checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Au6Cu4_complex_1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Au6Cu4_complex_1

```
Bond precision:  C-C = 0.0300 A          Wavelength=0.71073

Cell:            a=42.304(4)     b=12.4954(12)        c=39.273(3)
                 alpha=90        beta=102.817(2)      gamma=90
Temperature:     150 K
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	Calculated	Reported
Volume	20243(3)	20243(3)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C192 H188 Au6 Cu4 N8 [+ solvent]	?
Sum formula	C192 H188 Au6 Cu4 N8 [+ solvent]	C204 H220 Au6 Cu4 N10
Mr	4043.54	4247.85
Dx,g cm-3	1.327	1.394
Z	4	4
Mu (mm-1)	4.786	4.790
F000	7944.0	8416.0
F000’	7904.89	
h,k,lmax	50,15,47	50,15,47
Nref	18535	18484
Tmin,Tmax	0.568,0.682	0.559,0.745
Tmin’	0.506	

```
Correction method= # Reported T Limits: Tmin=0.559 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 25.350

R(reflections)= 0.0992( 9837)     wR2(reflections)= 0.3082( 18484)

S = 1.068                 Npar= 954
```

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

```
PLAT234_ALERT_4_B Large Hirshfeld Difference C77      --C78      .       0.27 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C78      --C79      .       0.28 Ang.
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ..............       0.03 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).        14 Note
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...         1 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..         2 Check
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Alert level C

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.31 Report
PLAT213_ALERT_2_C Atom C16            has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C17            has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C21            has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C49            has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       4.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference Au2      --C73_a    .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Au3      --C24      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Au3      --C49      .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu1      --C25      .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu1      --C74      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu2      --C48      .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2       --C37      .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C10      --C11      .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C38      --C39      .       0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C49      --C50      .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C63      --C64      .       0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C73      --C74      .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C75      --C76      .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C82      --C83      .       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C83      --C86      .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C89      --C90      .       0.24 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C17 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C26 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C30 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C38 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C40 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C54 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C63 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Au1      0.101 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C17      - C20      .       1.42 Ang.
PLAT368_ALERT_2_C Short  C(sp2)-C(sp2) Bond  C1       - C2       .       1.23 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H31C     ..H32B     .       2.06 Ang.
                                          1-x,1-y,1-z  =      5_666 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N1       --H1A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N2       --H2A      .     Please Check
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PLAT420_ALERT_2_C D-H Bond Without Acceptor  N3       --H3A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N4       --H4A      .     Please Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -1.801 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        39 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         2 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H8B              -0.77 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H31A             -0.55 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H32A             -0.52 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H33B             -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H44B             -0.82 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H55B             -0.54 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H66A             -0.69 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H79B             -0.31 eA-3
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Alert level G

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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:C204 H220 Au6 Cu4 N10
           Atom count from the _atom_site data:  C192 H188 Au6 Cu4 N8
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  C204 H220 Au6 Cu4 N10
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         816.00    768.00   48.00
           H         880.00    752.00  128.00
           Au         24.00     24.00    0.00
           Cu         16.00     16.00    0.00
           N          40.00     32.00    8.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        17 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        43 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         4 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ    Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    559.12 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.         2 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        5 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records        6 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records        10 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        10 Report
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C61      -C70           0.22 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C75      -C84           0.16 Ang.
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C24 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C25 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for       C30 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C48 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C96 Check
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C22      - C23      .      1.42 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C46      - C47      .      1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C70      - C71      .      1.42 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C74      - C75      .      1.44 Ang.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       340 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.6 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
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PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        2.0 Sig(I)
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  55 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  33 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  50 ALERT type 2 Indicator that the structure model may be wrong or deficient
  12 ALERT type 3 Indicator that the structure quality may be low
  25 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_ABSTY02_Au6Cu4_complex_1
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT234_Au6Cu4_complex_1
;
PROBLEM: Large Hirshfeld Difference C77      --C78      .       0.27 Ang.
RESPONSE: ...
;
_vrf_PLAT342_Au6Cu4_complex_1
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............       0.03 Ang.
RESPONSE: ...
;
_vrf_PLAT910_Au6Cu4_complex_1
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min).         14 Note
RESPONSE: ...
;
_vrf_PLAT919_Au6Cu4_complex_1
;
PROBLEM: Reflection # Likely Affected by the Beamstop ...          1 Check
RESPONSE: ...
;
_vrf_PLAT934_Au6Cu4_complex_1
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          2 Check
RESPONSE: ...
;
_vrf_PLAT084_Au6Cu4_complex_1
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................       0.31 Report
RESPONSE: ...
;
_vrf_PLAT213_Au6Cu4_complex_1
;
PROBLEM: Atom C16             has ADP max/min Ratio .....        3.1 prolat
RESPONSE: ...
;
```

_vrf_PLAT220_Au6Cu4_complex_1
;
PROBLEM: NonSolvent   Resd 1 C   Ueq(max)/Ueq(min) Range   3.5 Ratio
RESPONSE: ...
;
_vrf_PLAT222_Au6Cu4_complex_1
;
PROBLEM: NonSolvent Resd 1 H   Uiso(max)/Uiso(min) Range   4.1 Ratio
RESPONSE: ...
;
_vrf_PLAT241_Au6Cu4_complex_1
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of   C16 Check
RESPONSE: ...
;
_vrf_PLAT242_Au6Cu4_complex_1
;
PROBLEM: Low   'MainMol' Ueq as Compared to Neighbors of   N2 Check
RESPONSE: ...
;
_vrf_PLAT250_Au6Cu4_complex_1
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.3 Note
RESPONSE: ...
;
_vrf_PLAT260_Au6Cu4_complex_1
;
PROBLEM: Large Average Ueq of Residue Including   Au1   0.101 Check
RESPONSE: ...
;
_vrf_PLAT360_Au6Cu4_complex_1
;
PROBLEM: Short C(sp3)-C(sp3) Bond C17   - C20   .   1.42 Ang.
RESPONSE: ...
;
_vrf_PLAT368_Au6Cu4_complex_1
;
PROBLEM: Short C(sp2)-C(sp2) Bond C1   - C2   .   1.23 Ang.
RESPONSE: ...
;
_vrf_PLAT413_Au6Cu4_complex_1
;
PROBLEM: Short Inter XH3 .. XHn   H31C   ..H32B   .   2.06 Ang.
RESPONSE: ...
;
_vrf_PLAT420_Au6Cu4_complex_1
;
PROBLEM: D-H Bond Without Acceptor N1   --H1A   .   Please Check
RESPONSE: ...
;
_vrf_PLAT905_Au6Cu4_complex_1
;
PROBLEM: Negative K value in the Analysis of Variance ...   -1.801 Report
RESPONSE: ...
;
_vrf_PLAT911_Au6Cu4_complex_1
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=   0.600   39 Report
RESPONSE: ...
;
_vrf_PLAT918_Au6Cu4_complex_1
;

```
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .          2 Check
RESPONSE: ...
;
_vrf_PLAT977_Au6Cu4_complex_1
;
PROBLEM: Check Negative Difference Density on H8B              -0.77 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 02/06/2021; check.def file version of 02/06/2021

Datablock Au6Cu4_complex_1 - ellipsoid plot