checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0032 A Wavelength=0.71073

Cell: a=9.948(2) b=15.335(3) c=15.460(3)
alpha=90 beta=101.58(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2310.5(8)	2310.5(8)
Space group	P 21/n	P 2(1)/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C52 H40 Cu2 F4 N4 O8, 2(H2 O)	C52 H40 Cu2 F4 N4 O8, 2(H2 O)
Sum formula	C52 H44 Cu2 F4 N4 O10	C52 H44 Cu2 F4 N4 O10
Mr	1088.01	1088.01
Dx,g cm-3	1.564	1.564
Z	2	2
Mu (mm-1)	1.003	1.004
F000	1116.0	1116.0
F000’	1117.85	
h,k,lmax	11,18,18	11,18,18
Nref	4062	4062
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 1.000 Theta(max)= 24.990

R(reflections)= 0.0329(3642) wR2(reflections)= 0.0868(4035)

S = 1.060 Npar= 405

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 C

PLAT213_ALERT_2_C Atom F1 has ADP max/min Ratio ..... 3.2 prola
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.3 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 4.3 Ratio

```
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu1    --  O3      ..        5.1 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu1    --  N2      ..        6.6 su
```

Alert level G

```
  ABSMU_01  Radiation type not identified. Calculation of
            _exptl_absorpt_correction_mu not performed.
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/n
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.         18
PLAT984_ALERT_1_G The Cu-f'=     0.320 Deviates from the B&C-Value      0.328
PLAT985_ALERT_1_G The Cu-f"=     1.265 Deviates from the B&C-Value      1.271
```

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

   2 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 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 19/04/2012; check.def file version of 14/04/2012

Datablock I - ellipsoid plot