

checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: = 0.0000 Å

Wavelength=0.99937

Cell: a=6.58904(8) b=8.60622(11) c=16.2523(2)
 alpha=89.7895(10) beta=89.4785(9) gamma=79.0643(11)
Temperature: 298 K

	Calculated	Reported
Volume	904.84(2)	904.84(2)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	2(C5 H5 Br N), Br4 Cu	2(C5 H5 Br N), Br4 Cu
Sum formula	C10 H10 Br6 Cu N2	C10 H10 Br6 Cu N2
Mr	701.15	701.15
Dx, g cm-3	2.573	2.573
Z	2	2
Mu (mm-1)	7.617	7.618
F000	646.0	646.0
F000'	620.49	
h, k, lmax		
Nref		
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness=

Theta(max)=

R(reflections)=

wR2(reflections)=

S =

Npar=

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

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.

● Alert level G

ABSMU_01 Radiation type not identified. Calculation of
_exptl_absorpt_correction_mu not performed.

PLAT431_ALERT_2_G	Short Inter HL..A Contact	Br2	..	Br13	..	3.42	Ang.
PLAT431_ALERT_2_G	Short Inter HL..A Contact	Br4	..	Br23	..	3.35	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br3	..	C12	..	3.25	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C25	..	C26	..	2.97	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C26	..	C26	..	2.68	Ang.
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Cu1	(I)				1.53	
PLAT981_ALERT_1_G	No non-zero f" Anomalous Scattering Values Found					?	
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value					C	
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value					Br	
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value					Cu	
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value					N	
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value					C	
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value					Br	
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value					Cu	
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value					N	

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

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

59 **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

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

5 ALERT type 2 Indicator that the structure model may be wrong or deficient

2 ALERT type 3 Indicator that the structure quality may be low

57 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

PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
missing. This is required for a full paper submission (but is
optional for an electronic paper).

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
2 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should always 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 the submission requirements of the journal and these should be commented upon in the discussion or experimental section of a paper - after all, they might represent an interesting feature.

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

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# 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_DIFF003_I
;
PROBLEM: _diffrn_measurement_device_type 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 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 16/02/2011; check.def file version of 16/02/2011

Datablock I - ellipsoid plot

