checkCIF/PLATON report

Structure factors have been supplied for datablock(s) xray072

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: xray072

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Bond precision:  C-C = 0.0096 A          Wavelength=1.54178

Cell:            a=8.0879(6)    b=7.0547(5)          c=8.2312(6)
                 alpha=90       beta=103.020(2)      gamma=90
Temperature:     200 K

                Calculated                Reported
Volume          457.58(6)                 457.58(6)
Space group     P 21/m                    P 1 21/m 1
Hall group      -P 2yb                    -P 2yb
Moiety formula  C9 H11 I                  0.5(C18 H22 I2)
Sum formula     C9 H11 I                  C9 H11 I
Mr              246.08                    246.08
Dx,g cm-3       1.786                     1.786
Z               2                         2
Mu (mm-1)       26.888                    26.888
F000            236.0                     236.0
F000'           236.07
h,k,lmax        9,8,10                    9,8,10
Nref            978                       953
Tmin,Tmax       0.006,0.063               0.308,0.753
Tmin'           0.001

Correction method= # Reported T Limits: Tmin=0.308 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.974          Theta(max)= 72.065

R(reflections)= 0.0544( 953)      wR2(reflections)= 0.1481( 953)

S = 1.123                 Npar= 61
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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 C

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PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .....         C7 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .....         C8 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .....         C9 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..........    0.00956 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        18 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.41A   From I1           2.11 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.38A   From I1           1.64 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.80A   From I1          -1.61 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.98A   From C7           0.48 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.81A   From C7          -0.76 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.90A   From C9          -0.74 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.82A   From C7          -0.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7A           -0.68 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7B           -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7C           -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9A           -0.74 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9B           -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9C           -0.34 eA-3
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Alert level G

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PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.11 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H7B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9C        Constrained at        0.5 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1  )      10.50 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C5       - C9       .       1.51 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          7 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          9 Note
PLAT940_ALERT_3_G Fsqd Refinement With I > n * Sigma(I) Only .....     Please Check
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  18 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 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
  11 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 16/05/2021; check.def file version of 13/05/2021

Datablock xray072 - ellipsoid plot