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 = 0.0132 A Wavelength=1.54178

Cell: a=29.2846(9) b=29.2846(9) c=9.9941(4)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	8570.8(6)	8570.8(5)
Space group	P 4/n	P4/n
Hall group	-P 4a	?
Moiety formula	4(C30 H14 Cd Cl2 Cu2 O13), 2(C44 H36 Cu N8), 2(O0.50)	?
Sum formula	C208 H128 Cd4 Cl8 Cu10 N16 O53	C104 H64 Cd2 Cl4 Cu5 N8 O26.50
Mr	5068.00	2533.93
Dx,g cm-3	0.982	0.982
Z	1	2
Mu (mm-1)	3.597	3.597
F000	2530.0	2530.0
F000’	2520.41	
h,k,lmax	32,32,11	32,30,10
Nref	6152	5869
Tmin,Tmax	0.682,0.698	0.533,0.715
Tmin’	0.464	

Correction method= MULTI-SCAN

Data completeness= 0.954 Theta(max)= 58.920

R(reflections)= 0.0688(2937) wR2(reflections)= 0.1508(5869)

S = 1.044 Npar= 350

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
THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575

```
           Calculated sin(theta_max)/wavelength =    0.5555
PLAT023_ALERT_3_B Resolution (too) Low [sin(theta)/Lambda < 0.6]..      58.92 Deg.
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low .......      0.954
PLAT049_ALERT_1_B Calculated Density less than 1.0 gcm-3 .........     0.9819
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O010   --  C023_f  ..        9.2 su
```

Alert level C

```
PLAT045_ALERT_1_C Calculated and Reported Z Differ by ............       0.50 Ratio
PLAT048_ALERT_1_C MoietyFormula Not Given ........................          ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....          ?
PLAT220_ALERT_2_C Large Non-Solvent    O     Ueq(max)/Ueq(min) ...        3.4 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu02   --  O007    ..        6.0 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu02   --  O010    ..        9.6 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu02   --  C023_f  ..        6.5 su
PLAT234_ALERT_4_C Large Hirshfeld Difference Cd01   --  Cl4A    ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C024   --  C030    ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C032   --  C033    ..       0.17 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C038
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       Cd01
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       Cu02
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C033
PLAT311_ALERT_2_C Isolated Disordered Oxygen Atom (No H's ?) .....      *O039
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0132 Ang
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C019   -   C026   ...       1.54 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C020   -   C027   ...       1.53 Ang.
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Alert level G

```
REFLT03_ALERT_1_G ALERT: Expected hkl max differ from CIF values
           From the CIF: _diffrn_reflns_theta_max           58.92
           From the CIF: _reflns_number_total               5869
           From the CIF: _diffrn_reflns_limit_ max hkl   32.   29.   10.
           From the CIF: _diffrn_reflns_limit_ min hkl  -32.  -30.   -8.
           TEST1: Expected hkl limits for theta max
           Calculated maximum hkl   32.   32.   11.
           Calculated minimum hkl  -32.  -32.  -11.
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....         39
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................          5 Perc.
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................        100 Perc.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         55
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.16 Ratio
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        482
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
PLAT951_ALERT_5_G Reported and Calculated Kmax Values Differ by ..          2
```

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

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

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  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   9 ALERT type 4 Improvement, methodology, query or suggestion
   3 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).
```

```
   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