checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:    C-C = 0.0069 A            Wavelength=1.54184

Cell:              a=5.27903(15)     b=13.2092(9)      c=16.7456(6)
                   alpha=90          beta=90           gamma=90
Temperature:       123 K

                   Calculated                Reported
Volume             1167.70(10)               1167.70(9)
Space group        P 21 21 21                P 21 21 21
Hall group         P 2ac 2ab                 P 2ac 2ab
Moiety formula     C18 H11.40 Se0.30         C18 H11.40 Se0.30
Sum formula        C18 H11.40 Se0.30         C18 H11.40 Se0.30
Mr                 251.51                    251.55
Dx,g cm-3          1.431                     1.431
Z                  4                         4
Mu (mm-1)          1.643                     1.645
F000               518.7                     519.0
F000'              518.93
h,k,lmax           6,16,21                   6,16,21
Nref               2430[ 1439]               1832
Tmin,Tmax          0.789,0.877               0.622,1.000
Tmin'              0.477

Correction method= MULTI-SCAN

Data completeness= 1.27/0.75       Theta(max)= 75.616

R(reflections)= 0.0618( 1568)      wR2(reflections)= 0.1813( 1832)

S = 1.049                    Npar= Npar = 184
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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

     Crystal system given = orthorhombic
PLAT915_ALERT_3_B Low Friedel Pair Coverage .... 45 %

Alert level C

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) .... 7.56 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.0069 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #   1 Note
          C18 H11.40 Se0.30

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   6 Note
PLAT301_ALERT_3_G Main Residue Disorder .... Percentage =   24 Note
PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C1   -C6   1.44 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   1 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....   ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   47 Note

   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
   5 **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

   1 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
   5 ALERT type 3 Indicator that the structure quality may be low
   4 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*, 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 05/02/2014; check.def file version of 05/02/2014