checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 091209f

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: 091209f

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Bond precision:  C-C = 0.0120 A          Wavelength=0.71073

Cell:            a=7.6243(4)     b=29.1960(16)     c=13.5000(7)
                 alpha=90        beta=90           gamma=90
Temperature:     90 K
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	Calculated	Reported
Volume	3005.1(3)	3005.1(3)
Space group	P n m a	Pnma
Hall group	-P 2ac 2n	?
Moiety formula	C20 H11 Au4 Fe2 N12 O2	?
Sum formula	C20 H11 Au4 Fe2 N12 O2	C20 H11 Au4 Fe2 N12 O2
Mr	1350.99	1350.97
Dx,g cm-3	2.986	2.986
Z	4	4
Mu (mm-1)	20.434	20.434
F000	2396.0	2396.0
F000’	2370.73	
h,k,lmax	10,38,18	10,38,18
Nref	3811	3808
Tmin,Tmax	0.035,0.360	0.048,0.428
Tmin’	0.000	

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Correction method= # Reported T Limits: Tmin=0.048 Tmax=0.428
AbsCorr = EMPIRICAL

Data completeness= 0.999          Theta(max)= 28.310

R(reflections)= 0.0396( 3586)     wR2(reflections)= 0.1212( 3808)

S = 1.413                 Npar= 186
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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 N5              has ADP max/min Ratio .....       4.5 oblate
PLAT213_ALERT_2_B Atom C2              has ADP max/min Ratio .....       4.7 oblate
PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of .       130 Ang**3
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...         2 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....         2 Check
PLAT939_ALERT_3_B Large Value of Not (SHELXL) Weight Optimized S .    253.51 Check
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Alert level C

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PLAT220_ALERT_2_C Non-Solvent  Resd 1  N   Ueq(max)/Ueq(min) Range       3.2 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range       5.5 Ratio
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.012 Ang.
PLAT355_ALERT_3_C Long   O-H (X0.82,N0.98A)  O1       - H3       .      1.01 Ang.
PLAT355_ALERT_3_C Long   O-H (X0.82,N0.98A)  O1       - H3_i     .      1.01 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #         1 Note
            C20 H11 Au4 Fe2 N12 O2
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     5.307 Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         2 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.71A   From Au1            2.36 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.72A   From Au2            2.28 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.03A   From C2             1.98 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.76A   From Au1            1.85 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  2.91A   From N2             1.68 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.83A   From C1            -1.80 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.80A   From Au2           -1.76 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.02A   From Au2           -1.75 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.17A   From Au2           -1.75 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.21A   From Au2           -1.67 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.19A   From C9            -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.21A   From Au2           -1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.23A   From C10           -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.19A   From Au2           -1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.31A   From Au2           -1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.31A   From Au2           -1.51 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1              -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6              -0.32 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         1 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     33.24 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of H4         Constrained at       0.5 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.18 Ratio
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2018 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         3 Note
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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
  27 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  24 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 20/08/2018; check.def file version of 20/08/2018

Datablock 091209f - ellipsoid plot