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 = 0.0184 A          Wavelength=0.71073

Cell:            a=21.6328(9)     b=21.6328(9)     c=21.6328(9)
                 alpha=90         beta=90          gamma=90
Temperature:     296 K
```

	Calculated	Reported
Volume	10123.7(13)	10123.7(7)
Space group	P 21 3	P2(1)3
Hall group	P 2ac 2ab 3	?
Moiety formula	C72 H60 Cu3 N18, B O40 W12	?
Sum formula	C72 H60 B Cu3 N18 O40 W12	C72 H72 B Cu3 N18 O45 W12
Mr	4224.92	4317.11
Dx,g cm-3	2.772	2.832
Z	4	4
Mu (mm-1)	14.274	14.281
F000	7672.0	7880.0
F000’	7642.84	
h,k,lmax	25,25,25	25,25,25
Nref	3246[5984]	5991
Tmin,Tmax	0.030,0.037	0.113,0.138
Tmin’	0.015	

```
Correction method= MULTI-SCAN

Data completeness= 1.85/1.00      Theta(max)= 25.040

R(reflections)= 0.0415( 4737)     wR2(reflections)= 0.0844( 5991)

S = 0.953                 Npar= 388
```

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 B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 1

Alert level C

```
CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
            calculated from the _atom_site* data lies outside
            the range 0.99 <> 1.01
           From the CIF: _cell_formula_units_Z                  4
           From the CIF: _chemical_formula_weight          4317.11
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01   72.00  864.79
           H         1.01   60.00   60.48
           N        14.01   18.00  252.13
           O        16.00   40.00  639.96
           B        10.81    1.00   10.81
           W       183.85   12.00 2206.20
           Cu       63.55    3.00  190.64
           Calculated formula weight             4225.01
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT043_ALERT_1_C Check Reported Molecular Weight .............    4317.11
PLAT044_ALERT_1_C Calculated and Reported Dx Differ ............          ?
PLAT048_ALERT_1_C MoietyFormula Not Given ......................          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...        ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....        ?
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C4
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C10
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C22
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C24
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O3
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        N4
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C3
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C11
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C17
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C17    -C22         1.36 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds .............     0.0184 Ang
PLAT731_ALERT_1_C Bond    Calc   1.349(16), Rep    1.349(7) ......         2 su-Ra
             C1   -C2      1.555   1.555                  #        43
PLAT731_ALERT_1_C Bond    Calc     1.36(2), Rep    1.359(7) ......         3 su-Ra
             N3   -C8      1.555   1.555                  #        48
PLAT731_ALERT_1_C Bond    Calc     1.36(2), Rep    1.359(7) ......         3 su-Ra
             C5   -C6      1.555   1.555                  #        51
PLAT731_ALERT_1_C Bond    Calc     1.36(2), Rep    1.359(7) ......         3 su-Ra
             C6   -C7      1.555   1.555                  #        53
PLAT731_ALERT_1_C Bond    Calc     1.36(2), Rep    1.359(7) ......         3 su-Ra
             C7   -C8      1.555   1.555                  #        55
PLAT731_ALERT_1_C Bond    Calc   1.341(19), Rep    1.341(8) ......         2 su-Ra
             C9   -C10     1.555   1.555                  #        63
PLAT731_ALERT_1_C Bond    Calc   1.347(18), Rep    1.347(7) ......         3 su-Ra
             N6   -C16     1.555   1.555                  #        68
PLAT731_ALERT_1_C Bond    Calc     1.35(2), Rep    1.347(7) ......         3 su-Ra
             C13  -C14     1.555   1.555                  #        72
PLAT731_ALERT_1_C Bond    Calc   1.348(19), Rep    1.347(7) ......         3 su-Ra
             C14  -C15     1.555   1.555                  #        74
PLAT731_ALERT_1_C Bond    Calc     1.35(2), Rep    1.347(7) ......         3 su-Ra
             C15  -C16     1.555   1.555                  #        76
PLAT731_ALERT_1_C Bond    Calc   1.361(17), Rep    1.360(7) ......         2 su-Ra
             C18  -C19     1.555   1.555                  #        82
PLAT731_ALERT_1_C Bond    Calc   1.361(19), Rep    1.360(7) ......         3 su-Ra
             C21  -C22     1.555   1.555                  #        88
PLAT732_ALERT_1_C Angle   Calc    125.3(9), Rep    125.3(3) ......      3.00 su-Ra
             B1   -O2   -W1      1.555   1.555   1.555      #        68
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C72 H72 B1 Cu3 N18 O45 W12
           Atom count from the _atom_site data:  C72 H60 B1 Cu3 N18 O40 W12
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C72 H72 B Cu3 N18 O45 W12
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        288.00    288.00    0.00
          H        288.00    240.00   48.00
          B          4.00      4.00    0.00
          Cu        12.00     12.00    0.00
          N         72.00     72.00    0.00
          O        180.00    160.00   20.00
          W         48.00     48.00    0.00
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
           _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max           25.04
          From the CIF: _reflns_number_total               5991
          Count of symmetry unique reflns         3246
          Completeness (_total/calc)            184.57%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      2745
          Fraction of Friedel pairs measured     0.846
          Are heavy atom types Z>Si present        yes
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         10
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....         29
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          6 Units
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .        301 A**3
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.16 Ratio
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        254
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
  31 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  12 **ALERT level G** = General information/check it is not something unexpected

  21 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 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
   5 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.
```

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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

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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