

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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 = 0.0023 Å	Wavelength=0.71073
Cell:	a=14.5651(7)	b=22.8720(8) c=10.4529(5)
	alpha=90	beta=124.370(3) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	2874.2(2)	2874.2(2)
Space group	C c	Cc
Hall group	C -2yc	C-2yc
Moiety formula	C30 H27 N5 Si, C4 H8 O	C30 H27 N5 Si, C4 H8 O
Sum formula	C34 H35 N5 O Si	C34 H35 N5 O Si
Mr	557.76	557.76
Dx,g cm-3	1.289	1.289
Z	4	4
Mu (mm-1)	0.119	0.119
F000	1184.0	1184.0
F000'	1184.70	
h,k,lmax	20,32,14	20,32,14
Nref	8388[4202]	7879
Tmin,Tmax	0.940,0.988	0.962,0.995
Tmin'	0.940	

Correction method= # Reported T Limits: Tmin=0.962 Tmax=0.995
AbsCorr = INTEGRATION

Data completeness= 1.88/0.94 Theta(max)= 29.990

R(reflections)= 0.0331(7318) wR2(reflections)= 0.0831(7879)

S = 1.052 Npar= 377

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

PLAT410_ALERT_2_A Short Intra H...H Contact H34B .. H33D .. 1.78 Ang.

Author Response: Only the disorder position of atom C33 of the THF molecule (with site occupancy 0.17) was refined, together with the H atoms H33C and H33D. The close intramolecular contacts to H atoms at the neighboring C atoms C32 and C34 are just simulated. Refinement of alternative H positions at C32 and C34 for the disordered part has been omitted for simplicity.

Alert level B

PLAT410_ALERT_2_B Short Intra H...H Contact H32A .. H33D .. 1.86 Ang.

Author Response: Only the disorder position of atom C33 of the THF molecule (with site occupancy 0.17) was refined, together with the H atoms H33C and H33D. The close intramolecular contacts to H atoms at the neighboring C atoms C32 and C34 are just simulated. Refinement of alternative H positions at C32 and C34 for the disordered part has been omitted for simplicity.

Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.2 Ratio

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF		Please Do !
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High .	0.300	Report
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group Cc	Ic	Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder Percentage =	20	Note
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 and s.u.	0.30	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 4 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
 - 5 ALERT type 4 Improvement, methodology, query or suggestion
 - 1 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.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

7 **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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
```

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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 30/03/2016; check.def file version of 30/03/2016

