checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Au8Cu6_complex_4

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: Au8Cu6_complex_4

Bond precision: C-C = 0.0171 A   Wavelength=0.71073

Cell: a=22.9670(12)   b=28.1979(16)   c=39.221(2)
               alpha=90   beta=92.129(2)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	25383(2)	25383(2)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C192 H184 Au8 Cu6 N8 [+ solvent]	?
Sum formula	C192 H184 Au8 Cu6 N8 [+ solvent]	C204 H216 Au8 Cu6 N10
Mr	4560.54	4764.83
Dx,g cm-3	1.193	1.247
Z	4	4
Mu (mm-1)	5.130	5.134
F000	8792.0	9264.0
F000'	8741.08	
h,k,lmax	28,35,49	28,35,49
Nref	26525	25796
Tmin,Tmax	0.545,0.774	0.496,0.745
Tmin'	0.535	

Correction method= # Reported T Limits: Tmin=0.496 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.973   Theta(max)= 26.583

R(reflections)= 0.0584(13490)   wR2(reflections)= 0.2032(25796)

S = 1.018   Npar= 953

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

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PLAT213_ALERT_2_B Atom C43              has ADP max/min Ratio .....      4.7 prolat
PLAT213_ALERT_2_B Atom C46              has ADP max/min Ratio .....      4.1 prolat
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of    C54 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).     16 Note
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...      2 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..      9 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
PLAT213_ALERT_2_C Atom C7               has ADP max/min Ratio .....      3.2 prolat
PLAT213_ALERT_2_C Atom C9               has ADP max/min Ratio .....      3.1 prolat
PLAT213_ALERT_2_C Atom C16              has ADP max/min Ratio .....      3.4 prolat
PLAT213_ALERT_2_C Atom C17              has ADP max/min Ratio .....      3.2 prolat
PLAT213_ALERT_2_C Atom C18              has ADP max/min Ratio .....      3.2 prolat
PLAT213_ALERT_2_C Atom C32              has ADP max/min Ratio .....      3.2 prolat
PLAT213_ALERT_2_C Atom C37              has ADP max/min Ratio .....      4.0 prolat
PLAT213_ALERT_2_C Atom C38              has ADP max/min Ratio .....      3.8 prolat
PLAT213_ALERT_2_C Atom C39              has ADP max/min Ratio .....      3.8 prolat
PLAT213_ALERT_2_C Atom C40              has ADP max/min Ratio .....      4.0 prolat
PLAT213_ALERT_2_C Atom C41              has ADP max/min Ratio .....      3.5 prolat
PLAT213_ALERT_2_C Atom C42              has ADP max/min Ratio .....      3.2 prolat
PLAT213_ALERT_2_C Atom C45              has ADP max/min Ratio .....      3.8 prolat
PLAT220_ALERT_2_C NonSolvent    Resd 1   C    Ueq(max)/Ueq(min) Range    4.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1   H    Uiso(max)/Uiso(min) Range    5.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference Au4       --C48       .    0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Au5       --C73       .    0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu3       --C47       .    0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5        --C10       .    0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C6        --C7        .    0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29       --C34       .    0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30       --C31       .    0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C35       --C38       .    0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C47       --C48       .    0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C54       --C55       .    0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C63       --C64       .    0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C70       --C71       .    0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C73       --C74       .    0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C75       --C84       .    0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C76       --C77       .    0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C83       --C86       .    0.19 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    Cu3 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    C38 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C46 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C73 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C77 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    C30 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C35 Check
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PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      C37 Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      C76 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....     3.1 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Au1   0.110 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............  0.01711 Ang.
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
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 ...  -6.559 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600     347 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .       4 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H31A         -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H31B         -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H81A         -0.39 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 H216 Au8 Cu6 N10
            Atom count from the _atom_site data:  C192 H184 Au8 Cu6 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 H216 Au8 Cu6 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       864.00    736.00  128.00
            Au       32.00     32.00    0.00
            Cu       24.00     24.00    0.00
            N        40.00     32.00    8.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...      29 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
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       3 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records       4 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records       6 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records       6 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu3      --C48     .    6.2 s.u.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C75      -C84     .   1.43 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C75      -C84     0.21 Ang.
PLAT343_ALERT_2_G Unusual         Angle Range in Main Residue for      C1 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for     C23 Check
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 sp?     Angle Range in Main Residue for     C49 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for     C72 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for     C73 Check
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C26      - C27     .   1.44 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C46      - C47     .   1.46 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C50      - C51     .   1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C70      - C71     .   1.45 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C74      - C75     .   1.47 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C90      - C95     .   1.45 Ang.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........       ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............     241 Note
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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       365 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....        1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........      3.3 Low
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
  58 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  36 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  59 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
  23 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 02/06/2021; check.def file version of 02/06/2021

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NOMOVE FORCED

Prob = 50
Temp = 100

PLATON-Jun 4 02:23:30 2021 - (20621)

Z -101 Au8Cu6_complex_4 C 2/c   R = 0.06   RES= 0 -90 X