

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 = 0.0187 Å	Wavelength=0.71073
Cell:	a=12.402 (8)	b=32.754 (19) c=14.532 (9)
	alpha=90	beta=106.895 (11) gamma=90
Temperature:	296 K	
	Calculated	Reported
Volume	5648 (6)	5648 (6)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C30 H24 Co N6, Ag10 I11, 2(H0.50 O0.50) [+ solvent]	Ag10 I11, C30 H24 Co N6, H O
Sum formula	C30 H25 Ag10 Co I11 N6 O [+ solvent]	C30 H25 Ag10 Co I11 N6 O
Mr	3019.09	3019.09
Dx, g cm ⁻³	3.551	3.550
Z	4	4
Mu (mm ⁻¹)	9.713	9.713
F000	5340.0	5340.0
F000'	5286.50	
h, k, lmax	14, 38, 17	14, 38, 17
Nref	4988	3794
Tmin, Tmax	0.112, 0.379	0.796, 1.000
Tmin'	0.047	

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

AbsCorr = MULTII-SCAN

Data completeness= 0.761

Theta(max)= 24.993

R(reflections)= 0.0758(1726)

wR2(reflections)=
0.2180(3794)

S = 0.936

Npar= 242

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 A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.761 Why?

Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for I2 --I3 . 7.3 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for I3 --I4 . 8.2 s.u.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of I2 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of I3 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of I4 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of I5 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of I6 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Ag1 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Ag2 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Ag3 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Ag4 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Ag5 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Ag6 Check
PLAT245_ALERT_2_B U(iso) H1A Smaller than U(eq) O1 by 0.100 Ang**2
PLAT420_ALERT_2_B D-H Bond Without Acceptor O1 --H1A . Please Check
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.594 1193 Report

Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 45% Check
PLAT234_ALERT_4_C Large Hirshfeld Difference N2 --C10 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N3 --C11 . 0.19 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C14 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of I1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including I1 0.125 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1 0.111 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01871 Ang.
PLAT741_ALERT_1_C Bond Calc 0.000(4), Rep 0.00000 Missing s.u.
AG1 -AG1 1_555 2_755 # 27 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.898 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.02A From O1 0.70 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
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

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.10	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I1 --Ag1 .	17.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I1 --Ag2 .	23.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I2 --Ag1 .	22.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I2 --Ag3 .	27.8	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I2 --Ag4 .	18.4	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I2 --Ag5 .	35.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I3 --Ag1 .	29.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I3 --Ag2 .	37.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I3 --Ag3 .	35.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I3 --Ag5 .	42.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I4 --Ag2 .	34.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I4 --Ag3 .	35.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I4 --Ag5 .	37.3	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I4 --Ag6 .	36.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I5 --Ag3 .	39.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I5 --Ag5 .	45.3	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I5 --Ag6 .	30.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I5 --Ag5_a .	40.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I6 --Ag3 .	34.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I6 --Ag4 .	16.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I6 --Ag5 .	31.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I6 --Ag5_a .	31.2	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT415_ALERT_2_G	Short Inter D-H...H-X H1A ..H8 .	2.12	Ang.
	-x,y,1/2-z =	2_555	Check
PLAT415_ALERT_2_G	Short Inter D-H...H-X H1A ..H9 .	2.10	Ang.
	-x,y,1/2-z =	2_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C9	2.14	Ang.
	-x,y,1/2-z =	2_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C8	2.47	Ang.
	-x,y,1/2-z =	2_555	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	498	A**3
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	0.00	Deg.
	I1 -I1 -I3 2_755 1_555 2_755 #	1	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	0.00	Deg.
	I1 -I1 -AG1 2_755 1_555 1_555 #	2	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	0.00	Deg.
	I1 -I1 -AG1 2_755 1_555 2_755 #	3	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	0.00	Deg.
	I1 -I1 -AG2 2_755 1_555 1_555 #	4	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	0.00	Deg.
	I1 -I1 -AG2 2_755 1_555 2_755 #	5	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	0.00	Deg.
	AG1 -I1 -AG1 1_555 1_555 2_755 #	8	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	0.00	Deg.
	AG1 -I2 -AG1 1_555 1_555 2_755 #	16	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (III) .	3.65	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2	Note
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
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	3	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1300	Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	2.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	0 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
53 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
16 ALERT type 4 Improvement, methodology, query or suggestion
2 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: ...
;
_vrf_PLAT029_I
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.761 Why?
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 1 - ellipsoid plot

