checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_288

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: exp_288

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Bond precision:    C-C = 0.0048 A             Wavelength=0.71073

Cell:              a=13.9224(14)    b=7.4694(7)         c=16.2302(14)
                   alpha=90         beta=98.394(9)      gamma=90
Temperature:       293 K

                   Calculated                  Reported
Volume             1669.7(3)                   1669.7(3)
Space group        P 21/c                      P 1 21/c 1
Hall group         -P 2ybc                     -P 2ybc
Moiety formula     C15 H21 Co O6               C15 H21 Co O6
Sum formula        C15 H21 Co O6               C15 H21 Co O6
Mr                 356.25                      356.25
Dx,g cm-3          1.417                       1.417
Z                  4                           4
Mu (mm-1)          1.052                       1.052
F000               744.0                       744.0
F000'              745.75
h,k,lmax           18,9,21                     18,9,21
Nref               4130                        3790
Tmin,Tmax                                      0.002,1.000
Tmin'

Correction method= # Reported T Limits: Tmin=0.002 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.918          Theta(max)= 28.273

R(reflections)= 0.0504( 2677)     wR2(reflections)= 0.1352( 3790)

S = 1.018                    Npar= 205
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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 A

EXPT005_ALERT_1_A _exptl_crystal_description is missing
          Crystal habit description.
          The following tests will not be performed.
          CRYSR_01
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value ....   Please Do !

Alert level B

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low .   0.951 Why?

Alert level C

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...   Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...   Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...   Please Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C8 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   4.917 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   146 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..   1 Check

Alert level G

PLAT012_ALERT_1_G No   _shelx_res_checksum Found in CIF ......   Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)   293 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Co1   (III)   .   3.06 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   194 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   2.2 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   2 Info

   2 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
   7 **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

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 05/12/2020; check.def file version of 05/12/2020

NOMOVE FORCED

Prob = 50
Temp = 293

10 Y

PLATON-Jan 17 23:44:37 2021 — (51220)

Z 148   exp_288   P 1 21/c 1   R = 0.05   RES= 0 −60 X