

checkCIF/PLATON report (publication check)

No syntax errors found.
Please wait while processing
[report](#)

[CIF dictionary](#)
[Interpreting this](#)

Datablock: bim140p_1a

Bond precision: C-C = 0.0182 Å Wavelength=0.71073
 Cell: a=11.290(5) b=13.493(5) c=17.961(5)
 alpha=69.453(5) beta=75.682(5) gamma=80.616(5)
 Temperature: 100 K

	Calculated	Reported
Volume	2473.7(16)	2473.7(16)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	2(C50 H44 Cl Np O6 P4), C14 Np O2	?
Sum formula	C100 H88 Cl6 Np3 O14 P8	C100 H88 Cl6 Np3 O14 P8
Mr	2685.32	2685.16
Dx, g cm ⁻³	1.803	1.803
Z	1	1
Mu (mm ⁻¹)	3.481	3.481
F000	1301.0	1301.0
F000'	1268.59	
h, k, lmax	13, 16, 21	13, 16, 21
Nref	9072	8931
Tmin, Tmax	0.665, 0.933	0.308, 1.000
Tmin'	0.494	

Correction method= MULTI-SCAN
 Data completeness= 0.984 Theta(max)= 25.350
 R(reflections)= 0.0610(6172) wR2(reflections)= 0.1489(8931)
 S = 1.033 Npar= 592

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 C

[PLAT213 ALERT 2 C](#) Atom C13 has ADP max/min Ratio
 3.40 oblat
[PLAT213 ALERT 2 C](#) Atom C14 has ADP max/min Ratio
 3.20 oblat

[PLAT213 ALERT 2 C](#) Atom C33 has ADP max/min Ratio
3.60 oblat
[PLAT250 ALERT 2 C](#) Large U3/U1 Ratio for Average U(i,j) Tensor
2.18
[PLAT342 ALERT 3 C](#) Low Bond Precision on C-C Bonds (x 1000) Ang ..
18
[PLAT048 ALERT 1 C](#) MoietyFormula Not Given
?
[PLAT153 ALERT 1 C](#) The su's on the Cell Axes are Equal (x 100000)
500 Ang.
[PLAT234 ALERT 4 C](#) Large Hirshfeld Difference C29 -- C30 ..
0.15 Ang.
[PLAT234 ALERT 4 C](#) Large Hirshfeld Difference C34 -- C35 ..
0.16 Ang.
[PLAT234 ALERT 4 C](#) Large Hirshfeld Difference C40 -- C41 ..
0.16 Ang.

●Alert level G

[PLAT083 ALERT 2 G](#) SHELXL Second Parameter in WGHT Unusually Large.
16.79
[PLAT860 ALERT 3 G](#) Note: Number of Least-Squares Restraints
26
[PLAT154 ALERT 1 G](#) The su's on the Cell Angles are Equal (x 10000)
500 Deg.

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

3 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
2 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

checkCIF publication errors

●Alert level A

[PUBL006 ALERT 1 A](#) `_publ_requested_journal` is missing
e.g. 'Acta Crystallographica Section C'
[PUBL008 ALERT 1 A](#) `_publ_section_title` is missing. Title of paper.
[PUBL010 ALERT 1 A](#) `_publ_author_address` is missing. Author(s)
address(es).
[PUBL012 ALERT 1 A](#) `_publ_section_abstract` is missing.
Abstract of paper in English.

●Alert level G

[PUBL013 ALERT 1 G](#) The `_publ_section_comment` (discussion of study) is missing. This is required for a full paper submission (but is optional for an electronic paper).
[PUBL017 ALERT 1 G](#) The `_publ_section_references` section is missing or

empty.

4 **ALERT level A** = Data missing that is essential or data in wrong format

2 **ALERT level G** = General alerts. Data that may be required is missing

checkCIF/PLATON report (publication check)

No syntax errors found.
Please wait while processing
[report](#)

[CIF dictionary](#)
[Interpreting this](#)

Datablock: cas09mha

Bond precision: C-C = 0.0069 Å Wavelength=0.69410
 Cell: a=16.6871(16) b=14.5034(14) c=17.0076(16)
 alpha=90 beta=116.056(1) gamma=90
 Temperature: 100 K

	Calculated	Reported
Volume	3697.8(6)	3697.8(6)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C18 H17 N P), C14 Np O2	?
Sum formula	C36 H34 C14 N2 Np O2 P2	C36 H34 C14 N2 Np O2 P2
Mr	967.44	967.39
Dx, g cm ⁻³	1.738	1.738
Z	4	4
Mu (mm ⁻¹)	0.000	3.220
F000	1884.0	1884.0
F000'	1883.70	
h, k, lmax	22, 19, 22	22, 19, 22
Nref	9231	9201
Tmin, Tmax		0.194, 1.000
Tmin'		

Correction method= MULTI-SCAN
 Data completeness= 0.997 Theta(max)= 27.610
 R(reflections)= 0.0386(7916) wR2(reflections)= 0.1005(9201)
 S = 1.035 Npar= 436

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 C

[PLAT048 ALERT 1 C](#) MoietyFormula Not Given
 ?
[PLAT480 ALERT 4 C](#) Long H...A H-Bond Reported H1N .. CL2 ..
 2.89 Ang.

PLAT731 ALERT 1 C	Bond	Calc	0.86(4),	Rep	0.859(19)
2.11 su-Ra						
	N1	-H1N	1.555	1.555		
PLAT731 ALERT 1 C	Bond	Calc	0.86(4),	Rep	0.853(19)
2.11 su-Ra						
	N1	-H2N	1.555	1.555		
PLAT731 ALERT 1 C	Bond	Calc	0.85(4),	Rep	0.849(19)
2.11 su-Ra						
	N2	-H4N	1.555	1.555		
PLAT735 ALERT 1 C	D-H	Calc	0.86(4),	Rep	0.859(19)
2.11 su-Ra						
	N1	-H1N	1.555	1.555		
PLAT735 ALERT 1 C	D-H	Calc	0.86(4),	Rep	0.859(19)
2.11 su-Ra						
	N1	-H1N	1.555	1.555		
PLAT735 ALERT 1 C	D-H	Calc	0.86(4),	Rep	0.853(19)
2.11 su-Ra						
	N1	-H2N	1.555	1.555		
PLAT735 ALERT 1 C	D-H	Calc	0.85(4),	Rep	0.849(19)
2.11 su-Ra						
	N2	-H4N	1.555	1.555		

Alert level G

ABSMU_01 Radiation type not identified. Calculation of
 _exptl_absorpt_correction_mu not performed.

[PLAT860 ALERT 3 G](#) Note: Number of Least-Squares Restraints
 4

[PLAT092 ALERT 4 G](#) Check: Wavelength given is not Cu,Mo or Ag Ka ..
 0.69 Ang.

[PLAT128 ALERT 4 G](#) Non-standard setting of Space-group P21/c
 P21/n

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

0 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

3 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

[PUBL006 ALERT 1 A](#) _publ_requested_journal is missing
 e.g. 'Acta Crystallographica Section C'

[PUBL008 ALERT 1 A](#) _publ_section_title is missing. Title of paper.

[PUBL010 ALERT 1 A](#) _publ_author_address is missing. Author(s)
 address(es).

[PUBL012 ALERT 1 A](#) _publ_section_abstract is missing.
 Abstract of paper in English.

●Alert level G

[PUBL013 ALERT 1 G](#) The `_publ_section_comment` (discussion of study) is missing. This is required for a full paper submission (but is optional for an electronic paper).

[PUBL017 ALERT 1 G](#) The `_publ_section_references` section is missing or empty.

4 **ALERT level A** = Data missing that is essential or data in wrong format

2 **ALERT level G** = General alerts. Data that may be required is missing