checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound_1_mo_3z_yellow

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: Compound_1_mo_3z_yellow

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Bond precision:  S- O = 0.0060 A         Wavelength=0.71073

Cell:             a=9.2021(3)     b=13.2434(5)     c=12.5610(3)
                  alpha=90        beta=90          gamma=90
Temperature:      293 K
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	Calculated	Reported
Volume	1530.77(8)	1530.77(8)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	H4 O28 S4 U4, H2 O, 4(Cs)	H O7 S U, Cs, H0.5 O0.25
Sum formula	Cs4 H6 O29 S4 U4	Cs H1.50 O7.25 S U
Mr	2082.05	520.51
Dx,g cm-3	4.517	4.517
Z	2	8
Mu (mm-1)	26.156	26.156
F000	1780.0	1780.0
F000’	1703.56	
h,k,lmax	11,17,16	11,17,16
Nref	1826	1824
Tmin,Tmax	0.296,0.593	0.430,1.000
Tmin’	0.200	

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Correction method= # Reported T Limits: Tmin=0.430 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 27.495

R(reflections)= 0.0261( 1560)     wR2(reflections)= 0.0648( 1824)

S = 1.055                 Npar= 109
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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

PLAT420_ALERT_2_B D-H Without Acceptor O8 --H8AA . Please Check
PLAT420_ALERT_2_B D-H Without Acceptor O8 --H8AB . Please Check

Alert level C

PLAT213_ALERT_2_C Atom O5 has ADP max/min Ratio ..... 3.2 prolat
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.3 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.391 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.86A From U1 2.13 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.86A From U1 2.10 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.92A From Cs2 1.56 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.96A From O8A 1.11 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8AA -0.35 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.25 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 11.45 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8AA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8AB Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 2 Note
PLAT794_ALERT_5_G Tentative Bond Valency for U1 (VI) . 6.24 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 18 Note
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 ... 3 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
21 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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 07/08/2019; check.def file version of 30/07/2019

Datablock Compound_1_mo_3z_yellow - ellipsoid plot