

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: C-C = 0.0078 Å Wavelength=0.40663

Cell: a=25.042(4) b=26.826(4) c=30.848(5)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	20723(6)	20724(6)
Space group	F m m m	Fmmm
Hall group	-F 2 2	?
Moiety formula	C21 H11 Cu2 O12	?
Sum formula	C21 H11 Cu2 O12	C42 H22 Cu4 O24
Mr	582.40	1164.76
Dx,g cm-3	0.747	0.747
Z	16	8
Mu (mm-1)	0.187	0.167
F000	4656.0	4656.0
F000'	4663.17	
h,k,lmax	27,29,34	25,29,33
Nref	4004	3497
Tmin,Tmax		0.906,0.993
Tmin'		

Correction method= MULTI-SCAN

Data completeness= 0.873 Theta(max)= 13.060

R(reflections)= 0.0762(2068) wR2(reflections)= 0.2520(3497)

S = 1.001 Npar= 166

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 Low 0.874

Author Response: Complete dataset could not be collected due to the limited availability of synchrotron beam time.

Alert level B

REFLT03_ALERT_3_B Reflection count < 90% complete (theta max?)
From the CIF: _diffrn_reflms_theta_max 13.06
From the CIF: _diffrn_reflms_theta_full 13.06
From the CIF: _reflms_number_total 3497
TEST2: Reflms within _diffrn_reflms_theta_max
Count of symmetry unique reflms 4004
Completeness (_total/calc) 87.34%

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5557

PLAT022_ALERT_3_B Ratio Unique / Expected Reflections (too) Low .. 0.873
PLAT023_ALERT_3_B Resolution (too) Low [sin(theta)/Lambda < 0.6].. 13.06 Deg.
PLAT049_ALERT_1_B Calculated Density less than 1.0 gcm-3 0.7467
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for 05
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for Cu01
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for Cu02
PLAT430_ALERT_2_B Short Inter D...A Contact 03 .. 05 .. 2.69 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact 03 .. 03 .. 2.70 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact 04 .. 07 .. 2.72 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact 04 .. 04 .. 2.72 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact 05 .. 05 .. 2.68 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact 07 .. 07 .. 2.74 Ang.

Alert level C

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.252

PLAT045_ALERT_1_C Calculated and Reported Z Differ by 2.00 Ratio
PLAT048_ALERT_1_C MoietyFormula Not Given ?
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu02 -- 05 .. 10.0 su
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for 04
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for 08
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C1
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C12
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.2
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0078 Ang

Alert level G

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

REFLT03_ALERT_1_G ALERT: Expected hkl max differ from CIF values
From the CIF: _diffrn_reflms_theta_max 13.06
From the CIF: _reflms_number_total 3497
From the CIF: _diffrn_reflms_limit_max hkl 21. 29. 25.
From the CIF: _diffrn_reflms_limit_min hkl -25. -25. -33.
TEST1: Expected hkl limits for theta max
Calculated maximum hkl 27. 29. 34.
Calculated minimum hkl -27. -29. -34.

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 6
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ?
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.18
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C2 -C7 0.15 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C9 .. C10 .. 2.54 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C9 .. C9 .. 3.03 Ang.

PLAT432_ALERT_2_G	Short Inter X...Y Contact	C10	..	C10	..	1.40	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C10	..	C11	..	2.39	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C10	..	C10	..	2.41	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C10	..	C10	..	2.78	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C11	..	C11	..	2.73	Ang.
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure						!
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				2	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)					1.19	Ratio
PLAT804_ALERT_5_G	ARU-Pack Problem in PLATON Analysis				73	Times
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints				21	
PLAT869_ALERT_4_G	ALERTS Related to the use of SQUEEZE Suppressed						!
PLAT950_ALERT_5_G	Reported and Calculated Hmax Values Differ by	..				2	

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

4 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
 8 ALERT type 3 Indicator that the structure quality may be low
 4 ALERT type 4 Improvement, methodology, query or suggestion
 3 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).

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 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: ...
;
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 18/07/2011; check.def file version of 04/07/2011

Datablock I - ellipsoid plot

