refine_ls_wR_factor_gt 0.1468
_refine_ls_goodness_of_fit_ref 1.028
_refine_ls_restrained_S_all 1.028
_refine_ls_shift/su_max 0.001
_refine_ls_shift/su_mean 0.000

_refine_diff_density_max 1.336
_refine_diff_density_min -0.627
_refine_diff_density_rms 0.088

_vrn_publ_code_void_volume 326.7
_vrn_publ_code_frame_time_sec 10.0
_vrn_publ_code_meas_time_hour 8.0

#=====

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Pd11 Pd Uani 0.36531(1) 0.50642(3) -0.02736(1) 1.000 0.0262(1) . .
N11 N Uani 0.32979(9) 0.3988(3) -0.01676(15) 1.000 0.0260(12) . .
N12 N Uani 0.38853(9) 0.4290(3) 0.04495(15) 1.000 0.0277(12) . .
N13 N Uani 0.40185(11) 0.6061(4) -0.04330(19) 1.000 0.0491(17) . .
C11 C Uani 0.41843(12) 0.4654(4) 0.0810(2) 1.000 0.0332(17) . .
C12 C Uani 0.41529(13) 0.5466(4) 0.1159(2) 1.000 0.0397(17) . .
C13 C Uani 0.44439(13) 0.5875(4) 0.1463(2) 1.000 0.0461(19) . .
C14 C Uani 0.47494(14) 0.5505(5) 0.1427(3) 1.000 0.055(2) . .
C15 C Uani 0.47736(14) 0.4713(5) 0.1089(3) 1.000 0.057(2) . .
C16 C Uani 0.44925(13) 0.4256(5) 0.0770(2) 1.000 0.0436(19) . .
C17 C Uani 0.38113(15) 0.5857(5) 0.1228(3) 1.000 0.062(2) . .
C18 C Uani 0.3822(2) 0.6273(6) 0.1785(3) 1.000 0.074(3) . .
C19 C Uani 0.36699(19) 0.6672(7) 0.0845(3) 1.000 0.085(3) . .
C110 C Uani 0.45237(14) 0.3339(6) 0.0413(3) 1.000 0.062(3) . .
C111 C Uani 0.48081(16) 0.3443(7) 0.0135(3) 1.000 0.085(3) . .
C112 C Uani 0.4565(2) 0.2324(6) 0.0730(4) 1.000 0.092(4) . .
C113 C Uani 0.37089(12) 0.3570(4) 0.06010(18) 1.000 0.0286(16) . .
C114 C Uani 0.37981(14) 0.2975(4) 0.1109(2) 1.000 0.0432(17) . .
C115 C Uani 0.33762(11) 0.3371(4) 0.02353(18) 1.000 0.0274(16) . .

C116	C	Uani	0.31584(12)	0.2556(4)	0.0380(2)	1.000	0.0353(17)	. .
C117	C	Uani	0.29714(11)	0.3909(4)	-0.05185(18)	1.000	0.0274(16)	. .
C118	C	Uani	0.29437(12)	0.3417(4)	-0.10090(19)	1.000	0.0322(17)	. .
C119	C	Uani	0.26308(13)	0.3391(4)	-0.1347(2)	1.000	0.0364(17)	. .
C120	C	Uani	0.23596(12)	0.3851(4)	-0.1207(2)	1.000	0.0375(17)	. .
C121	C	Uani	0.23955(12)	0.4338(4)	-0.0724(2)	1.000	0.0343(17)	. .
C122	C	Uani	0.27030(12)	0.4380(4)	-0.03659(19)	1.000	0.0301(17)	. .
C123	C	Uani	0.32446(13)	0.2921(4)	-0.1162(2)	1.000	0.0392(19)	. .
C124	C	Uani	0.32271(15)	0.2962(5)	-0.1757(2)	1.000	0.053(2)	. .
C125	C	Uani	0.32911(16)	0.1790(5)	-0.0968(2)	1.000	0.057(2)	. .
C126	C	Uani	0.27309(13)	0.4933(4)	0.01597(19)	1.000	0.0390(17)	. .
C127	C	Uani	0.25039(14)	0.4452(6)	0.0486(2)	1.000	0.055(2)	. .
C128	C	Uani	0.26601(19)	0.6100(5)	0.0076(3)	1.000	0.067(3)	. .
C129	C	Uani	0.4227(2)	0.6634(6)	0.0003(3)	1.000	0.079(3)	. .
C130	C	Uani	0.4223(2)	0.5481(8)	-0.0718(4)	1.000	0.120(5)	. .
C131	C	Uani	0.3839(2)	0.6873(7)	-0.0810(3)	1.000	0.101(4)	. .
C132	C	Uani	0.3539(3)	0.6594(8)	-0.1116(5)	1.000	0.127(5)	. .
C133	C	Uani	0.3316(2)	0.7469(8)	-0.1409(4)	1.000	0.112(4)	. .
C134	C	Uani	0.33673(14)	0.5839(5)	-0.0889(2)	1.000	0.0492(19)	. .

H13	H	Uiso	0.44317	0.64268	0.17023	1.000	0.0551	. .
H14	H	Uiso	0.49444	0.58033	0.16396	1.000	0.0658	. .
H15	H	Uiso	0.49867	0.44659	0.10684	1.000	0.0678	. .
H17	H	Uiso	0.36561	0.52474	0.11672	1.000	0.0745	. .
H18	H	Uiso	0.39222	0.69702	0.18230	1.000	0.1117	. .
H18'	H	Uiso	0.39541	0.58004	0.20463	1.000	0.1117	. .
H18"	H	Uiso	0.35960	0.63138	0.18408	1.000	0.1117	. .
H19	H	Uiso	0.34498	0.68671	0.08936	1.000	0.1277	. .
H19'	H	Uiso	0.36509	0.64059	0.04862	1.000	0.1277	. .
H19"	H	Uiso	0.38147	0.72867	0.09000	1.000	0.1277	. .
H110	H	Uiso	0.43131	0.32902	0.01367	1.000	0.0746	. .
H111	H	Uiso	0.47907	0.41127	-0.00516	1.000	0.1275	. .
H111'	H	Uiso	0.47977	0.28703	-0.01184	1.000	0.1275	. .
H111"	H	Uiso	0.50193	0.34118	0.03961	1.000	0.1275	. .
H112	H	Uiso	0.45658	0.17306	0.04921	1.000	0.1380	. .
H112'	H	Uiso	0.43801	0.22473	0.09062	1.000	0.1380	. .
H112"	H	Uiso	0.47742	0.23412	0.09954	1.000	0.1380	. .
H114	H	Uiso	0.40124	0.32209	0.13154	1.000	0.0644	. .
H114'	H	Uiso	0.38126	0.22286	0.10336	1.000	0.0644	. .
H114"	H	Uiso	0.36275	0.30869	0.13105	1.000	0.0644	. .
H116	H	Uiso	0.30809	0.27817	0.06914	1.000	0.0528	. .
H116'	H	Uiso	0.32828	0.19016	0.04589	1.000	0.0528	. .
H116"	H	Uiso	0.29676	0.24445	0.00851	1.000	0.0528	. .
H119	H	Uiso	0.26025	0.30513	-0.16785	1.000	0.0437	. .
H120	H	Uiso	0.21487	0.38325	-0.14450	1.000	0.0451	. .
H121	H	Uiso	0.22079	0.46493	-0.06327	1.000	0.0410	. .
H123	H	Uiso	0.34450	0.33239	-0.09812	1.000	0.0467	. .
H124	H	Uiso	0.30488	0.25042	-0.19413	1.000	0.0799	. .
H124'	H	Uiso	0.34386	0.27285	-0.18257	1.000	0.0799	. .
H124"	H	Uiso	0.31827	0.36812	-0.18829	1.000	0.0799	. .
H125	H	Uiso	0.33225	0.17746	-0.05834	1.000	0.0849	. .
H125'	H	Uiso	0.34863	0.14906	-0.10674	1.000	0.0849	. .
H125"	H	Uiso	0.30945	0.13806	-0.11296	1.000	0.0849	. .
H126	H	Uiso	0.29646	0.48557	0.03657	1.000	0.0468	. .
H127	H	Uiso	0.22722	0.45447	0.02999	1.000	0.0826	. .
H127'	H	Uiso	0.25417	0.47975	0.08302	1.000	0.0826	. .
H127"	H	Uiso	0.25525	0.37042	0.05359	1.000	0.0826	. .
H128	H	Uiso	0.28230	0.64108	-0.01000	1.000	0.1006	. .
H128'	H	Uiso	0.26749	0.64404	0.04175	1.000	0.1006	. .
H128"	H	Uiso	0.24369	0.61973	-0.01451	1.000	0.1006	. .

H129 H Uiso 0.43641 0.61406 0.02459 1.000 0.1181 . .
 H129' H Uiso 0.40866 0.70295 0.01905 1.000 0.1181 . .
 H129" H Uiso 0.43701 0.71176 -0.01360 1.000 0.1181 . .
 H130 H Uiso 0.43533 0.59701 -0.08786 1.000 0.1791 . .
 H130' H Uiso 0.40804 0.50635 -0.09953 1.000 0.1791 . .
 H130" H Uiso 0.43717 0.50180 -0.04740 1.000 0.1791 . .
 H131 H Uiso 0.38055 0.74972 -0.06026 1.000 0.1213 . .
 H131' H Uiso 0.39841 0.70837 -0.10463 1.000 0.1213 . .
 H132 H Uiso 0.36018 0.61997 -0.14108 1.000 0.1531 . .
 H133 H Uiso 0.31989 0.78101 -0.11661 1.000 0.1678 . .
 H133' H Uiso 0.31540 0.71703 -0.17062 1.000 0.1678 . .
 H133" H Uiso 0.34524 0.79852 -0.15405 1.000 0.1678 . .
 H134 H Uiso 0.32673 0.53264 -0.11637 1.000 0.0594 . .
 H134' H Uiso 0.31844 0.61872 -0.07673 1.000 0.0594 . .

F21 F Uani 0.02751(10) 0.7862(3) 0.1981(2) 1.000 0.116(2) . .
 F22 F Uani 0.05001(11) 0.9317(4) 0.1988(3) 1.000 0.144(3) . .
 F23 F Uani 0.03907(13) 0.8728(7) 0.2645(3) 1.000 0.171(4) . .
 F24 F Uani 0.16976(10) 0.9705(3) 0.2560(2) 1.000 0.0853(18) . .
 F25 F Uani 0.19908(9) 0.8312(3) 0.2674(2) 1.000 0.092(2) . .
 F26 F Uani 0.18203(10) 0.8986(4) 0.33007(17) 1.000 0.0881(19) . .
 F27 F Uani 0.21469(14) 0.5573(4) 0.1632(2) 1.000 0.104(2) . .
 F210 F Uani 0.20870(9) 0.1832(3) 0.33816(14) 1.000 0.0579(11) . .
 F211 F Uani 0.20837(8) 0.2970(3) 0.39799(13) 1.000 0.0556(11) . .
 F212 F Uani 0.25159(8) 0.2777(3) 0.36632(16) 1.000 0.0696(15) . .
 F213 F Uani 0.12550(9) 0.4127(3) 0.49578(13) 1.000 0.0711(15) . .
 F214 F Uani 0.16183(7) 0.4951(3) 0.46462(12) 1.000 0.0544(13) . .
 F215 F Uani 0.12183(9) 0.5785(3) 0.48464(13) 1.000 0.0639(14) . .
 F216 F Uani 0.00071(9) 0.4703(4) 0.3248(2) 1.000 0.089(2) . .
 F217 F Uani 0.01374(8) 0.3170(3) 0.30801(17) 1.000 0.0739(15) . .
 F218 F Uani 0.01428(9) 0.3568(5) 0.38677(16) 1.000 0.113(2) . .
 F219 F Uani 0.04955(9) 0.1385(3) 0.12701(17) 1.000 0.0709(14) . .
 F220 F Uani 0.05405(11) 0.1579(3) 0.20875(19) 1.000 0.0850(17) . .
 F221 F Uani 0.09739(10) 0.1248(3) 0.18084(19) 1.000 0.0789(16) . .
 F224 F Uani 0.07506(13) 0.5732(5) 0.0505(2) 1.000 0.117(2) . .
 F281 F Uani 0.2354(2) 0.6405(6) 0.2241(3) 0.517(14) 0.045(3) . .
 F282 F Uani 0.2585(4) 0.5551(16) 0.2367(5) 0.483(14) 0.116(9) . .
 F291 F Uani 0.2601(4) 0.5031(16) 0.2131(12) 0.517(14) 0.183(12) . .
 F292 F Uani 0.2434(2) 0.4411(11) 0.1822(3) 0.483(14) 0.076(4) . .
 F2221 F Uani 0.0475(11) 0.4614(14) 0.0232(5) 0.59(5) 0.114(7) . .
 F2222 F Uani 0.0317(6) 0.4632(19) 0.0343(13) 0.41(5) 0.077(7) . .
 F2231 F Uani 0.0367(8) 0.5996(16) 0.0774(6) 0.59(5) 0.100(7) . .
 F2232 F Uani 0.0241(6) 0.549(5) 0.0662(15) 0.41(5) 0.121(15) . .
 C21 C Uani 0.11763(11) 0.6382(4) 0.25887(17) 1.000 0.0256(14) . .
 C22 C Uani 0.08669(12) 0.6884(4) 0.24420(18) 1.000 0.0292(17) . .
 C23 C Uani 0.08375(12) 0.7960(4) 0.2391(2) 1.000 0.0360(17) . .
 C24 C Uani 0.11158(13) 0.8596(4) 0.2489(2) 1.000 0.0372(17) . .
 C25 C Uani 0.14239(12) 0.8126(4) 0.2653(2) 1.000 0.0341(17) . .
 C26 C Uani 0.14511(12) 0.7047(4) 0.27009(18) 1.000 0.0309(17) . .
 C27 C Uani 0.05040(15) 0.8443(5) 0.2224(3) 1.000 0.053(2) . .
 C28 C Uani 0.17300(15) 0.8781(5) 0.2789(3) 1.000 0.052(2) . .
 C29 C Uani 0.15768(11) 0.4677(4) 0.26974(19) 1.000 0.0293(16) . .
 C210 C Uani 0.17773(12) 0.5057(4) 0.2370(2) 1.000 0.0349(17) . .
 C211 C Uani 0.21058(13) 0.4745(5) 0.2429(2) 1.000 0.0428(19) . .
 C212 C Uani 0.22470(13) 0.4028(4) 0.2806(2) 1.000 0.0407(17) . .
 C213 C Uani 0.20521(12) 0.3602(4) 0.3120(2) 1.000 0.0335(17) . .
 C214 C Uani 0.17234(11) 0.3924(4) 0.30648(19) 1.000 0.0284(16) . .
 C215 C Uani 0.23167(18) 0.5253(8) 0.2093(3) 1.000 0.077(3) . .
 C216 C Uani 0.21862(13) 0.2801(4) 0.3530(2) 1.000 0.043(2) . .
 C217 C Uani 0.10351(11) 0.4799(4) 0.31305(19) 1.000 0.0286(16) . .

C218	C	Uani	0.12173(11)	0.4949(4)	0.36466(19)	1.000	0.0316(16)	. .
C219	C	Uani	0.10862(12)	0.4749(4)	0.40838(19)	1.000	0.0319(16)	. .
C220	C	Uani	0.07609(13)	0.4415(5)	0.4025(2)	1.000	0.0410(19)	. .
C221	C	Uani	0.05711(12)	0.4275(5)	0.3517(2)	1.000	0.0407(19)	. .
C222	C	Uani	0.07056(12)	0.4456(4)	0.3077(2)	1.000	0.0341(16)	. .
C223	C	Uani	0.12936(14)	0.4894(5)	0.4627(2)	1.000	0.0422(19)	. .
C224	C	Uani	0.02156(14)	0.3943(7)	0.3433(3)	1.000	0.059(3)	. .
C225	C	Uani	0.09854(11)	0.4553(4)	0.20810(18)	1.000	0.0259(16)	. .
C226	C	Uani	0.09349(12)	0.3471(4)	0.2075(2)	1.000	0.0377(17)	. .
C227	C	Uani	0.07632(14)	0.2944(4)	0.1632(2)	1.000	0.0458(19)	. .
C228	C	Uani	0.06342(13)	0.3476(4)	0.1165(2)	1.000	0.0402(17)	. .
C229	C	Uani	0.06828(12)	0.4538(4)	0.1157(2)	1.000	0.0345(17)	. .
C230	C	Uani	0.08555(11)	0.5066(4)	0.16053(18)	1.000	0.0305(14)	. .
C231	C	Uani	0.07010(19)	0.1798(5)	0.1676(3)	1.000	0.068(3)	. .
C232	C	Uani	0.05322(16)	0.5144(5)	0.0674(2)	1.000	0.051(2)	. .
B2	B	Uani	0.11932(13)	0.5101(5)	0.2622(2)	1.000	0.0283(17)	. .

H22	H	Uiso	0.06713	0.64706	0.23757	1.000	0.0350	. .
H24	H	Uiso	0.10961	0.93317	0.24445	1.000	0.0447	. .
H26	H	Uiso	0.16653	0.67480	0.28147	1.000	0.0373	. .
H210	H	Uiso	0.16861	0.55425	0.21000	1.000	0.0421	. .
H212	H	Uiso	0.24726	0.38288	0.28487	1.000	0.0483	. .
H214	H	Uiso	0.15949	0.36194	0.32856	1.000	0.0343	. .
H218	H	Uiso	0.14387	0.51957	0.37006	1.000	0.0379	. .
H220	H	Uiso	0.06706	0.42862	0.43236	1.000	0.0489	. .
H222	H	Uiso	0.05715	0.43450	0.27336	1.000	0.0410	. .
H226	H	Uiso	0.10217	0.30833	0.23871	1.000	0.0457	. .
H228	H	Uiso	0.05162	0.31165	0.08606	1.000	0.0482	. .
H230	H	Uiso	0.08856	0.57998	0.15859	1.000	0.0363	. .

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Pd11	0.0208(2)	0.0293(2)	0.0265(2)	0.0004(2)	0.0012(1)	-0.0017(2)
N11	0.022(2)	0.028(2)	0.025(2)	-0.0025(18)	-0.0009(16)	-0.0009(17)
N12	0.022(2)	0.031(2)	0.028(2)	-0.0040(18)	0.0013(17)	0.0008(17)
N13	0.041(3)	0.059(3)	0.050(3)	-0.017(3)	0.016(2)	-0.016(2)
C11	0.025(3)	0.034(3)	0.035(3)	-0.004(2)	-0.005(2)	-0.003(2)
C12	0.033(3)	0.034(3)	0.047(3)	-0.005(3)	-0.002(2)	0.001(2)
C13	0.038(3)	0.038(3)	0.054(4)	-0.012(3)	-0.007(3)	-0.002(3)
C14	0.035(3)	0.057(4)	0.061(4)	-0.016(3)	-0.013(3)	-0.008(3)
C15	0.025(3)	0.070(5)	0.066(4)	-0.014(3)	-0.009(3)	0.007(3)
C16	0.027(3)	0.051(4)	0.046(3)	-0.012(3)	-0.006(2)	0.002(2)
C17	0.041(3)	0.042(4)	0.090(5)	-0.040(4)	-0.014(3)	0.004(3)
C18	0.086(5)	0.067(5)	0.074(5)	0.008(4)	0.028(4)	0.011(4)
C19	0.075(5)	0.127(7)	0.053(4)	-0.003(5)	0.015(4)	0.037(5)
C110	0.029(3)	0.076(5)	0.076(5)	-0.033(4)	-0.001(3)	0.005(3)
C111	0.043(4)	0.119(7)	0.091(6)	-0.031(5)	0.011(4)	0.020(4)
C112	0.080(6)	0.058(5)	0.146(8)	-0.040(5)	0.042(6)	0.003(4)
C113	0.031(3)	0.028(3)	0.024(2)	-0.006(2)	0.000(2)	0.006(2)
C114	0.049(3)	0.041(3)	0.031(3)	0.007(2)	-0.009(2)	-0.003(3)
C115	0.028(3)	0.029(3)	0.024(2)	-0.005(2)	0.003(2)	0.000(2)
C116	0.034(3)	0.033(3)	0.038(3)	0.004(2)	0.006(2)	-0.005(2)
C117	0.023(2)	0.028(3)	0.028(3)	0.004(2)	-0.001(2)	-0.004(2)

C118	0.032(3)	0.037(3)	0.024(3)	-0.001(2)	-0.001(2)	-0.002(2)
C119	0.038(3)	0.042(3)	0.025(3)	-0.003(2)	-0.002(2)	0.000(2)
C120	0.024(3)	0.047(3)	0.035(3)	0.005(2)	-0.007(2)	-0.003(2)
C121	0.028(3)	0.039(3)	0.033(3)	0.000(2)	0.001(2)	0.000(2)
C122	0.029(3)	0.032(3)	0.029(3)	0.001(2)	0.006(2)	-0.006(2)
C123	0.034(3)	0.051(4)	0.031(3)	-0.012(2)	0.004(2)	0.001(2)
C124	0.047(4)	0.071(4)	0.043(3)	-0.003(3)	0.013(3)	0.008(3)
C125	0.064(4)	0.058(4)	0.046(4)	-0.002(3)	0.009(3)	0.021(3)
C126	0.033(3)	0.049(3)	0.031(3)	-0.011(3)	-0.001(2)	0.006(3)
C127	0.038(3)	0.092(5)	0.035(3)	-0.008(3)	0.009(3)	0.007(3)
C128	0.086(5)	0.055(4)	0.053(4)	-0.017(3)	-0.001(4)	0.011(4)
C129	0.087(6)	0.081(6)	0.064(5)	-0.002(4)	0.009(4)	-0.031(5)
C130	0.091(7)	0.123(8)	0.171(10)	-0.057(7)	0.085(7)	-0.032(6)
C131	0.110(7)	0.088(6)	0.095(6)	0.062(5)	0.001(5)	-0.041(5)
C132	0.098(7)	0.100(7)	0.157(10)	0.079(7)	-0.029(7)	-0.029(6)
C133	0.084(6)	0.125(8)	0.115(8)	0.080(7)	-0.004(5)	-0.002(6)
C134	0.045(3)	0.065(4)	0.034(3)	0.012(3)	0.001(3)	0.016(3)
F2221	0.23(2)	0.080(7)	0.022(4)	-0.007(4)	0.010(9)	-0.011(12)
F2231	0.163(18)	0.097(10)	0.037(5)	0.018(6)	0.013(8)	0.091(10)
F21	0.048(2)	0.046(2)	0.214(6)	-0.021(3)	-0.052(3)	0.012(2)
F22	0.056(3)	0.066(3)	0.283(8)	0.079(4)	-0.021(4)	0.008(2)
F23	0.075(4)	0.272(9)	0.153(6)	-0.068(6)	0.000(4)	0.091(5)
F24	0.063(3)	0.054(2)	0.134(4)	0.027(2)	0.012(3)	-0.027(2)
F25	0.046(2)	0.067(3)	0.173(5)	-0.037(3)	0.047(3)	-0.023(2)
F26	0.068(3)	0.115(4)	0.076(3)	-0.024(3)	0.005(2)	-0.058(3)
F27	0.116(4)	0.115(4)	0.100(4)	0.021(3)	0.063(3)	-0.031(3)
F210	0.061(2)	0.0363(19)	0.074(2)	0.0013(18)	0.0099(19)	0.0121(17)
F211	0.058(2)	0.065(2)	0.0410(19)	0.0091(17)	0.0051(16)	0.0273(18)
F212	0.0283(18)	0.082(3)	0.091(3)	0.022(2)	-0.0026(18)	0.0169(18)
F213	0.078(3)	0.091(3)	0.0353(19)	0.0226(19)	-0.0065(18)	-0.042(2)
F214	0.0346(17)	0.082(3)	0.0411(18)	0.0088(18)	-0.0028(14)	-0.0110(17)
F215	0.059(2)	0.081(3)	0.048(2)	-0.018(2)	0.0041(18)	-0.005(2)
F216	0.0261(19)	0.106(4)	0.136(4)	0.005(3)	0.019(2)	0.005(2)
F217	0.0334(19)	0.099(3)	0.087(3)	0.003(3)	0.0087(19)	-0.023(2)
F218	0.045(2)	0.235(6)	0.061(3)	0.026(3)	0.018(2)	-0.056(3)
F219	0.068(2)	0.046(2)	0.096(3)	-0.022(2)	0.013(2)	-0.0155(19)
F220	0.096(3)	0.064(3)	0.096(3)	-0.001(2)	0.024(3)	-0.024(2)
F221	0.064(2)	0.033(2)	0.137(4)	0.000(2)	0.017(2)	0.0045(18)
F224	0.105(4)	0.151(5)	0.085(3)	0.068(4)	0.003(3)	-0.022(4)
F281	0.060(5)	0.034(4)	0.049(4)	0.004(3)	0.026(3)	-0.017(4)
F291	0.092(13)	0.143(15)	0.37(3)	0.172(19)	0.17(2)	0.089(12)
C21	0.025(2)	0.034(3)	0.019(2)	0.007(2)	0.0074(19)	0.003(2)
C22	0.031(3)	0.029(3)	0.027(3)	0.001(2)	0.005(2)	-0.002(2)
C23	0.033(3)	0.034(3)	0.039(3)	-0.001(2)	0.004(2)	0.004(2)
C24	0.044(3)	0.030(3)	0.037(3)	-0.001(2)	0.008(2)	-0.002(2)
C25	0.033(3)	0.034(3)	0.035(3)	0.000(2)	0.007(2)	-0.006(2)
C26	0.028(3)	0.037(3)	0.029(3)	0.001(2)	0.009(2)	0.000(2)
C27	0.038(3)	0.032(3)	0.083(5)	-0.003(3)	-0.002(3)	0.011(3)
C28	0.041(3)	0.048(4)	0.069(4)	-0.006(3)	0.016(3)	-0.015(3)
C29	0.024(2)	0.034(3)	0.030(3)	-0.001(2)	0.006(2)	0.001(2)
C210	0.032(3)	0.038(3)	0.038(3)	0.005(3)	0.015(2)	0.002(2)
C211	0.030(3)	0.054(4)	0.051(3)	0.000(3)	0.023(3)	-0.001(3)
C212	0.025(3)	0.049(3)	0.049(3)	-0.009(3)	0.010(2)	0.005(2)
C213	0.027(3)	0.034(3)	0.037(3)	-0.006(2)	0.002(2)	0.001(2)
C214	0.022(2)	0.032(3)	0.033(3)	-0.002(2)	0.010(2)	0.000(2)
C215	0.045(4)	0.127(8)	0.068(5)	0.030(5)	0.033(4)	0.002(5)
C216	0.030(3)	0.043(4)	0.052(4)	-0.001(3)	0.000(3)	0.011(2)
C217	0.022(2)	0.030(3)	0.035(3)	0.009(2)	0.009(2)	0.005(2)
C218	0.024(2)	0.034(3)	0.036(3)	0.008(2)	0.005(2)	0.001(2)
C219	0.026(2)	0.038(3)	0.032(3)	0.004(2)	0.007(2)	-0.004(2)
C220	0.031(3)	0.059(4)	0.036(3)	0.006(3)	0.014(2)	-0.003(3)

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C221 0.021(3) 0.065(4) 0.036(3) 0.011(3) 0.006(2) -0.002(2)
C222 0.021(2) 0.051(3) 0.029(3) 0.008(2) 0.003(2) -0.001(2)
C223 0.043(3) 0.054(4) 0.030(3) 0.005(3) 0.009(2) -0.011(3)
C224 0.026(3) 0.109(6) 0.043(4) 0.009(4) 0.011(3) -0.013(4)
C225 0.017(2) 0.031(3) 0.031(3) 0.002(2) 0.008(2) 0.0044(19)
C226 0.033(3) 0.036(3) 0.041(3) 0.004(2) 0.002(2) 0.005(2)
C227 0.042(3) 0.035(3) 0.057(4) -0.005(3) 0.004(3) 0.000(3)
C228 0.034(3) 0.045(3) 0.040(3) -0.012(3) 0.005(2) 0.000(2)
C229 0.028(3) 0.043(3) 0.034(3) -0.002(2) 0.010(2) 0.000(2)
C230 0.030(2) 0.032(3) 0.031(2) -0.002(2) 0.010(2) 0.000(2)
C231 0.067(5) 0.047(4) 0.085(5) -0.008(4) 0.006(4) 0.003(4)
C232 0.057(4) 0.066(4) 0.027(3) 0.003(3) 0.006(3) -0.002(4)
B2 0.021(3) 0.036(3) 0.028(3) 0.004(3) 0.006(2) 0.001(2)
F292 0.042(5) 0.157(11) 0.044(5) 0.005(5) 0.040(4) -0.004(6)
F282 0.112(16) 0.18(2) 0.078(7) -0.072(10) 0.066(9) -0.117(16)
F2222 0.076(13) 0.080(10) 0.049(15) 0.016(10) -0.043(9) -0.013(9)
F2232 0.067(12) 0.22(4) 0.084(19) 0.08(2) 0.036(11) 0.076(15)

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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

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Pd11 N11 2.078(4) . . yes
Pd11 N12 2.152(4) . . yes
Pd11 N13 2.091(5) . . yes
Pd11 C134 2.023(6) . . yes
F2221 C232 1.310(15) . . yes
F2222 C232 1.27(3) . . yes
F2222 F2232 1.45(6) . . yes
F2231 C232 1.34(3) . . yes
F2232 C232 1.28(3) . . yes
F21 C27 1.258(8) . . yes
F22 C27 1.274(9) . . yes
F23 C27 1.335(10) . . yes
F24 C28 1.317(8) . . yes
F25 C28 1.327(8) . . yes
F26 C28 1.325(9) . . yes
F27 C215 1.312(9) . . yes
F210 C216 1.336(6) . . yes
F211 C216 1.349(6) . . yes
F212 C216 1.331(6) . . yes
F213 C223 1.338(7) . . yes
F214 C223 1.336(7) . . yes
F215 C223 1.343(7) . . yes
F216 C224 1.318(9) . . yes

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F217 C224 1.339(9) . . yes
 F218 C224 1.324(9) . . yes
 F219 C231 1.309(9) . . yes
 F220 C231 1.409(9) . . yes
 F221 C231 1.310(9) . . yes
 F224 C232 1.325(9) . . yes
 F281 C215 1.523(13) . . yes
 F282 C215 1.238(18) . . yes
 F291 C215 1.19(2) . . yes
 F292 C215 1.431(15) . . yes
 N11 C117 1.455(6) . . yes
 N11 C115 1.294(6) . . yes
 N12 C11 1.452(6) . . yes
 N12 C113 1.291(6) . . yes
 N13 C130 1.449(11) . . yes
 N13 C131 1.505(10) . . yes
 N13 C129 1.459(9) . . yes
 C11 C12 1.405(7) . . no
 C11 C16 1.400(8) . . no
 C12 C13 1.387(8) . . no
 C12 C17 1.549(8) . . no
 C13 C14 1.374(8) . . no
 C14 C15 1.360(10) . . no
 C15 C16 1.397(9) . . no
 C16 C110 1.520(10) . . no
 C17 C19 1.470(11) . . no
 C17 C18 1.535(11) . . no
 C110 C111 1.520(10) . . no
 C110 C112 1.527(11) . . no
 C13 H13 0.9501 . . no
 C113 C115 1.509(7) . . no
 C113 C114 1.497(7) . . no
 C14 H14 0.9501 . . no
 C115 C116 1.482(7) . . no
 C15 H15 0.9503 . . no
 C117 C122 1.398(7) . . no
 C117 C118 1.404(7) . . no
 C17 H17 1.0005 . . no
 C18 H18' 0.9796 . . no
 C118 C123 1.529(7) . . no
 C18 H18 0.9795 . . no
 C18 H18" 0.9803 . . no
 C118 C119 1.393(7) . . no
 C119 C120 1.387(7) . . no
 C19 H19" 0.9799 . . no
 C19 H19' 0.9798 . . no
 C19 H19 0.9803 . . no
 C120 C121 1.380(7) . . no
 C121 C122 1.399(7) . . no
 C122 C126 1.521(7) . . no
 C123 C124 1.534(7) . . no
 C123 C125 1.531(8) . . no
 C126 C128 1.528(8) . . no
 C126 C127 1.530(8) . . no
 C131 C132 1.364(15) . . no
 C132 C134 1.406(13) . . no
 C132 C133 1.540(15) . . no
 C110 H110 0.9995 . . no
 C111 H111 0.9795 . . no
 C111 H111" 0.9801 . . no
 C111 H111' 0.9801 . . no

C112 H112' 0.9818 . . no
 C112 H112 0.9800 . . no
 C112 H112" 0.9791 . . no
 C114 H114" 0.9803 . . no
 C114 H114 0.9801 . . no
 C114 H114' 0.9796 . . no
 C116 H116 0.9795 . . no
 C116 H116' 0.9804 . . no
 C116 H116" 0.9800 . . no
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 C121 H121 0.9496 . . no
 C22 C23 1.386(7) . . no
 C23 C24 1.387(7) . . no
 C123 H123 1.0001 . . no
 C23 C27 1.486(8) . . no
 C124 H124" 0.9803 . . no
 C24 C25 1.388(7) . . no
 C124 H124' 0.9792 . . no
 C124 H124 0.9793 . . no
 C125 H125 0.9795 . . no
 C25 C28 1.494(8) . . no
 C125 H125' 0.9804 . . no
 C125 H125" 0.9798 . . no
 C25 C26 1.389(7) . . no
 C126 H126 1.0001 . . no
 C127 H127' 0.9790 . . no
 C127 H127" 0.9805 . . no
 C127 H127 0.9799 . . no
 C128 H128" 0.9806 . . no
 C128 H128' 0.9788 . . no
 C128 H128 0.9807 . . no
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 C129 H129' 0.9796 . . no
 C129 H129 0.9792 . . no
 C129 H129" 0.9805 . . no
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 C29 C214 1.396(7) . . no
 C130 H130 0.9792 . . no
 C130 H130' 0.9812 . . no
 C130 H130" 0.9784 . . no
 C131 H131' 0.9888 . . no
 C131 H131 0.9909 . . no
 C132 H132 0.9999 . . no
 C133 H133' 0.9800 . . no
 C133 H133 0.9812 . . no
 C133 H133" 0.9795 . . no
 C134 H134 0.9895 . . no
 C134 H134' 0.9901 . . no
 C22 H22 0.9502 . . no
 C24 H24 0.9498 . . no
 C26 H26 0.9502 . . no
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 C211 C215 1.514(10) . . no
 C211 C212 1.374(8) . . no
 C212 C213 1.383(7) . . no
 C213 C216 1.493(7) . . no
 C213 C214 1.398(7) . . no

C217 C222 1.410(7) . . no
 C217 B2 1.648(7) . . yes
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 C218 C219 1.390(7) . . no
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 C221 C224 1.500(8) . . no
 C225 C226 1.400(7) . . no
 C225 B2 1.633(7) . . yes
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 C227 C228 1.390(7) . . no
 C227 C231 1.498(8) . . no
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 C214 H214 0.9500 . . no
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 C220 H220 0.9492 . . no
 C222 H222 0.9504 . . no
 C226 H226 0.9503 . . no
 C228 H228 0.9504 . . no
 C230 H230 0.9501 . . no

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 N11 Pd11 N12 76.67(15) . . . yes
 N11 Pd11 N13 174.94(17) . . . yes
 N11 Pd11 C134 97.1(2) . . . yes
 N12 Pd11 N13 104.66(17) . . . yes
 N12 Pd11 C134 169.74(19) . . . yes
 N13 Pd11 C134 82.2(2) . . . yes
 F2232 F2222 C232 55.5(16) . . . yes
 F2222 F2232 C232 55(2) . . . yes
 C115 N11 C117 119.6(4) . . . yes
 Pd11 N11 C117 123.3(3) . . . yes
 Pd11 N11 C115 117.1(3) . . . yes
 Pd11 N12 C113 115.0(3) . . . yes
 C11 N12 C113 119.4(4) . . . yes
 Pd11 N12 C11 124.4(3) . . . yes
 Pd11 N13 C131 106.1(4) . . . yes
 Pd11 N13 C129 118.7(4) . . . yes
 Pd11 N13 C130 108.7(5) . . . yes
 C130 N13 C131 106.3(6) . . . yes
 C129 N13 C130 110.1(6) . . . yes
 C129 N13 C131 106.2(5) . . . yes
 N12 C11 C12 117.7(4) . . . yes
 N12 C11 C16 119.7(4) . . . yes
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 C11 C12 C13 116.9(5) . . . no

C13 C12 C17 120.8(5) . . . no
C11 C12 C17 122.2(5) . . . no
C12 C13 C14 121.8(5) . . . no
C13 C14 C15 120.3(6) . . . no
C14 C15 C16 121.5(6) . . . no
C15 C16 C110 120.8(5) . . . no
C11 C16 C15 117.1(5) . . . no
C11 C16 C110 122.0(5) . . . no
C18 C17 C19 108.4(6) . . . no
C12 C17 C18 112.9(6) . . . no
C12 C17 C19 112.7(6) . . . no
C16 C110 C111 113.9(6) . . . no
C16 C110 C112 110.0(6) . . . no
C111 C110 C112 109.1(6) . . . no
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N12 C113 C115 115.3(4) . . . yes
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C12 C13 H13 119.12 . . . no
C13 C14 H14 119.81 . . . no
C15 C14 H14 119.93 . . . no
C113 C115 C116 118.7(4) . . . no
N11 C115 C113 115.7(4) . . . yes
C14 C15 H15 119.26 . . . no
C16 C15 H15 119.19 . . . no
N11 C115 C116 125.4(4) . . . yes
N11 C117 C122 118.6(4) . . . yes
C118 C117 C122 122.9(4) . . . no
C18 C17 H17 107.50 . . . no
C12 C17 H17 107.51 . . . no
N11 C117 C118 118.4(4) . . . yes
C19 C17 H17 107.59 . . . no
C117 C118 C123 121.2(4) . . . no
C119 C118 C123 121.5(4) . . . no
H18' C18 H18" 109.45 . . . no
H18 C18 H18" 109.48 . . . no
C17 C18 H18' 109.50 . . . no
C17 C18 H18" 109.42 . . . no
C117 C118 C119 117.3(5) . . . no
C17 C18 H18 109.44 . . . no
H18 C18 H18' 109.54 . . . no
C118 C119 C120 121.2(5) . . . no
C17 C19 H19 109.48 . . . no
H19 C19 H19' 109.48 . . . no
H19 C19 H19" 109.45 . . . no
H19' C19 H19" 109.48 . . . no
C17 C19 H19" 109.46 . . . no
C17 C19 H19' 109.47 . . . no
C119 C120 C121 120.2(5) . . . no
C120 C121 C122 121.2(5) . . . no
C121 C122 C126 119.3(5) . . . no
C117 C122 C121 117.2(4) . . . no
C117 C122 C126 123.5(4) . . . no
C124 C123 C125 109.8(4) . . . no
C118 C123 C124 113.1(4) . . . no
C118 C123 C125 110.9(4) . . . no
C122 C126 C128 110.7(5) . . . no
C127 C126 C128 110.5(5) . . . no
C122 C126 C127 112.3(4) . . . no
N13 C131 C132 116.8(8) . . . yes
C131 C132 C133 117.7(9) . . . no

C133 C132 C134 113.8(9) . . . no
C131 C132 C134 114.5(10) . . . no
Pd11 C134 C132 114.1(6) . . . yes
C16 C110 H110 107.89 . . . no
C112 C110 H110 107.98 . . . no
C111 C110 H110 107.91 . . . no
C110 C111 H111" 109.45 . . . no
C110 C111 H111 109.50 . . . no
H111' C111 H111 109.50 . . . no
H111" C111 H111 109.49 . . . no
H111' C111 H111" 109.44 . . . no
C110 C111 H111' 109.44 . . . no
C110 C112 H112 109.51 . . . no
H112' C112 H112" 109.42 . . . no
H112' C112 H112 109.33 . . . no
H112" C112 H112 109.54 . . . no
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C110 C112 H112" 109.60 . . . no
C113 C114 H114' 109.46 . . . no
H114' C114 H114" 109.48 . . . no
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C113 C114 H114 109.47 . . . no
C113 C114 H114" 109.45 . . . no
C115 C116 H116" 109.47 . . . no
C115 C116 H116' 109.46 . . . no
H116' C116 H116 109.47 . . . no
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H116' C116 H116" 109.43 . . . no
H116" C116 H116 109.49 . . . no
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C119 C120 H120 119.87 . . . no
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C122 C121 H121 119.38 . . . no
C120 C121 H121 119.37 . . . no
C22 C21 B2 119.7(4) . . . yes
C22 C21 C26 115.3(5) . . . no
C26 C21 B2 125.0(4) . . . yes
C21 C22 C23 122.3(5) . . . no
C24 C23 C27 119.3(5) . . . no
C22 C23 C27 119.8(5) . . . no
C22 C23 C24 120.9(5) . . . no
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C124 C123 H123 107.62 . . . no
C118 C123 H123 107.60 . . . no
H124' C124 H124" 109.50 . . . no
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H124' C124 H124 109.58 . . . no
H124" C124 H124 109.51 . . . no
C123 C124 H124' 109.42 . . . no
C123 C124 H124" 109.38 . . . no
C23 C24 C25 118.1(5) . . . no
C123 C125 H125 109.49 . . . no
H125' C125 H125 109.48 . . . no
H125" C125 H125 109.51 . . . no
H125' C125 H125" 109.44 . . . no
C123 C125 H125' 109.43 . . . no
C123 C125 H125" 109.47 . . . no
C26 C25 C28 119.3(5) . . . no
C24 C25 C26 120.6(5) . . . no

C24 C25 C28 120.1(5) . . . no
C21 C26 C25 122.7(5) . . . no
C128 C126 H126 107.73 . . . no
C127 C126 H126 107.71 . . . no
C122 C126 H126 107.72 . . . no
F21 C27 F23 102.1(6) . . . yes
F21 C27 C23 116.6(5) . . . yes
C126 C127 H127" 109.42 . . . no
C126 C127 H127 109.44 . . . no
F21 C27 F22 110.5(6) . . . yes
H127' C127 H127 109.54 . . . no
H127" C127 H127 109.43 . . . no
H127' C127 H127" 109.50 . . . no
C126 C127 H127' 109.49 . . . no
F23 C27 C23 110.4(6) . . . yes
F22 C27 F23 100.8(7) . . . yes
F22 C27 C23 114.6(5) . . . yes
H128' C128 H128 109.51 . . . no
H128" C128 H128 109.36 . . . no
C126 C128 H128' 109.56 . . . no
C126 C128 H128" 109.45 . . . no
H128' C128 H128" 109.52 . . . no
F24 C28 F26 104.7(5) . . . yes
F24 C28 C25 113.7(5) . . . yes
F25 C28 F26 104.8(6) . . . yes
F25 C28 C25 112.5(5) . . . yes
F26 C28 C25 112.4(5) . . . yes
C126 C128 H128 109.44 . . . no
F24 C28 F25 108.0(5) . . . yes
C210 C29 C214 115.4(4) . . . no
H129' C129 H129" 109.46 . . . no
H129' C129 H129 109.57 . . . no
H129" C129 H129 109.51 . . . no
C214 C29 B2 124.6(4) . . . yes
N13 C129 H129' 109.44 . . . no
C210 C29 B2 120.0(4) . . . yes
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N13 C129 H129" 109.37 . . . no
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N13 C130 H130" 109.47 . . . no
N13 C130 H130 109.42 . . . no
H130" C130 H130 109.69 . . . no
H130' C130 H130 109.44 . . . no
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N13 C131 H131 108.11 . . . no
C132 C131 H131 107.94 . . . no
N13 C131 H131' 108.24 . . . no
H131' C131 H131 107.32 . . . no
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Pd11 C134 H134' 108.73 . . . no

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H134' C134 H134 107.65 . . . no
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C23 C22 H22 118.86 . . . no
C23 C24 H24 120.94 . . . no
C25 C24 H24 120.98 . . . no
C21 C26 H26 118.62 . . . no
C25 C26 H26 118.66 . . . no
C29 C210 C211 122.0(5) . . . no
C210 C211 C215 119.3(6) . . . no
C212 C211 C215 119.4(5) . . . no
C210 C211 C212 121.2(5) . . . no
C211 C212 C213 118.3(5) . . . no
C212 C213 C214 120.5(5) . . . no
C212 C213 C216 121.3(5) . . . no
C214 C213 C216 118.2(5) . . . no
C29 C214 C213 122.5(4) . . . no
F282 C215 C211 111.1(9) . . . yes
F292 C215 C211 105.4(8) . . . yes
F282 C215 F292 98.9(11) . . . yes
F27 C215 F282 131.1(11) . . . yes
F27 C215 F292 87.5(6) . . . yes
F281 C215 C211 108.0(6) . . . yes
F291 C215 C211 122.4(14) . . . yes
F27 C215 F281 86.1(7) . . . yes
F27 C215 F291 117.8(16) . . . yes
F27 C215 C211 113.7(6) . . . yes
F281 C215 F291 99.6(12) . . . yes
F210 C216 F211 105.3(4) . . . yes
F210 C216 F212 106.5(4) . . . yes
F211 C216 F212 106.4(4) . . . yes
F211 C216 C213 111.7(4) . . . yes
F210 C216 C213 113.0(4) . . . yes
F212 C216 C213 113.4(4) . . . yes
C222 C217 B2 123.0(4) . . . yes
C218 C217 B2 120.8(4) . . . yes
C218 C217 C222 116.0(4) . . . no
C217 C218 C219 122.3(4) . . . no
C218 C219 C223 120.3(5) . . . no
C220 C219 C223 118.7(5) . . . no
C218 C219 C220 121.0(5) . . . no
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C220 C221 C222 120.8(5) . . . no
C220 C221 C224 120.1(5) . . . no
C222 C221 C224 119.1(5) . . . no
C217 C222 C221 121.7(5) . . . no
F213 C223 F214 106.3(5) . . . yes
F213 C223 F215 106.1(4) . . . yes
F213 C223 C219 113.0(5) . . . yes
F214 C223 F215 105.4(5) . . . yes
F214 C223 C219 113.7(4) . . . yes
F215 C223 C219 111.7(5) . . . yes
F216 C224 F217 104.9(6) . . . yes
F216 C224 F218 108.8(6) . . . yes
F217 C224 F218 104.6(7) . . . yes
F217 C224 C221 112.8(5) . . . yes
F218 C224 C221 112.5(6) . . . yes
F216 C224 C221 112.7(7) . . . yes
C226 C225 C230 115.3(4) . . . no
C230 C225 B2 125.8(5) . . . yes
C226 C225 B2 118.9(4) . . . yes

C225	C226	C227	122.6(5)	. . .	no
C228	C227	C231	120.5(5)	. . .	no
C226	C227	C228	120.9(5)	. . .	no
C226	C227	C231	118.6(5)	. . .	no
C227	C228	C229	117.9(5)	. . .	no
C230	C229	C232	119.4(5)	. . .	no
C228	C229	C230	121.0(5)	. . .	no
C228	C229	C232	119.5(5)	. . .	no
C225	C230	C229	122.3(5)	. . .	no
F219	C231	F221	111.2(6)	. . .	yes
F219	C231	C227	115.2(6)	. . .	yes
F220	C231	F221	102.7(5)	. . .	yes
F220	C231	C227	111.8(5)	. . .	yes
F221	C231	C227	113.1(6)	. . .	yes
F219	C231	F220	101.5(6)	. . .	yes
F2221	C232	F2231	126.2(17)	. . .	yes
F2221	C232	F224	90.3(16)	. . .	yes
F2222	C232	F2232	69(3)	. . .	yes
F2231	C232	F224	91.1(13)	. . .	yes
F2231	C232	C229	113.2(8)	. . .	yes
F224	C232	C229	112.8(5)	. . .	yes
F2222	C232	F224	119.6(14)	. . .	yes
F2232	C232	F224	120(3)	. . .	yes
F2222	C232	C229	113.5(14)	. . .	yes
F2221	C232	C229	115.5(10)	. . .	yes
F2232	C232	C229	115(2)	. . .	yes
C29	C210	H210	118.95	. . .	no
C211	C210	H210	119.01	. . .	no
C213	C212	H212	120.95	. . .	no
C211	C212	H212	120.79	. . .	no
C29	C214	H214	118.72	. . .	no
C213	C214	H214	118.80	. . .	no
C217	C218	H218	118.84	. . .	no
C219	C218	H218	118.82	. . .	no
C221	C220	H220	120.88	. . .	no
C219	C220	H220	120.96	. . .	no
C217	C222	H222	119.15	. . .	no
C221	C222	H222	119.19	. . .	no
C225	C226	H226	118.69	. . .	no
C227	C226	H226	118.76	. . .	no
C229	C228	H228	121.03	. . .	no
C227	C228	H228	121.03	. . .	no
C225	C230	H230	118.85	. . .	no
C229	C230	H230	118.83	. . .	no
C21	B2	C225	112.0(4)	. . .	yes
C217	B2	C225	111.3(4)	. . .	yes
C29	B2	C217	111.9(4)	. . .	yes
C29	B2	C225	105.6(4)	. . .	yes
C21	B2	C217	104.9(4)	. . .	yes
C21	B2	C29	111.3(4)	. . .	yes

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N12 Pd11 N13 C130 85.8(5) no
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N13 Pd11 C134 C132 1.3(6) no
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Pd11 N11 C117 C122 -99.5(5) no
C115 N11 C117 C118 -103.7(5) no
C115 N11 C117 C122 80.0(6) no
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C11 N12 C113 C115 170.4(4) no
Pd11 N12 C11 C16 -94.7(5) no
C113 N12 C11 C12 -87.1(6) no
Pd11 N12 C11 C12 80.0(5) no
C113 N12 C11 C16 98.2(6) no
Pd11 N13 C131 C132 -25.5(9) no
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H110 C110 C112 H112' -62.13 no
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C22 C21 B2 C225 52.1(6) no
C26 C21 B2 C29 -10.5(6) no
C26 C21 B2 C217 110.7(5) no
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C26 C21 C22 C23 2.6(7) no
B2 C21 C22 C23 -177.9(4) no
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C23 C24 C25 C26 1.9(7) no
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C24 C25 C28 F24 -24.2(8) no
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H126 C126 C127 H127 177.52 no
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H132	C132	C133	H133	167.14		no
C131	C132	C134	H134'	105.10		no
H132	C132	C134	Pd11	94.08		no
H132	C132	C134	H134'	-144.42		no
H132	C132	C134	H134	-27.50		no
C131	C132	C133	H133"	38.89		no
C131	C132	C133	H133	-81.06		no
C134	C132	C133	H133'	-62.87		no
C134	C132	C133	H133"	177.00		no
C134	C132	C133	H133	57.05		no
H132	C132	C133	H133'	47.22		no
H132	C132	C133	H133"	-72.91		no
C133	C132	C134	H134	82.56		no
C133	C132	C134	H134'	-34.36		no
C29	C210	C211	C212	1.5(8)		no
C29	C210	C211	C215	-174.9(6)		no
C210	C211	C212	C213	1.5(8)		no
C210	C211	C215	F291	178.8(16)		no
C215	C211	C212	C213	177.8(6)		no
C210	C211	C215	F281	64.3(8)		no
C212	C211	C215	F291	2.4(18)		no
C212	C211	C215	F281	-112.1(7)		no
C210	C211	C215	F27	-29.4(10)		no
C212	C211	C215	F27	154.2(6)		no
C211	C212	C213	C214	-2.2(8)		no
C211	C212	C213	C216	178.6(5)		no
C212	C213	C216	F210	-102.9(6)		no
C214	C213	C216	F211	-40.5(6)		no
C214	C213	C216	F210	77.9(6)		no
C214	C213	C216	F212	-160.7(5)		no
C216	C213	C214	C29	179.2(5)		no
C212	C213	C214	C29	0.0(8)		no
C212	C213	C216	F211	138.7(5)		no
C212	C213	C216	F212	18.5(7)		no
C222	C217	B2	C225	-21.6(7)		no
C222	C217	C218	C219	1.6(7)		no
B2	C217	C218	C219	176.9(5)		no
C218	C217	B2	C29	45.5(7)		no
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C218	C217	B2	C21	-75.3(6)		no
C222	C217	B2	C29	-139.5(5)		no
C218	C217	B2	C225	163.4(5)		no
C222	C217	B2	C21	99.7(5)		no
B2	C217	C222	C221	-175.5(5)		no
C217	C218	C219	C223	178.3(5)		no
C217	C218	C219	C220	-1.9(8)		no
C223	C219	C220	C221	-179.5(5)		no
C218	C219	C223	F213	-137.8(5)		no
C218	C219	C223	F214	-16.5(8)		no
C218	C219	C223	F215	102.7(6)		no
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