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

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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
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  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
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  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
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_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 09:14:42

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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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# The loop structure below should contain the names and adresses of all
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_publ_author_address

   'Meetsma, Auke'
;
 ? # author related footnote
;
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
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```
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;

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# 4. TEXT

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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 dynamic disorder (dynamic
 means that the smeared electron density is due to fluctuations of
 the atomic positions within each unit cell). The smeared electron
 density for F222...F224 has been described by two site occupancy
 factors, each with a value of 0.5, with separately refined displacement
 parameters.
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 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.

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 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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```

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Edited by A.J.C Wilson, Kluwer Academic Publishers,
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Spek, A.L. (1990). Acta Cryst. A46, C-34.

Spek, A.L. (1994). Am. Crystallogr. Assoc.-Abstracts, 22, 66.
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Fig. 1. Chemical structural diagram (scheme 1) of the title compound

Fig. 2. Perspective PLUTO drawing of the molecule illustrating the
configuration and the adopted numbering scheme.

Fig. 3. Molecular packing viewed down unit cell axes.

Fig. 4. 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_formula_sum
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_symmetry_Int_Tables_number 14

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

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_cell_length_b 15.7270(7)
_cell_length_c 36.571(2)
_cell_angle_alpha 90
_cell_angle_beta 91.951(1)
_cell_angle_gamma 90
_cell_volume 7406.3(6)
_cell_formula_units_Z 4

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 6429
_cell_measurement_theta_min 2.26
_cell_measurement_theta_max 24.27
_cell_special_details
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 The final unit cell was obtained from the xyz centroids of
   6429 reflections after integration using the SAINT software
   package (Bruker, 2000).
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_exptl_crystal_size_rad ?
_exptl_crystal_density_meas ?
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_exptl_absorpt_coefficient_mu 0.357
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;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
;
_diffrn_measurement_method 'phi and omega scans'
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;
 Crystal into the cold nitrogen stream of the low-temparature unit
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;
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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
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_diffrn_reflns_limit_h_min -15
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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 11677
_reflns_threshold_expression I>2\s(I)


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_computing_structure_solution
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 DIRDIF-99 (Beurskens et al., 1999)
;
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_computing_molecular_graphics
;
 PLUTO (Meetsma, 2003)
 PLATON (Spek, 1994)
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_computing_publication_material 'PLATON (Spek, 1990)'

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

# 8. REFINEMENT DATA


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 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
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```

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_atom_sites_solution_hydrogens geom
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_chemical_absolute_configuration ?

_refine_ls_abs_structure_Flack ?
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_refine_ls_wR_factor_gt 0.1932
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_refine_ls_shift/su_mean 0.000

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N12 N Uani 0.2261(3) 0.4983(2) 0.14384(10) 1.000 0.0344(11) . .
N13 N Uani 0.4682(4) 0.4548(3) 0.09152(14) 1.000 0.0547(16) . .
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C12 C Uani 0.3960(4) 0.7653(3) 0.13530(14) 1.000 0.0496(18) . .
C13 C Uani 0.4623(5) 0.8358(3) 0.13828(15) 1.000 0.060(2) . .
C14 C Uani 0.5311(5) 0.8446(3) 0.16765(15) 1.000 0.0571(19) . .
C15 C Uani 0.5361(4) 0.7834(3) 0.19477(14) 1.000 0.0501(17) . .
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C17 C Uani 0.3201(6) 0.7559(4) 0.10285(17) 1.000 0.073(3) . .
C18 C Uani 0.3616(10) 0.7865(6) 0.0670(2) 1.000 0.143(5) . .
C19 C Uani 0.2152(7) 0.7991(5) 0.1115(3) 1.000 0.111(4) . .
C110 C Uani 0.4784(4) 0.6433(3) 0.22219(13) 1.000 0.0483(17) . .
C111 C Uani 0.5238(7) 0.6708(5) 0.25850(17) 1.000 0.091(3) . .
C112 C Uani 0.5383(7) 0.5646(4) 0.20872(19) 1.000 0.086(3) . .
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C118 C Uani 0.2009(3) 0.3451(3) 0.14263(12) 1.000 0.0351(12) . .
C119 C Uani 0.1582(4) 0.2737(3) 0.12492(13) 1.000 0.0378(16) . .
C120 C Uani 0.0920(3) 0.2826(3) 0.09481(13) 1.000 0.0370(14) . .
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C145 C Uani 0.7777(9) 0.7570(7) 0.1238(3) 1.000 0.132(4) . .
C146 C Uani 0.8012(9) 0.6286(7) 0.1492(5) 1.000 0.186(8) . .


H13 H Uiso 0.45974 0.87819 0.11974 1.000 0.0714 . .
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H17 H Uiso 0.30573 0.69368 0.09998 1.000 0.0878 . .
H18 H Uiso 0.36194 0.84881 0.06655 1.000 0.2147 . .
H18' H Uiso 0.31729 0.76518 0.04667 1.000 0.2147 . .
H18" H Uiso 0.43257 0.76537 0.06440 1.000 0.2147 . .
H19 H Uiso 0.19065 0.77739 0.13478 1.000 0.1665 . .
H19' H Uiso 0.16376 0.78632 0.09191 1.000 0.1665 . .
H19" H Uiso 0.22516 0.86073 0.11322 1.000 0.1665 . .
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H112" H Uiso 0.53209 0.51817 0.22640 1.000 0.1289 . .
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H136 H Uiso 0.40529 0.25342 0.01236 1.000 0.0873 . .
H137 H Uiso 0.32558 0.34213 -0.03137 1.000 0.1096 . .
H138 H Uiso 0.31080 0.48786 -0.02124 1.000 0.1123 . .
H139 H Uiso 0.37833 0.54867 0.03389 1.000 0.0936 . .
H142 H Uiso 0.66255 0.52677 0.09361 1.000 0.0975 . .
H142' H Uiso 0.62590 0.52362 0.13497 1.000 0.0975 . .
H143 H Uiso 0.61025 0.67809 0.09419 1.000 0.0936 . .
H143' H Uiso 0.60651 0.66852 0.13758 1.000 0.0936 . .
H144 H Uiso 0.78430 0.64660 0.09628 1.000 0.1125 . .
H145 H Uiso 0.75150 0.78966 0.10265 1.000 0.1975 . .
H145' H Uiso 0.85334 0.76287 0.12615 1.000 0.1975 . .
H145" H Uiso 0.74628 0.77854 0.14604 1.000 0.1975 . .
H146 H Uiso 0.86860 0.65612 0.15393 1.000 0.2777 . .
H146' H Uiso 0.81190 0.56814 0.14403 1.000 0.2777 . .
H146" H Uiso 0.75849 0.63461 0.17067 1.000 0.2777 . .


F21 F Uani 1.2685(3) 0.14707(19) 0.05652(9) 1.000 0.0584(11) . .
F22 F Uani 1.2317(3) 0.0195(2) 0.03943(9) 1.000 0.0680(12) . .
F23 F Uani 1.3700(3) 0.0450(3) 0.07142(11) 1.000 0.0771(15) . .
F24 F Uani 1.2758(3) -0.0760(2) 0.20490(9) 1.000 0.0761(13) . .
F25 F Uani 1.2121(3) 0.0333(3) 0.22919(10) 1.000 0.0993(18) . .
F26 F Uani 1.3559(3) 0.0384(3) 0.20331(14) 1.000 0.119(2) . .
F27 F Uani 0.9579(3) -0.2315(3) 0.20573(13) 1.000 0.0971(17) . .
F28 F Uani 0.9620(9) -0.1662(4) 0.2543(2) 1.000 0.254(5) . .
F29 F Uani 0.8351(5) -0.2350(3) 0.2394(2) 1.000 0.159(3) . .
F210 F Uani 0.6727(4) 0.0884(4) 0.25690(18) 1.000 0.144(3) . .
F211 F Uani 0.5772(3) -0.0088(3) 0.24113(12) 1.000 0.0930(17) . .
F212 F Uani 0.5910(4) 0.0957(4) 0.20665(16) 1.000 0.164(3) . .
F213 F Uani 0.9590(3) 0.3516(2) 0.18538(9) 1.000 0.0597(11) . .
F214 F Uani 0.8081(3) 0.3153(3) 0.20034(10) 1.000 0.0779(14) . .
F215 F Uani 0.8289(4) 0.4209(2) 0.16444(12) 1.000 0.0994(18) . .
F216 F Uani 0.7123(3) 0.3524(3) 0.04244(9) 1.000 0.0761(14) . .
F217 F Uani 0.7174(4) 0.2259(3) 0.02376(11) 1.000 0.1072(18) . .
F218 F Uani 0.8493(3) 0.3057(3) 0.01985(8) 1.000 0.0687(13) . .
F219 F Uani 0.5830(3) -0.1040(3) 0.01558(14) 1.000 0.112(2) . .
F220 F Uani 0.5555(3) -0.0437(3) 0.06741(11) 1.000 0.0822(18) . .
F221 F Uani 0.6038(3) 0.0245(3) 0.02248(15) 1.000 0.106(2) . .
F2221 F Uani 1.0347(12) -0.2201(11) 0.0427(3) 0.500 0.093(6) . .
F2222 F Uani 0.9923(15) -0.2534(9) 0.0454(6) 0.500 0.131(8) . .
F2231 F Uani 1.0605(7) -0.1549(8) 0.0212(4) 0.500 0.086(4) . .
F2232 F Uani 0.9895(14) -0.1565(8) -0.0057(4) 0.500 0.110(6) . .
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F2241 F Uani 0.9062(9) -0.2621(6) 0.0147(3) 0.500 0.082(4) . .
F2242 F Uani 0.9336(14) -0.2130(17) -0.0069(4) 0.500 0.163(8) . .
C21 C Uani 1.0429(3) 0.0408(2) 0.12980(11) 1.000 0.0273(11) . .
C22 C Uani 1.1028(3) 0.0538(3) 0.09915(12) 1.000 0.0317(12) . .
C23 C Uani 1.2114(4) 0.0524(3) 0.10152(13) 1.000 0.0385(14) . .
C24 C Uani 1.2650(4) 0.0386(3) 0.13437(15) 1.000 0.0428(14) . .
C25 C Uani 1.2071(4) 0.0265(3) 0.16509(13) 1.000 0.0386(14) . .
C26 C Uani 1.0982(3) 0.0282(3) 0.16282(11) 1.000 0.0328(12) . .
C27 C Uani 1.2704(4) 0.0662(3) 0.06723(16) 1.000 0.0505(17) . .
C28 C Uani 1.2610(4) 0.0058(4) 0.20081(16) 1.000 0.0514(17) . .
C29 C Uani 0.8614(3) 0.0035(3) 0.16228(10) 1.000 0.0276(11) . .
C210 C Uani 0.8989(3) -0.0718(3) 0.17832(11) 1.000 0.0334(12) . .
C211 C Uani 0.8568(4) -0.1062(3) 0.20962(12) 1.000 0.0387(14) . .
C212 C Uani 0.7724(4) -0.0685(3) 0.22538(12) 1.000 0.0416(16) . .
C213 C Uani 0.7312(4) 0.0036(3) 0.20935(12) 1.000 0.0389(14) . .
C214 C Uani 0.7754(3) 0.0397(3) 0.17852(11) 1.000 0.0314(12) . .
C215 C Uani 0.9060(6) -0.1830(4) 0.22706(16) 1.000 0.065(2) . .
C216 C Uani 0.6414(5) 0.0442(4) 0.22664(18) 1.000 0.061(2) . .
C217 C Uani 0.8791(3) 0.1396(3) 0.11725(10) 1.000 0.0270(11) . .
C218 C Uani 0.8855(3) 0.2003(3) 0.14537(11) 1.000 0.0304(12) . .
C219 C Uani 0.8544(3) 0.2839(3) 0.14025(12) 1.000 0.0352(12) . .
C220 C Uani 0.8158(3) 0.3122(3) 0.10669(12) 1.000 0.0376(14) . .
C221 C Uani 0.8114(3) 0.2542(3) 0.07819(12) 1.000 0.0353(14) . .
C222 C Uani 0.8417(3) 0.1705(3) 0.08324(11) 1.000 0.0302(11) . .
C223 C Uani 0.8621(4) 0.3434(3) 0.17191(14) 1.000 0.0459(17) . .
C224 C Uani 0.7724(4) 0.2834(3) 0.04101(13) 1.000 0.0471(17) . .
C225 C Uani 0.8737(3) -0.0214(3) 0.09187(10) 1.000 0.0295(11) . .
C226 C Uani 0.7691(3) -0.0181(3) 0.08086(12) 1.000 0.0364(14) . .
C227 C Uani 0.7278(4) -0.0667(3) 0.05230(13) 1.000 0.0428(14) . .
C228 C Uani 0.7899(4) -0.1239(3) 0.03406(13) 1.000 0.0447(16) . .
C229 C Uani 0.8929(4) -0.1298(3) 0.04466(13) 1.000 0.0429(16) . .
C230 C Uani 0.9342(3) -0.0795(3) 0.07300(11) 1.000 0.0338(12) . .
C231 C Uani 0.6175(4) -0.0536(5) 0.04010(18) 1.000 0.064(2) . .
C232 C Uani 0.9628(5) -0.1886(4) 0.02465(17) 1.000 0.061(2) . .
B2 B Uani 0.9153(4) 0.0406(3) 0.12530(11) 1.000 0.0258(11) . .


H22 H Uiso 1.06893 0.06397 0.07609 1.000 0.0381 . .
H24 H Uiso 1.33869 0.03746 0.13579 1.000 0.0516 . .
H26 H Uiso 1.06081 0.02063 0.18453 1.000 0.0393 . .
H210 H Uiso 0.95507 -0.10037 0.16749 1.000 0.0399 . .
H212 H Uiso 0.74352 -0.09177 0.24674 1.000 0.0498 . .
H214 H Uiso 0.74611 0.09028 0.16838 1.000 0.0379 . .
H218 H Uiso 0.91223 0.18338 0.16879 1.000 0.0365 . .
H220 H Uiso 0.79316 0.36922 0.10330 1.000 0.0447 . .
H222 H Uiso 0.83721 0.13267 0.06300 1.000 0.0361 . .
H226 H Uiso 0.72432 0.01902 0.09345 1.000 0.0433 . .
H228 H Uiso 0.76183 -0.15800 0.01472 1.000 0.0538 . .
H230 H Uiso 1.00575 -0.08490 0.07971 1.000 0.0406 . .


loop_
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_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
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_atom_site_aniso_U_12
Pd1 0.0362(2) 0.0279(2) 0.0487(2) -0.0073(2) -0.0016(1) -0.0070(1)
N11 0.042(2) 0.0229(18) 0.0380(19) -0.0005(14) -0.0122(16) -0.0019(15)
```

N12 0.0312(19) 0.0266(18) 0.045(2) -0.0003(15) -0.0032(16) -0.0029(15)
N13 0.048(3) 0.039(2) 0.078(3) -0.014(2) 0.017(2) -0.013(2)
C11 0.049(3) 0.023(2) 0.039(2) -0.0021(17) -0.012(2) -0.0043(19)
C12 0.069(4) 0.030(2) 0.048(3) 0.007(2) -0.023(2) -0.010(2)
C13 0.094(5) 0.034(3) 0.049(3) 0.015(2) -0.021(3) -0.021(3)
C14 0.077(4) 0.038(3) 0.055(3) 0.003(2) -0.016(3) -0.025(3)
C15 0.060(3) 0.043(3) 0.046(3) -0.004(2) -0.018(2) -0.016(2)
C16 0.046(3) 0.033(2) 0.033(2) -0.0028(18) -0.0108(19) -0.004(2)
C17 0.113(6) 0.037(3) 0.065(4) 0.016(3) -0.058(4) -0.019(3)
C18 0.246(13) 0.119(7) 0.058(4) 0.037(5) -0.079(6) -0.081(8)
C19 0.109(7) 0.068(5) 0.149(8) 0.014(5) -0.088(6) 0.004(4)
C110 0.062(3) 0.043(3) 0.039(3) 0.006(2) -0.013(2) -0.009(2)
C111 0.143(8) 0.081(5) 0.047(4) 0.007(3) -0.019(4) -0.008(5)
C112 0.129(7) 0.065(4) 0.062(4) 0.015(3) -0.015(4) 0.024(4)
C113 0.039(3) 0.031(2) 0.054(3) -0.007(2) -0.005(2) 0.004(2)
C114 0.048(3) 0.038(3) 0.094(4) -0.027(3) 0.001(3) 0.001(2)
C115 0.043(3) 0.028(2) 0.054(3) -0.005(2) -0.002(2) 0.0023(19)
C116 0.045(3) 0.044(3) 0.086(4) -0.022(3) 0.015(3) -0.004(2)
C117 0.028(2) 0.027(2) 0.043(2) -0.0050(17) 0.0015(17) -0.0022(17)
C118 0.036(2) 0.030(2) 0.039(2) -0.0012(18) -0.0029(18) -0.0039(18)
C119 0.041(3) 0.024(2) 0.048(3) 0.0007(18) -0.006(2) -0.0026(19)
C120 0.035(2) 0.029(2) 0.047(3) -0.0065(19) 0.0001(19) -0.0080(18)
C121 0.039(3) 0.042(3) 0.038(2) 0.001(2) -0.0048(19) -0.003(2)
C122 0.043(3) 0.031(2) 0.048(3) 0.003(2) -0.004(2) -0.003(2)
C123 0.056(3) 0.032(2) 0.045(3) -0.001(2) -0.013(2) -0.007(2)
C124 0.089(5) 0.081(5) 0.042(3) -0.013(3) -0.009(3) 0.030(4)
C125 0.055(3) 0.046(3) 0.049(3) 0.003(2) -0.012(2) 0.001(2)
C126 0.062(4) 0.043(3) 0.070(4) 0.013(3) -0.024(3) -0.008(3)
C127 0.068(5) 0.056(4) 0.170(9) 0.030(5) -0.037(5) 0.005(3)
C128 0.079(5) 0.070(4) 0.095(5) 0.030(4) -0.018(4) -0.007(4)
C129 0.032(3) 0.049(3) 0.077(4) -0.015(3) 0.008(2) -0.012(2)
C130 0.037(3) 0.050(3) 0.088(4) -0.019(3) 0.005(3) -0.006(2)
C131 0.032(3) 0.075(4) 0.084(4) -0.008(3) -0.002(3) -0.002(3)
C132 0.039(3) 0.056(4) 0.097(5) -0.013(3) 0.010(3) 0.005(3)
C133 0.043(3) 0.048(3) 0.078(4) -0.018(3) 0.015(3) -0.009(2)
C134 0.039(3) 0.043(3) 0.077(4) -0.014(3) 0.019(3) -0.012(2)
C135 0.065(4) 0.047(3) 0.070(4) -0.012(3) 0.025(3) -0.008(3)
C136 0.101(5) 0.063(4) 0.055(4) -0.018(3) 0.015(3) -0.012(4)
C137 0.136(7) 0.076(5) 0.063(4) -0.016(4) 0.005(4) -0.015(5)
C138 0.142(8) 0.082(5) 0.057(4) 0.002(4) 0.007(4) 0.007(5)
C139 0.110(6) 0.056(4) 0.069(4) -0.003(3) 0.020(4) -0.008(4)
C140 0.071(4) 0.053(3) 0.054(3) -0.015(3) 0.020(3) -0.012(3)
C141 0.055(4) 0.051(4) 0.110(5) -0.029(3) 0.028(4) -0.022(3)
C142 0.077(5) 0.075(5) 0.093(5) -0.034(4) 0.026(4) -0.028(4)
C143 0.087(5) 0.081(5) 0.067(4) -0.023(3) 0.027(3) -0.051(4)
C144 0.066(5) 0.105(6) 0.111(6) -0.031(5) 0.019(4) -0.002(5)
C145 0.161(9) 0.138(8) 0.096(6) -0.015(6) 0.008(6) -0.114(8)
C146 0.090(8) 0.084(7) 0.38(2) 0.011(10) -0.060(11) -0.016(6)
F2221 0.089(9) 0.113(12) 0.074(7) -0.052(8) -0.046(7) 0.074(9)
F2222 0.135(15) 0.053(7) 0.210(19) 0.002(8) 0.067(14) 0.039(8)
F2231 0.068(6) 0.099(8) 0.093(7) -0.044(6) 0.024(5) 0.022(5)
F2232 0.164(14) 0.086(7) 0.084(8) 0.022(6) 0.084(10) 0.060(8)
F2241 0.089(7) 0.059(5) 0.098(8) -0.050(5) -0.001(6) 0.004(5)
F2242 0.123(13) 0.27(2) 0.090(9) -0.134(13) -0.080(9) 0.143(15)
F21 0.067(2) 0.0462(18) 0.0635(19) 0.0110(14) 0.0243(16) -0.0038(15)
F22 0.082(2) 0.065(2) 0.059(2) -0.0144(16) 0.0327(18) -0.0214(18)
F23 0.0442(18) 0.088(3) 0.101(3) 0.017(2) 0.0308(18) 0.0121(18)
F24 0.118(3) 0.060(2) 0.0491(18) 0.0134(16) -0.0135(19) 0.026(2)
F25 0.103(3) 0.145(4) 0.0470(19) -0.036(2) -0.040(2) 0.071(3)
F26 0.080(3) 0.140(4) 0.133(4) 0.066(3) -0.075(3) -0.044(3)
F27 0.097(3) 0.085(3) 0.111(3) 0.048(3) 0.030(3) 0.050(3)

```
F28 0.449(14) 0.088(4) 0.207(7) 0.007(4) -0.251(9) 0.060(6)
F29 0.171(6) 0.081(3) 0.231(7) 0.099(4) 0.107(5) 0.044(4)
F210 0.100(4) 0.164(5) 0.168(5) -0.115(5) 0.012(4) 0.021(4)
F211 0.078(3) 0.098(3) 0.107(3) 0.009(2) 0.061(2) -0.007(2)
F212 0.117(4) 0.229(7) 0.154(5) 0.133(5) 0.105(4) 0.124(4)
F213 0.0560(19) 0.058(2) 0.065(2) -0.0193(16) 0.0010(15) -0.0129(15)
F214 0.082(2) 0.084(3) 0.070(2) -0.0441(19) 0.0367(19) -0.026(2)
F215 0.149(4) 0.043(2) 0.103(3) -0.030(2) -0.042(3) 0.035(2)
F216 0.074(2) 0.092(3) 0.063(2) 0.0356(19) 0.0107(17) 0.048(2)
F217 0.164(4) 0.080(3) 0.072(2) 0.034(2) -0.077(3) -0.030(3)
F218 0.066(2) 0.103(3) 0.0378(16) 0.0284(17) 0.0128(14) 0.0289(19)
F219 0.053(2) 0.135(4) 0.144(4) -0.087(3) -0.047(2) 0.024(2)
F220 0.0325(17) 0.129(4) 0.085(3) -0.015(2) -0.0005(17) -0.0005(19)
F221 0.068(3) 0.117(4) 0.130(4) 0.015(3) -0.044(3) 0.020(3)
C21 0.031(2) 0.0196(19) 0.031(2) 0.0022(15) -0.0029(16) 0.0004(16)
C22 0.035(2) 0.026(2) 0.034(2) 0.0024(16) 0.0005(17) 0.0011(17)
C23 0.036(2) 0.029(2) 0.051(3) 0.0007(19) 0.008(2) -0.0012(18)
C24 0.029(2) 0.031(2) 0.068(3) 0.000(2) -0.005(2) 0.0000(19)
C25 0.036(2) 0.032(2) 0.047(3) -0.0007(19) -0.0109(19) 0.0019(19)
C26 0.035(2) 0.033(2) 0.030(2) 0.0026(17) -0.0067(17) -0.0013(18)
C27 0.047(3) 0.041(3) 0.065(3) 0.002(2) 0.022(3) -0.002(2)
C28 0.042(3) 0.051(3) 0.060(3) 0.004(3) -0.018(2) 0.006(2)
C29 0.030(2) 0.030(2) 0.0226(18) 0.0002(15) -0.0029(15) -0.0033(16)
C210 0.037(2) 0.031(2) 0.032(2) 0.0041(17) -0.0005(17) -0.0006(18)
C211 0.048(3) 0.036(2) 0.032(2) 0.0080(18) 0.0003(19) -0.007(2)
C212 0.057(3) 0.039(3) 0.029(2) 0.0032(19) 0.005(2) -0.018(2)
C213 0.041(3) 0.040(2) 0.036(2) -0.0067(19) 0.0070(19) -0.012(2)
C214 0.036(2) 0.030(2) 0.028(2) 0.0006(16) -0.0008(17) -0.0035(18)
C215 0.101(5) 0.044(3) 0.051(3) 0.026(3) 0.002(3) 0.003(3)
C216 0.062(4) 0.049(3) 0.073(4) -0.007(3) 0.029(3) -0.009(3)
C217 0.026(2) 0.033(2) 0.0220(18) 0.0024(15) 0.0015(15) -0.0008(16)
C218 0.030(2) 0.033(2) 0.028(2) 0.0013(16) -0.0003(16) -0.0012(17)
C219 0.031(2) 0.033(2) 0.042(2) -0.0025(19) 0.0065(18) -0.0032(18)
C220 0.035(2) 0.031(2) 0.047(3) 0.0064(19) 0.0059(19) 0.0043(18)
C221 0.030(2) 0.040(3) 0.036(2) 0.0129(18) 0.0029(18) 0.0051(18)
C222 0.029(2) 0.036(2) 0.0257(19) 0.0019(16) 0.0020(16) 0.0041(17)
C223 0.044(3) 0.037(3) 0.057(3) -0.015(2) 0.005(2) -0.001(2)
C224 0.050(3) 0.050(3) 0.041(3) 0.017(2) -0.003(2) 0.011(2)
C225 0.033(2) 0.030(2) 0.0253(19) 0.0029(16) -0.0040(16) -0.0017(17)
C226 0.032(2) 0.044(3) 0.033(2) -0.0063(19) -0.0008(17) 0.0025(19)
C227 0.034(2) 0.052(3) 0.042(2) -0.012(2) -0.004(2) 0.000(2)
C228 0.047(3) 0.047(3) 0.039(2) -0.017(2) -0.013(2) 0.002(2)
C229 0.046(3) 0.041(3) 0.041(2) -0.009(2) -0.009(2) 0.009(2)
C230 0.032(2) 0.036(2) 0.033(2) -0.0033(18) -0.0062(17) 0.0053(18)
C231 0.035(3) 0.087(5) 0.070(4) -0.031(3) -0.010(3) 0.008(3)
C232 0.061(4) 0.061(4) 0.059(4) -0.025(3) -0.017(3) 0.023(3)
B2 0.027(2) 0.030(2) 0.0202(19) 0.0016(16) -0.0028(16) -0.0001(18)

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

# 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_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Pd1 N11 2.085(3) . . yes
 Pd1 N12 2.143(4) . . yes
 Pd1 N13 2.104(5) . . yes
 Pd1 C141 2.015(7) . . yes
 F2221 F2231 1.34(2) . . yes
 F2221 C232 1.224(16) . . yes
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 F2222 C232 1.319(19) . . yes
 F2222 F2241 1.56(2) . . yes
 F2231 C232 1.376(12) . . yes
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 F2232 C232 1.277(16) . . yes
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 F2241 C232 1.408(12) . . yes
 F2242 C232 1.261(17) . . yes
 F21 C27 1.331(6) . . yes
 F22 C27 1.337(6) . . yes
 F23 C27 1.330(6) . . yes
 F24 C28 1.308(7) . . yes
 F25 C28 1.306(7) . . yes
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 F27 C215 1.293(8) . . yes
 F28 C215 1.239(11) . . yes
 F29 C215 1.317(9) . . yes
 F210 C216 1.357(9) . . yes
 F211 C216 1.300(8) . . yes
 F212 C216 1.257(9) . . yes
 F213 C223 1.333(6) . . yes
 F214 C223 1.345(6) . . yes
 F215 C223 1.317(6) . . yes
 F216 C224 1.335(7) . . yes
 F217 C224 1.299(7) . . yes
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 F219 C231 1.266(9) . . yes
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 N11 C11 1.452(6) . . yes
 N11 C113 1.279(6) . . yes
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 N13 C129 1.453(7) . . yes
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C116 H116' 0.9794 . . no
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C120 H120 0.9500 . . no
C121 H121 0.9497 . . no
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C124 H124" 0.9801 . . no
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C217 B2 1.649(7) . . yes
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C220 C221 1.385(6) . . no
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 C229 C230 1.395(6) . . no
 C229 C232 1.499(8) . . no
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 C214 H214 0.9504 . . no
 C218 H218 0.9502 . . no
 C220 H220 0.9498 . . no
 C222 H222 0.9499 . . no
 C226 H226 0.9507 . . no
 C228 H228 0.9493 . . no
 C230 H230 0.9497 . . no

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 F2222 F2241 F2242 101.8(13) . . . yes
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 C11 N11 C113 120.8(4) . . . yes
 Pd1 N11 C113 118.4(3) . . . yes
 C115 N12 C117 123.2(4) . . . yes
 Pd1 N12 C115 116.4(3) . . . yes
 Pd1 N12 C117 120.4(3) . . . yes
 Pd1 N13 C129 116.4(4) . . . yes
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C129 N13 C141 127.0(5) . . . yes
C140 N13 C141 118.3(5) . . . yes
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N11 C11 C12 116.5(4) . . . yes
C12 C11 C16 123.8(5) . . . no
C11 C12 C13 117.1(5) . . . no
C11 C12 C17 122.1(5) . . . no
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C12 C17 C19 109.8(6) . . . no
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C12 C17 H17 106.80 . . . no
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C17 C18 H18 109.56 . . . no
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H18 C18 H18" 109.42 . . . no
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C17 C18 H18' 109.55 . . . no
C17 C18 H18" 109.56 . . . no
H18 C18 H18' 109.38 . . . no
C17 C19 H19" 109.42 . . . no
C17 C19 H19' 109.42 . . . no
H19 C19 H19' 109.48 . . . no
H19 C19 H19" 109.54 . . . no
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H19' C19 H19" 109.50 . . . no
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C119 C120 C121 120.5(4) . . . no
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C121 C122 C126 120.7(4) . . . no
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C122 C126 C128 109.8(5) . . . no
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C135 C140 C139 123.1(6) . . . no
N13 C140 C135 107.8(5) . . . yes
N13 C140 C139 129.2(6) . . . yes
Pd1 C141 C142 130.7(5) . . . yes
Pd1 C141 N13 72.8(3) . . . yes
N13 C141 C142 122.4(6) . . . yes
C141 C142 C143 112.3(6) . . . no
C142 C143 C144 115.4(7) . . . no
C143 C144 C146 113.3(9) . . . no
C145 C144 C146 102.7(9) . . . no
C143 C144 C145 116.6(8) . . . no
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C110 C111 H111' 109.47 . . . no
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C120 C119 H119 119.58 . . . no
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C122 C121 H121 119.23 . . . no
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C21 C26 C25 122.3(4) . . . no
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C128 C126 H126 107.86 . . . no
C122 C126 H126 107.78 . . . no
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C126 C127 H127' 109.52 . . . no
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H128' C128 H128 109.41 . . . no
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C126 C128 H128' 109.46 . . . no
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C212 C213 C216 118.0(4) . . . no
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F27 C215 F28 108.2(7) . . . yes
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F217 C224 F218 107.9(4) . . . yes
F218 C224 C221 112.0(4) . . . yes
C226 C225 C230 115.6(4) . . . no
C226 C225 B2 118.8(4) . . . yes
C230 C225 B2 125.7(4) . . . yes
C225 C226 C227 122.7(4) . . . no
C228 C227 C231 120.3(5) . . . no
C226 C227 C231 119.2(5) . . . no
C226 C227 C228 120.4(5) . . . no
C227 C228 C229 118.4(4) . . . no
C228 C229 C232 119.7(5) . . . no
C228 C229 C230 120.8(4) . . . no
C230 C229 C232 119.5(5) . . . no
C225 C230 C229 122.2(4) . . . no
F219 C231 F221 100.8(5) . . . yes
F219 C231 F220 114.0(5) . . . yes
F219 C231 C227 115.7(5) . . . yes
F220 C231 F221 100.2(5) . . . yes
F220 C231 C227 112.9(5) . . . yes
F221 C231 C227 111.4(5) . . . yes
F2221 C232 F2241 100.5(10) . . . yes
F2221 C232 F2242 124.5(13) . . . yes
F2221 C232 F2232 114.0(11) . . . yes
F2222 C232 F2242 111.3(15) . . . yes
F2222 C232 C229 111.2(10) . . . yes
F2231 C232 F2232 59.6(10) . . . yes
F2221 C232 C229 116.3(8) . . . yes
F2222 C232 F2231 96.0(11) . . . yes
F2222 C232 F2232 136.4(12) . . . yes
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 C211 C210 H210 118.86 . . . no
 C211 C212 H212 120.90 . . . no
 C213 C212 H212 120.80 . . . no
 C213 C214 H214 119.11 . . . no
 C29 C214 H214 119.06 . . . no
 C217 C218 H218 118.71 . . . no
 C219 C218 H218 118.81 . . . no
 C219 C220 H220 121.30 . . . no
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 C221 C222 H222 118.85 . . . no
 C217 C222 H222 118.89 . . . no
 C225 C226 H226 118.66 . . . no
 C227 C226 H226 118.68 . . . no
 C227 C228 H228 120.82 . . . no
 C229 C228 H228 120.81 . . . no
 C229 C230 H230 118.93 . . . no
 C225 C230 H230 118.91 . . . no
 C21 B2 C217 106.9(3) . . . yes
 C21 B2 C225 112.1(3) . . . yes
 C29 B2 C225 105.4(3) . . . yes
 C217 B2 C225 110.2(3) . . . yes
 C29 B2 C217 110.9(3) . . . yes
 C21 B2 C29 111.5(3) . . . yes

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_geom_torsion_atom_site_label_4
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_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
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 N12 Pd1 N11 C113 4.9(3) . . . . no
 N13 Pd1 N11 C11 5.4(7) . . . . no
 N13 Pd1 N11 C113 -174.2(5) . . . . no
 C141 Pd1 N11 C11 -2.1(4) . . . . no
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 N11 Pd1 N12 C115 -3.3(3) . . . . no
 N11 Pd1 N12 C117 173.0(3) . . . . no
 N13 Pd1 N12 C115 176.3(3) . . . . no
 N13 Pd1 N12 C117 -7.4(4) . . . . no
 N11 Pd1 N13 C129 111.0(5) . . . . no
 N11 Pd1 N13 C140 -120.7(5) . . . . no
 N11 Pd1 N13 C141 -10.0(7) . . . . no
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C141 Pd1 N13 C140 -110.7(6) . . . . no
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N11 Pd1 C141 C142 57.8(7) . . . . no
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F2231 F2221 F2222 C232 -18(3) . . . . no
C232 F2221 F2222 F2241 27.2(17) . . . . no
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C232 F2221 F2231 F2232 -26.8(11) . . . . no
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F2231 F2221 C232 F2241 141.0(10) . . . . no
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F2241 F2222 C232 F2242 -31.0(12) . . . . no
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F2232 F2231 C232 C229 -102.6(9) . . . . no
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F2232 F2231 C232 F2242 27.4(15) . . . . no
F2221 F2231 C232 C229 109.0(9) . . . . no
F2232 F2231 C232 F2221 148.4(12) . . . . no
F2221 F2231 F2232 F2242 -8(2) . . . . no
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F2221 F2231 C232 F2232 -148.4(12) . . . . no
C232 F2231 F2232 F2242 -33.4(16) . . . . no
F2231 F2232 C232 F2221 -30.4(12) . . . . no
F2242 F2232 C232 F2221 116.3(17) . . . . no
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F2242 F2232 C232 F2231 146.7(16) . . . . no
F2231 F2232 C232 F2241 -139.3(9) . . . . no
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F2242 F2241 C232 F2222 -142.2(16) . . . . no
F2222 F2241 C232 F2231 74.6(16) . . . . no
F2242 F2241 C232 F2231 -67.6(18) . . . . no
F2222 F2241 C232 F2232 134.6(13) . . . . no
F2222 F2241 C232 C229 -106.4(11) . . . . no
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F2241 F2242 C232 F2232 170.9(18) . . . . no
F2232 F2242 C232 F2221 -96.1(18) . . . . no
F2232 F2242 C232 C229 97.0(12) . . . . no
F2232 F2242 C232 F2241 -170.9(18) . . . . no
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C113 N11 C11 C12 -99.2(5) . . . . no
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Pd1 N11 C113 C114 176.6(4) . . . . no
Pd1 N11 C113 C115 -5.6(6) . . . . no
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C117 N12 C115 C116 3.8(8) . . . . no
Pd1 N13 C129 C130 -46.1(7) . . . . no
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Pd1 N13 C140 C135 -131.9(4) . . . . no
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C129 N13 C141 Pd1 -106.0(6) . . . . no
C129 N13 C141 C142 21.8(10) . . . . no
C140 N13 C129 C134 -1.2(6) . . . . no
C140 N13 C141 C142 -122.5(7) . . . . no
N11 C11 C12 C17 1.7(7) . . . . no
N11 C11 C16 C15 178.6(4) . . . . no
C16 C11 C12 C13 -0.4(8) . . . . no

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C11 C12 C17 C19 90.4(7) . . . . no
C13 C12 C17 C18 36.9(8) . . . . no
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C11 C12 C17 C18 -142.9(6) . . . . no
C11 C12 C13 C14 -0.2(8) . . . . no
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C11 C16 C110 C111 -158.2(5) . . . . no
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H110 C110 C112 H112' 64.66 . . . . no
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C16 C110 C112 H112" -171.75 . . . . no
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C111 C110 C112 H112' -179.76 . . . . no
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C16 C110 C111 H111 -63.55 . . . . no
C112 C110 C111 H111' -58.05 . . . . no
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C117 C118 C119 H119 -178.49 . . . . no
C119 C118 C123 H123 139.19 . . . . no
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H119 C119 C120 C121 179.09 . . . . no
H120 C120 C121 C122 179.23 . . . . no
C119 C120 C121 H121 179.15 . . . . no
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C26 C21 C22 C23 1.3(6) . . . . no
B2 C21 C22 C23 -178.4(4) . . . . no

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C26 C21 B2 C29 -12.3(5) . . . . no
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C26 C21 B2 C225 -130.2(4) . . . . no
H121 C121 C122 C126 1.94 . . . . no
H121 C121 C122 C117 -178.23 . . . . no
C22 C21 B2 C29 167.3(4) . . . . no
C22 C21 C26 C25 -1.5(6) . . . . no
B2 C21 C26 C25 178.1(4) . . . . no
C22 C21 B2 C217 -71.3(4) . . . . no
C22 C21 B2 C225 49.5(5) . . . . no
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C121 C122 C126 H126 148.51 . . . . no
C21 C22 C23 C24 -0.4(7) . . . . no
C21 C22 C23 C27 179.5(4) . . . . no
H123 C123 C125 H125 174.10 . . . . no
C27 C23 C24 C25 179.8(4) . . . . no
C22 C23 C27 F22 -46.5(6) . . . . no
C118 C123 C124 H124' -175.91 . . . . no
C22 C23 C27 F21 74.1(6) . . . . no
H123 C123 C125 H125' 54.13 . . . . no
H123 C123 C125 H125" -65.95 . . . . no
C22 C23 C24 C25 -0.3(7) . . . . no
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C118 C123 C125 H125" 52.67 . . . . no
C118 C123 C124 H124" 64.16 . . . . no
C22 C23 C27 F23 -166.1(4) . . . . no
C24 C23 C27 F21 -106.0(5) . . . . no
C24 C23 C27 F22 133.4(5) . . . . no
C24 C23 C27 F23 13.8(6) . . . . no
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H123 C123 C124 H124' -58.88 . . . . no
C118 C123 C125 H125 -67.27 . . . . no
C124 C123 C125 H125' -62.01 . . . . no
C124 C123 C125 H125" 177.91 . . . . no
C124 C123 C125 H125 57.96 . . . . no
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C118 C123 C124 H124 -55.86 . . . . no
H123 C123 C124 H124" -178.81 . . . . no
C125 C123 C124 H124' 57.28 . . . . no
C23 C24 C25 C28 176.1(5) . . . . no
C23 C24 C25 C26 0.0(7) . . . . no
C26 C25 C28 F25 -33.8(7) . . . . no
C26 C25 C28 F26 -154.7(5) . . . . no
C24 C25 C28 F25 150.1(5) . . . . no
C24 C25 C28 F24 -87.3(6) . . . . no
C24 C25 C26 C21 0.9(7) . . . . no
C24 C25 C28 F26 29.2(7) . . . . no
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C28 C25 C26 C21 -175.1(4) . . . . no
C122 C126 C127 H127 163.89 . . . . no
C127 C126 C128 H128" -59.03 . . . . no
C127 C126 C128 H128 -179.04 . . . . no
H126 C126 C128 H128' -56.83 . . . . no
C122 C126 C127 H127" -76.15 . . . . no
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C128 C126 C127 H127' 167.31 . . . . no
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H126 C126 C127 H127' -74.82 . . . . no
H126 C126 C127 H127" 165.07 . . . . no
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C127 C126 C128 H128' 61.06 . . . . no
H126 C126 C128 H128 63.08 . . . . no
H126 C126 C128 H128" -176.92 . . . . no
B2 C29 C214 C213 178.0(4) . . . . no
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C214 C29 B2 C225 -102.0(5) . . . . no
C214 C29 B2 C21 136.2(4) . . . . no
C214 C29 B2 C217 17.2(6) . . . . no
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C210 C29 B2 C225 74.6(5) . . . . no
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H133 C133 C134 C129 -179.35 . . . . no
H133 C133 C134 C135 -1.03 . . . . no
C134 C135 C136 H136 -1.71 . . . . no
C140 C135 C136 H136 -179.23 . . . . no
C135 C136 C137 H137 -179.49 . . . . no
H136 C136 C137 H137 0.53 . . . . no
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H142' C142 C143 C144 74.59 . . . . no
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H142' C142 C143 H143' -47.18 . . . . no
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H143 C143 C144 C146 178.11 . . . . no

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C146 C144 C145 H145' 54.49 . . . . no
C145 C144 C146 H146' -157.82 . . . . no
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C146 H146' F215 0.9800 2.4400 3.331(12) 151.00 . yes
C116 H116 F213 0.9800 2.4700 3.386(6) 155.00 1_455 yes
C212 H212 F214 0.9500 2.5300 3.462(6) 166.00 2_645 yes

#===END of Crystallographic Information File
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