checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Au10Cu4

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: Au10Cu4

Bond precision: C-C = 0.0206 A Wavelength=0.71073

Cell: a=18.240(4) b=25.481(5) c=31.410(5)
alpha=89.152(6) beta=83.396(6) gamma=78.725(6)
Temperature: 120 K

	Calculated	Reported
Volume	14221(5)	14221(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C248 H240 Au10 Cu4 N8 P4 [+ solvent]	?
Sum formula	C248 H240 Au10 Cu4 N8 P4 [+ solvent]	C260 H272 Au10 Cu4 N10 P4
Mr	5680.19	5884.56
Dx,g cm-3	1.327	1.374
Z	2	2
Mu (mm-1)	5.492	5.495
F000	5500.0	5736.0
F000’	5466.59	
h,k,lmax	21,30,37	21,30,37
Nref	52055	51935
Tmin,Tmax	0.821,0.947	0.555,0.745
Tmin’	0.644	

Correction method= # Reported T Limits: Tmin=0.555 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.350

R(reflections)= 0.0664(31898) wR2(reflections)= 0.2072(51935)

S = 1.039 Npar= 2443

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

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Au5 3.11 eA-3

Author Response: Residual electron density does not make chemical sense. Residual elect resides too close to heavy metal atom center.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Au2 2.81 eA-3

Author Response: Residual electron density does not make chemical sense. Residual elect resides too close to heavy metal atom center.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Au6 2.72 eA-3

Author Response: Residual electron density does not make chemical sense. Residual elect resides too close to heavy metal atom center.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Au3 2.56 eA-3

Author Response: Residual electron density does not make chemical sense. Residual elect resides too close to heavy metal atom center.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Au1 2.16 eA-3

Author Response: Residual electron density does not make chemical sense. Residual elect resides too close to heavy metal atom center.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Au4 2.13 eA-3

Author Response: Residual electron density does not make chemical sense. Residual elect resides too close to heavy metal atom center.

Alert level B

PLAT213_ALERT_2_B Atom C23 has ADP max/min Ratio ..... 4.4 prolat
PLAT213_ALERT_2_B Atom C126 has ADP max/min Ratio ..... 4.2 prolat
PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 6.2 Ratio
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C197 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C226 Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02057 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 36 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 3 Check

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Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the

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           _exptl_absorpt_process_details field.
           Absorption correction given as MULTI-SCAN
PLAT213_ALERT_2_C Atom N1              has ADP max/min Ratio .....       3.1 oblate
PLAT213_ALERT_2_C Atom C5              has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom C14             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom C21             has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom C22             has ADP max/min Ratio .....       4.0 prolat
PLAT213_ALERT_2_C Atom C90             has ADP max/min Ratio .....       3.9 prolat
PLAT213_ALERT_2_C Atom C123            has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom C156            has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom C226            has ADP max/min Ratio .....       3.6 prolat
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       5.6 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C123 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C126 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C156 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C198 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C215 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C218 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C222 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C246 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C69 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C89 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C113 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C117 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C128 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C141 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C155 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C157 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C161 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C165 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C185 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C189 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C193 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C196 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C214 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C217 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C221 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C224 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C245 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C165     - C166     .       1.39 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C165     - C168     .       1.40 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C165     - C167     .       1.67 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C185     - C188     .       1.65 Ang.
PLAT370_ALERT_2_C Short  C(sp2)-C(sp1) Bond  C63      - C64      .       1.20 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H10A     ..H20G     .       2.13 Ang.
                                                  1+x,y,z  =      1_655 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N1       --H1B      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N2       --H2B      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N3       --H3A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N4       --H4B      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N5       --H5A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N6       --H6B      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N7       --H7A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N8       --H8A      .     Please Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -2.951 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        84 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         8 Note
PLAT977_ALERT_2_C Check Negative Difference Density on H2B             -0.50 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H20E            -0.68 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H23F            -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H30A            -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H66A            -0.43 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:C260 H272 Au10 Cu4 N10 P4
           Atom count from the _atom_site data:  C248 H240 Au10 Cu4 N8 P4
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    2
           From the CIF: _chemical_formula_sum  C260 H272 Au10 Cu4 N10 P4
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        520.00    496.00   24.00
           H        544.00    480.00   64.00
           Au        20.00     20.00    0.00
           Cu         8.00      8.00    0.00
           N         20.00     16.00    4.00
           P          8.00      8.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         16 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         48 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          8 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      37.11 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.006 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          3 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
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C1 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C2 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C39 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C40 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C49 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C50 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C88 Check
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C14      - C15      .       1.45 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C26      - C27      .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C62      - C63      .       1.45 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C74      - C75      .       1.46 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C86      - C87      .       1.42 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C98      - C99      .       1.48 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C110     - C111     .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C122     - C123     .       1.45 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C134     - C135     .       1.46 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C146     - C147     .       1.45 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C170     - C171     .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C182     - C183     .       1.43 Ang.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       379 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 !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        11 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.0 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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6 **ALERT level A** = Most likely a serious problem - resolve or explain
8 **ALERT level B** = A potentially serious problem, consider carefully

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 60 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 41 ALERT level G = General information/check it is not something unexpected

  6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 92 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
  7 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
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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 22/03/2021; check.def file version of 19/03/2021

Datablock Au10Cu4 - ellipsoid plot