checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_0905_1_0m

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: cu_0905_1_0m

Bond precision: C-C = 0.0079 A Wavelength=1.54178

Cell: a=18.0897(9) b=9.4109(6) c=21.7652(11)
alpha=90 beta=100.338(4) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	3645.2(4)	3645.2(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C42 H48 O10	C42 H48 O10
Sum formula	C42 H48 O10	C42 H48 O10
Mr	712.80	712.80
Dx,g cm-3	1.299	1.299
Z	4	4
Mu (mm-1)	0.751	0.751
F000	1520.0	1520.0
F000'	1524.84	
h,k,lmax	22,11,26	22,11,26
Nref	7188	6995
Tmin,Tmax	0.893,0.914	0.010,0.087
Tmin'	0.893	

Correction method= # Reported T Limits: Tmin=0.010 Tmax=0.087
AbsCorr = NONE

Data completeness= 0.973 Theta(max)= 72.101

R(reflections)= 0.1174(5137) wR2(reflections)= 0.2696(6995)

S = 1.075 Npar= 489

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 C

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PLAT082_ALERT_2_C High R1 Value ..................................       0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.27 Report
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O006 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O00M Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O00F Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C02O Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00791 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H02O     ..H02P     .       1.97 Ang.
                                                    x,y,z  =      1_555 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C42 H48 O10
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     39.856 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.278 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.247 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        112 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          4 Note
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          8 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      10.76 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O00F     --C0       .        7.2 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         4% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H1B      ..H02W     .       2.11 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H3A      ..H02S     .       2.10 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H01M     ..H2B      .       1.87 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H02M     ..H01K     .       2.11 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H02W     ..H0A      .       2.07 Ang.
                                                    x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        100 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         63 Note
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         81 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.3 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          2 Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
20 **ALERT level G** = General information/check it is not something unexpected

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  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 17 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
  5 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 18/05/2022; check.def file version of 17/05/2022

Datablock cu_0905_1_0m - ellipsoid plot