

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: jod1062s

Bond precision: C-C = 0.0028 Å

Wavelength=0.71073

Cell: a=9.1519(6) b=12.3000(8) c=13.0848(9)
 alpha=86.445(2) beta=71.574(2) gamma=73.180(2)
Temperature: 100 K

	Calculated	Reported
Volume	1336.93(16)	1336.93(15)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C29 H33 Br N2 O2 Pd	?
Sum formula	C29 H33 Br N2 O2 Pd	C29 H33 Br N2 O2 Pd
Mr	627.87	627.88
Dx,g cm-3	1.560	1.560
Z	2	2
Mu (mm-1)	2.217	2.217
F000	636.0	636.0
F000'	633.63	
h,k,lmax	12,16,17	12,16,17
Nref	6963	6304
Tmin,Tmax	0.715,0.856	0.715,0.860
Tmin'	0.544	

Correction method= MULTI-SCAN

Data completeness= 0.905

Theta(max)= 28.760

R(reflections)= 0.0228(5906)

wR2(reflections)= 0.0557(6304)

S = 1.051

Npar= 329

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Pd1	--	Br1	..	10.96	su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Pd1	--	C13	..	10.58	su

Alert level C

PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Pd1	--	N1	..	5.63	su
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PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Pd1 -- C8 .. 5.25 su
PLAT420_ALERT_2_C D-H Without Acceptor N1 - H01B ... ?

● **Alert level G**

HYDTR01_ALERT_1_G Extra text has been found in the _refine_ls_hydrogen_treatment fi
Explanatory text should be in the _publ_section_refinement field.
Hydrogen treatment given as NH2 free with SADI, rigid methyls, other
Hydrogen treatment identified as riding
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 1
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal (x 10000) 200 Deg.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2

0 **ALERT level A** = In general: serious problem
2 **ALERT level B** = Potentially serious problem
3 **ALERT level C** = Check and explain
4 **ALERT level G** = General alerts; check

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/10/2010; check.def file version of 11/10/2010

