checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 200721d

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: 200721d

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Bond precision:    Y- O = 0.0061 A              Wavelength=0.71073

Cell:              a=6.8217(5)      b=9.5882(6)          c=10.5206(8)
                   alpha=90         beta=105.445(8)      gamma=90
Temperature:       373 K

                   Calculated               Reported
Volume             663.28(9)                663.28(8)
Space group        P 21/c                   P 1 21/c 1
Hall group         -P 2ybc                  -P 2ybc
Moiety formula     Mo4 O15 Y2               0.5(Mo8 O30 Y4)
Sum formula        Mo4 O15 Y2               Mo4 O15 Y2
Mr                 801.58                   801.58
Dx,g cm-3          4.014                    4.014
Z                  2                        2
Mu (mm-1)          12.389                   12.389
F000               732.0                    732.0
F000'              707.48
h,k,lmax           8,11,13                  8,11,13
Nref               1355                     1349
Tmin,Tmax          0.557,0.781              0.087,1.000
Tmin'              0.533

Correction method= # Reported T Limits: Tmin=0.087 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996            Theta(max)= 26.367


R(reflections)= 0.0431( 1207)               wR2(reflections)=
                                            0.1066( 1349)

S = 1.045                   Npar= 98
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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
PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE.   293 Degree

Alert level C
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   3 Report
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.67Ang From Mo2   -2.38 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.65Ang From Mo2   -2.04 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.61Ang From Mo1   -1.91 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.56Ang From Mo1   -1.73 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.89Ang From Y1   -1.60 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.03Ang From O1   .   1.03 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.75Ang From O3   .   0.96 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.89Ang From O3   .   -1.07 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From O5   .   -0.91 eA-3

Alert level G
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mo1   (VI)   .   5.83 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mo2   (VI)   .   5.97 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y1   (III)   .   3.29 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   4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   3.5 Low

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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 28/11/2022; check.def file version of 28/11/2022