

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 = 0.0375 A Wavelength=0.71073

Cell: a=19.780(1) b=19.780(1) c=20.291(1)
 alpha=90 beta=90 gamma=90
Temperature: 170 K

	Calculated	Reported
Volume	7938.8(9)	7938.8(9)
Space group	I 4 2 2	I 4 2 2
Hall group	I 4 2	I 4 2
Moiety formula	C48 H56 N32 S8 Zn4, 8(C H3)	C56 H80 N32 S8 Zn4
Sum formula	C56 H80 N32 S8 Zn4	C56 H80 N32 S8 Zn4
Mr	1719.56	1719.48
Dx, g cm-3	0.719	0.719
Z	2	2
Mu (mm-1)	0.731	0.731
F000	1776.0	1776.0
F000'	1780.52	
h,k,lmax	25,25,25	25,25,25
Nref	4292[2423]	4242
Tmin,Tmax	0.803,0.803	0.693,0.901
Tmin'	0.803	

Correction method= # Reported T Limits: Tmin=0.693 Tmax=0.901
AbsCorr = NUMERICAL

Data completeness= 1.75/0.99 Theta(max)= 26.873

R(reflections)= 0.1616(1360) wR2(reflections)= 0.4359(4242)

S = 1.145 Npar= 104

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.

[IMAGE] **Alert level A**

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

[IMAGE] **Alert level B**

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 32% Check
PLAT031_ALERT_4_B Refined Extinction Parameter Within Range 2.273 Sigma
PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 0.7194 Check
PLAT082_ALERT_2_B High R1 Value 0.16 Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.44 Report
PLAT234_ALERT_4_B Large Hirshfeld Difference C3 --C10 0.28 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.0375 Ang.
PLAT413_ALERT_2_B Short Inter XH3 .. XHn H1 ..H12B 1.92 Ang.
PLAT930_ALERT_2_B Check Twin Law (1-1 -1) [1-1 -1] Estimated BASF 0.47

[IMAGE] **Alert level C**

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
rot
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.139
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.600
From the CIF: _refine_ls_abs_structure_Flack_su 0.110
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.139 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.01 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 --C2 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2 --N3 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N3 --C4 0.22 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.4 Note
PLAT420_ALERT_2_C D-H Without Acceptor N4 --H4A Please Check
PLAT420_ALERT_2_C D-H Without Acceptor N4 --H4B Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 10.797 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.304 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.330 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.156 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 0.60 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 4 Check

[IMAGE] **Alert level G**

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.600 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report

PLAT300_ALERT_4_G	Atom Site Occupancy of H11A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12F	Constrained at	0.5	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C10	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C3 - C10	.	1.65	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C10 - C11	.	1.60	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C12		3.06	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2 ..C12		2.94	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C3 ..C12		2.27	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C10 ..C12		1.84	Ang.
PLAT722_ALERT_1_G	Angle Calc 140.00, Rep 141.10 Dev...		1.10	Degree
	H12A -C12 -H12D 1.555 1.555 1.555	#	47	Check
PLAT722_ALERT_1_G	Angle Calc 140.00, Rep 141.10 Dev...		1.10	Degree
	H12B -C12 -H12E 1.555 1.555 1.555	#	52	Check
PLAT722_ALERT_1_G	Angle Calc 140.00, Rep 141.10 Dev...		1.10	Degree
	H12C -C12 -H12F 1.555 1.555 1.555	#	58	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.12	Ratio
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C10 --C12		1.84	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		18	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..		!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		20	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
PLAT931_ALERT_5_G	Found Twin Law () [1 -1 -1] Est. BASF		0.48	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		4	Note

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

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

checkCIF publication errors

[IMAGE] Alert level A

PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_sectiontitle is missing. Title of paper.
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

[IMAGE] Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

3 **ALERT level A** = Data missing that is essential or data in wrong format
1 **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_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT602_I
;
PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure      ! Info
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 30/01/2018; check.def file version of 30/01/2018

Datablock I - ellipsoid plot

