checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound_3_mo_3z_greenplate

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_3_mo_3z_greenplate

Bond precision: S- O = 0.0300 A Wavelength=0.71073

Cell: a=7.5829(3) b=14.4441(11) c=14.6458(14)
alpha=93.737(7) beta=99.535(5) gamma=99.614(5)
Temperature: 293 K

	Calculated	Reported
Volume	1552.6(2)	1552.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Cs O24 S5 U2, 3(H2 O), 5(Cs)	Cs6 H6 O27 S5 U2
Sum formula	Cs6 H6 O27 S5 U2	Cs6 H6 O27 S5 U2
Mr	1871.87	1871.87
Dx,g cm-3	4.004	4.004
Z	2	2
Mu (mm-1)	17.779	17.779
F000	1632.0	1632.0
F000’	1591.75	
h,k,lmax	9,17,17	9,17,17
Nref	5443	5151
Tmin,Tmax	0.533,0.915	0.490,1.000
Tmin’	0.486	

Correction method= # Reported T Limits: Tmin=0.490 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.946 Theta(max)= 24.999

R(reflections)= 0.0829(3806) wR2(reflections)= 0.2215(5151)

S = 1.068 Npar= 365

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.69A From O24 4.20 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.71A From O6 3.98 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.48A From O15 3.84 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 2.22A From O25 3.68 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.98A From U1 -3.80 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.05A From U1 -3.67 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT975_ALERT_2_A Check Calcd Resid. Dens. 0.90A From O18 2.47 eA-3

Author Response: Due to small size and bad quality of the crystals.

Alert level B

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low . 0.946 Why?

Author Response: Due to small size and bad quality of the crystals.

PLAT213_ALERT_2_B Atom O12 has ADP max/min Ratio ..... 4.8 prolat
PLAT420_ALERT_2_B D-H Without Acceptor O25 --H25A . Please Check
PLAT420_ALERT_2_B D-H Without Acceptor O27 --H27A . Please Check
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.88A From O2 2.96 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.17A   From U2   2.68 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.05A   From U1   2.66 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.77A   From U2   2.63 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.81A   From Cs1   2.53 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.86A   From Cs2   2.51 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.93A   From U2   -3.14 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.86A   From U2   -2.88 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.99A   From U1   -2.59 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.02A   From U1   -2.58 eA-3

Author Response: Due to small size and bad quality of the crystals.

Alert level C

PLAT213_ALERT_2_C Atom O6   has ADP max/min Ratio .....   4.0 prolat
PLAT213_ALERT_2_C Atom O7   has ADP max/min Ratio .....   3.7 prolat
PLAT213_ALERT_2_C Atom O13   has ADP max/min Ratio .....   3.9 oblate
PLAT213_ALERT_2_C Atom O14   has ADP max/min Ratio .....   3.1 prolat
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O21 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   U2 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   S1 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   S3 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   S5 Check

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PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O25      0.116 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O26      0.111 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.531 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595        293 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.58A   From O14            2.50 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.85A   From Cs3            2.48 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.90A   From O18            2.47 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.66A   From Cs3            2.41 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.96A   From U1             2.32 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.16A   From U2             2.30 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.13A   From O22A           2.26 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.08A   From O3             2.17 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.99A   From Cs1            2.13 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.04A   From Cs5            2.12 eA-3
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Author Response: Due to small size and bad quality of the crystals.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.01A   From U2             2.09 eA-3
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Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.90A   From U2   2.08 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.14A   From U1   2.06 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.99A   From Cs3   1.96 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.95A   From U1   1.94 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.80A   From U2   -2.39 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.05A   From Cs4   -2.31 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.88A   From Cs1   -2.20 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.79A   From U2   -2.20 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.01A   From Cs6   -2.20 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.87A   From U1   -2.20 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.92A   From Cs1   -2.18 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.37A   From Cs6   -2.15 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.04A   From Cs4   -2.12 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.07A   From Cs3   -2.00 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.49A   From Cs5   -1.98 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.22A   From Cs1   -1.97 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.09A   From Cs3   -1.95 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.98A   From Cs5   -1.94 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.56A   From Cs4   -1.89 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.33A   From O17   -1.85 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.23A   From O19   -1.84 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.24A   From Cs3   -1.84 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.11A   From Cs2   -1.81 eA-3

Author Response: Due to small size and bad quality of the crystals.

PLAT977_ALERT_2_C Check Negative Difference Density on H25A   -0.59 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   10 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   1 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   6 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 132.52 Why ?
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds   6 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   7 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
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   9% Note
PLAT794_ALERT_5_G Tentative Bond Valency for U1   (VI)   .   6.03 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   15 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still   53% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...   8 Note

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

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 71 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
  4 ALERT type 4 Improvement, methodology, query or suggestion
  3 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_3_mo_3z_greenplate - ellipsoid plot

