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

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# CIF-file generated for C66H66BF24N3Pd CP826B
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# 0. AUDIT DETAILS

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 SHELXL97-2 & Manual Editing
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_audit_update_record
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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 choise 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)

_journal_date_recd_electronic ?

_journal_date_to_coeditor ?
_journal_date_from_coeditor ?
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_journal_date_accepted ?

_journal_date_printers_first ?
_journal_date_printers_final ?
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_journal_date_proofs_in ?

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# 3. TITLE AND AUTHOR LIST

_publ_section_title
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;
_publ_section_title_footnote
;
 ?
;

# The loop structure below should contain the names and adresses 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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   Groningen University, The Netherlands. (unpublished).

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

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   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

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; ?
;
_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety
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Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
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_chemical_formula_sum
'C66 H66 B F24.00 N3 Pd'
_chemical_formula_iupac ?
_chemical_formula_weight 1474.46
_chemical_compound_source 'see text'

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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
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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
 '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

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

loop_
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 x,y,z
 -x,y,1/2-z
 -x,-y,-z
 x,-y,1/2+z
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 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'
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_exptl_crystal_size_max 0.35
_exptl_crystal_size_mid 0.31
_exptl_crystal_size_min 0.23
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_exptl_crystal_density_diffrn 1.458
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000 6000
_exptl_absorpt_coefficient_mu 0.385
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_exptl_absorpt_process_details '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min 0.7829
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#===============================================================================

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_diffrn_radiation_monochromator 'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
;
_diffrn_measurement_method 'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
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;
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_diffrn_standards_interval_time ?

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_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number 47500
_diffrn_reflns_av_R_equivalents 0.0734
_diffrn_reflns_av_sigmaI/netI 0.0781
_diffrn_reflns_limit_h_min -49
_diffrn_reflns_limit_h_max 49
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_diffrn_reflns_limit_l_min -30
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_diffrn_measured_fraction_theta_full 0.999

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
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_reflns_number_gt 7997
_reflns_threshold_expression I>2\s(I)


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_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^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement. R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
 'calc w=1/[\s^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
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_chemical_absolute_configuration ?

_refine_ls_abs_structure_Flack ?
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_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

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_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
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# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
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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) . .
```

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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) . .
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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) . .
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H18" H Uiso 0.35960 0.63138 0.18408 1.000 0.1117 . .
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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 . .
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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 . .
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H116" H Uiso 0.29676 0.24445 0.00851 1.000 0.0528 . .
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H120 H Uiso 0.21487 0.38325 -0.14450 1.000 0.0451 . .
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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 . .
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H131 H Uiso 0.38055 0.74972 -0.06026 1.000 0.1213 . .
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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 . .


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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) . .
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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 . .


loop_
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_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
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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)

#===============================================================================

# 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
;

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_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
 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
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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
C119 H119 0.9490 . . no
C120 H120 0.9505 . . no
C21 C22 1.407(7) . . no
C21 C26 1.398(7) . . no
C21 B2 1.642(8) . . yes
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
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C124 H124 0.9793 . . no
C125 H125 0.9795 . . no
C25 C28 1.494(8) . . no
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C127 H127" 0.9805 . . no
C127 H127 0.9799 . . no
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C128 H128 0.9807 . . no
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C129 H129 0.9792 . . no
C129 H129" 0.9805 . . no
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C29 C214 1.396(7) . . no
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C130 H130" 0.9784 . . no
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C132 H132 0.9999 . . no
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C133 H133" 0.9795 . . no
C134 H134 0.9895 . . no
C134 H134' 0.9901 . . no
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C24 H24 0.9498 . . no
C26 H26 0.9502 . . no
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C213 C216 1.493(7) . . no
C213 C214 1.398(7) . . no

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C12 C17 H17 107.51 . . . no
N11 C117 C118 118.4(4) . . . yes
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C117 C118 C123 121.2(4) . . . no
C119 C118 C123 121.5(4) . . . no
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C17 C18 H18' 109.50 . . . no
C17 C18 H18" 109.42 . . . no
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C17 C18 H18 109.44 . . . no
H18 C18 H18' 109.54 . . . no
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H19 C19 H19' 109.48 . . . no
H19 C19 H19" 109.45 . . . no
H19' C19 H19" 109.48 . . . no
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C131 C132 C133 117.7(9) . . . no
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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
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C120 C121 H121 119.37 . . . no
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C22 C23 C24 120.9(5) . . . no
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C124 C123 H123 107.62 . . . no
C118 C123 H123 107.60 . . . no
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H124' C124 H124 109.58 . . . no
H124" C124 H124 109.51 . . . no
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H125' C125 H125 109.48 . . . no
H125" C125 H125 109.51 . . . no
H125' C125 H125" 109.44 . . . no
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F21 C27 C23 116.6(5) . . . yes
C126 C127 H127" 109.42 . . . no
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F21 C27 F22 110.5(6) . . . yes
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F22 C27 F23 100.8(7) . . . yes
F22 C27 C23 114.6(5) . . . yes
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C126 C128 H128' 109.56 . . . no
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F27 C215 F292 87.5(6) . . . yes
F281 C215 C211 108.0(6) . . . yes
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F27 C215 F281 86.1(7) . . . yes
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F27 C215 C211 113.7(6) . . . yes
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F216 C224 C221 112.7(7) . . . yes
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C226 C225 B2 118.9(4) . . . yes
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 F219 C231 F220 101.5(6) . . . yes
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 F2221 C232 F224 90.3(16) . . . yes
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 F2231 C232 F224 91.1(13) . . . yes
 F2231 C232 C229 113.2(8) . . . yes
 F224 C232 C229 112.8(5) . . . yes
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