

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision:	C-C = 0.0091 Å	Wavelength=0.71073	
Cell:	a=29.2509(11)	b=17.6371(6)	c=24.6865(9)
	alpha=90	beta=111.982(1)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	11809.9(7)	11809.9(7)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	Ag8 I12, 2(C36 H24 Co N6) [+ solvent]	2(C36 H24 Co N6), Ag8 I12	
Sum formula	C72 H48 Ag8 Co2 I12 N12 [+ solvent]	C72 H48 Ag8 Co2 I12 N12	
Mr	3584.84	3584.84	
Dx, g cm ⁻³	2.016	2.016	
Z	4	4	
Mu (mm ⁻¹)	4.740	4.740	
F000	6520.0	6520.0	
F000'	6473.30		
h, k, lmax	38, 23, 32	38, 23, 32	
Nref	29317	28862	
Tmin, Tmax	0.073, 0.241	0.796, 1.000	
Tmin'	0.047		

Correction method= # Reported T Limits: Tmin=0.796 Tmax=1.000

AbsCorr = MULTII-SCAN

Data completeness= 0.984

Theta(max)= 28.279

R(reflections)= 0.0445(15243)

wR2(reflections)=
0.1187(28862)

S = 0.857

Npar= 955

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

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	Ag1	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	Ag2	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	Ag3	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	Ag4	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	Ag5	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	Ag7	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	I2	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	I3	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	I4	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	I5	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	I6	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	I8	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	I9	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	I11	Check
PLAT342_ALERT_3_C	Low	Bond Precision on C-C Bonds		0.00906	Ang.
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance		6.624	Check
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance		2.173	Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L= 0.600		7	Report



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ		Please Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I1 --Ag2 .	8.8	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I1 --Ag3 .	20.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I2 --Ag1 .	45.8	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I2 --Ag2 .	33.4	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I3 --Ag1 .	86.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I3 --Ag2 .	131.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I3 --Ag3 .	94.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I3 --Ag4 .	62.3	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I4 --Ag1 .	179.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I4 --Ag2 .	121.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I4 --Ag4 .	47.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I4 --Ag5 .	57.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I5 --Ag3 .	84.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I5 --Ag4 .	46.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I5 --Ag6 .	68.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I6 --Ag4 .	64.8	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I6 --Ag5 .	65.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I6 --Ag6 .	106.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I6 --Ag7 .	96.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I7 --Ag5 .	23.4	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I7 --Ag7 .	29.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I8 --Ag5 .	28.8	s.u.

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I9	--Ag7	.	42.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I9	--Ag8	.	35.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I10	--Ag6	.	40.3 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I10	--Ag8	.	30.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I11	--Ag6	.	46.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I11	--Ag7	.	34.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I11	--Ag8	.	57.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I12	--Ag8	.	39.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I12	--Ag3_b	.	27.6 s.u.
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure				! Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1	(II)	.		1.95 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Co2	(II)	.		1.97 Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed				! Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600				448 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...				2 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity				2.6 Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities				Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
43 **ALERT level G** = General information/check it is not something unexpected

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

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
 _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.
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.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
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.

7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
```

```

RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form

```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock I - ellipsoid plot

