checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Au6Cu2

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: Au6Cu2

Bond precision: C-C = 0.0259 A Wavelength=0.71073

Cell: a=34.044(3) b=19.6078(18) c=40.167(3)
alpha=90 beta=105.596(3) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	25825(4)	25825(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C144 H138 Au6 Cu2 N6, 2(C6 H16 N) [+ solvent]	?
Sum formula	C156 H170 Au6 Cu2 N8 [+ solvent]	C168 H202 Au6 Cu2 N10
Mr	3465.93	3670.26
Dx,g cm-3	0.891	0.944
Z	4	4
Mu (mm-1)	3.584	3.587
F000	6776.0	7248.0
F000’	6734.33	
h,k,lmax	42,24,49	42,24,49
Nref	25439	25313
Tmin,Tmax	0.657,0.836	0.537,0.745
Tmin’	0.519	

Correction method= # Reported T Limits: Tmin=0.537 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 26.022

R(reflections)= 0.0932(18949) wR2(reflections)= 0.2675(25313)

S = 1.059 Npar= 764

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

PLAT974_ALERT_2_A Check Calcd Negative Resid. Density on Au2 -2.29 eA-3

Author Response: The negative Resid. Density is too close to heavy metal atom center to make any chemical sense.

Alert level B

PLAT213_ALERT_2_B Atom C32 has ADP max/min Ratio ..... 4.2 prolat
PLAT234_ALERT_4_B Large Hirshfeld Difference C7 --C14 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C15 --C16 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C30 --C31 . 0.30 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C31 --C32 . 0.28 Ang.
PLAT260_ALERT_2_B Large Average Ueq of Residue Including N4 0.438 Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02588 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C55 - C56 . 1.59 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 14 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 5 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
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.27 Report
PLAT213_ALERT_2_C Atom C15 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom C55 has ADP max/min Ratio ..... 3.6 prolat
PLAT213_ALERT_2_C Atom C59 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C60 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C61 has ADP max/min Ratio ..... 3.8 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference Au3 --C27 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Au4 --C70 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu1 --C26 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu1 --C50 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C27 --C28 . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C39 --C44 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C52 --C53 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C55 --C56 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C65 --C66 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C66 --C67 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C69 --C70 . 0.19 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C16 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C31 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C42 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C52 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C55 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C66 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C14 Check

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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        C43 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C56 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C65 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C67 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C71 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      0.124 Check
PLAT370_ALERT_2_C Short  C(sp2)-C(sp1) Bond  C69      - C70      .       1.15 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N1       --H1A      .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N2       --H2B      .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N3       --H3A      .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N4       --H4B      .     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.922 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         91 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         4 Check
PLAT974_ALERT_2_C Check Calcd Negative Resid. Density on       Au4      -1.29 eA-3
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Author Response: The negative Resid. Density is too close to heavy metal atom center to make any chemical sense.

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PLAT977_ALERT_2_C Check Negative Difference Density on H10A             -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15A             -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H30A             -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H54A             -0.48 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H76B             -0.34 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:C168 H202 Au6 Cu2 N10
           Atom count from the _atom_site data:  C156 H170 Au6 Cu2 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  C168 H202 Au6 Cu2 N10
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        672.00    624.00   48.00
           H        808.00    680.00  128.00
           Au        24.00     24.00    0.00
           Cu         8.00      8.00    0.00
           N         40.00     32.00    8.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         40 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         44 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
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     579.68 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         17 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         11 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         11 Report
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C39      -C44      .       1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C63      -C68      .       1.42 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C29      -C34            0.20 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C53      -C58            0.27 Ang.
PLAT343_ALERT_2_G Unusual         Angle Range in Main Residue for        C26 Check
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PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C2       - C3       .       1.53 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C24      - C25      .       1.42 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C28      - C29      .       1.48 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C44      - C49      .       1.46 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C52      - C53      .       1.46 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C68      - C69      .       1.45 Ang.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        396 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 !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         21 Note
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
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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  1 ALERT level A = Most likely a serious problem - resolve or explain
 10 ALERT level B = A potentially serious problem, consider carefully
 52 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 32 ALERT level G = General information/check it is not something unexpected

  6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 56 ALERT type 2 Indicator that the structure model may be wrong or deficient
 11 ALERT type 3 Indicator that the structure quality may be low
 21 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 05/12/2020; check.def file version of 05/12/2020

Datablock Au6Cu2 - ellipsoid plot