

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 = 0.0475 Å Wavelength=0.71073

Cell: a=20.065(2) b=20.065(2) c=19.1367(18)
 alpha=90 beta=90 gamma=90
Temperature: 170 K

	Calculated	Reported
Volume	7704.5(17)	7704.5(17)
Space group	I 4 2 2	I 4 2 2
Hall group	I 4 2	I 4 2
Moiety formula	C48 H64 N32 Ni4 S8, O	C48 H64 N32 Ni4 O S8
Sum formula	C48 H64 N32 Ni4 O S8	C48 H64 N32 Ni4 O S8
Mr	1596.55	1596.63
Dx, g cm ⁻³	0.688	0.688
Z	2	2
Mu (mm ⁻¹)	0.617	0.617
F000	1648.0	1648.0
F000'	1652.94	
h,k,lmax	23,23,22	23,23,22
Nref	3299[1883]	3261
Tmin,Tmax	0.831,0.831	0.441,0.688
Tmin'	0.831	

Correction method= # Reported T Limits: Tmin=0.441 Tmax=0.688
AbsCorr = NUMERICAL

Data completeness= 1.73/0.99 Theta(max)= 24.689

R(reflections)= 0.1743(794) wR2(reflections)= 0.4928(3261)

S = 1.102 Npar= 72

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

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.315
PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 0.315 Report
PLAT026_ALERT_3_A Ratio Observed / Unique Reflections (too) Low .. 24% Check
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) 0.49 Report
PLAT234_ALERT_4_A Large Hirshfeld Difference N3 --C4 0.32 Ang.
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

[IMAGE] Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 0.6882 Check
PLAT082_ALERT_2_B High R1 Value 0.17 Report
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 01 Check
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.0475 Ang.

[IMAGE] Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5877
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.17 Report
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C5 - C6 . 1.34 Ang.
PLAT363_ALERT_2_C Long C(sp3)-C(sp2) Bond C3 - C5 . 1.63 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N4 --H4A Please Check
PLAT420_ALERT_2_C D-H Without Acceptor N4 --H4B Please Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -4.862 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.471 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.386 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 0.70 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.588 14 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

[IMAGE] Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 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 . 0.700 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 4 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 4 Report
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 2 0.13 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 1 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 85 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note

6 **ALERT level A** = Most likely a serious problem - resolve or explain

5 **ALERT level B** = A potentially serious problem, consider carefully

17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

15 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
19 ALERT type 2 Indicator that the structure model may be wrong or deficient
12 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
1 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_section_title 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
```

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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_RINTA01_I
;
PROBLEM: The value of Rint is greater than 0.25
RESPONSE: ...
;
_vrf_PLAT020_I
;
PROBLEM: The Value of Rint is Greater Than 0.12 ..... 0.315 Report
RESPONSE: ...
;
_vrf_PLAT026_I
;
PROBLEM: Ratio Observed / Unique Reflections (too) Low .. 24% Check
RESPONSE: ...
;
_vrf_PLAT084_I
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.49 Report
RESPONSE: ...
;
_vrf_PLAT234_I
;
PROBLEM: Large Hirshfeld Difference N3 --C4 0.32 Ang.
RESPONSE: ...
;
_vrf_PLAT602_I
;
PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
RESPONSE: ...
;
# end Validation Reply Form

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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.

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