checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

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Bond precision:    C-C = 0.0041 A              Wavelength=0.71073

Cell:              a=17.1783(12)      b=15.058(3)       c=17.048(4)
                   alpha=90           beta=90           gamma=90
Temperature:       100 K

                   Calculated                 Reported
Volume             4409.8(14)                 4409.7(14)
Space group        P c c n                    P c c n
Hall group         -P 2ab 2ac                 -P 2ab 2ac
Moiety formula     C42 H48 Bi5 Co2 N4         C42 H48 Bi5 Co2 N4
Sum formula        C42 H48 Bi5 Co2 N4         C42 H48 Bi5 Co2 N4
Mr                 1771.60                    1771.60
Dx,g cm-3          2.668                      2.668
Z                  4                          4
Mu (mm-1)          20.646                     20.646
F000               3188.0                     3188.0
F000'              3115.38
h,k,lmax           26,23,26                   26,23,25
Nref               8407                       8349
Tmin,Tmax          0.097,0.356                0.035,0.108
Tmin'              0.001

Correction method= # Reported T Limits: Tmin=0.035 Tmax=0.108
AbsCorr = MULTI-SCAN

Data completeness= 0.993            Theta(max)= 33.129

R(reflections)= 0.0269( 7137)                   wR2(reflections)=
                                                0.0574( 8349)

S = 1.065                  Npar= 246
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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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PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......       3.309 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600           5 Report
                0  2  0,   2  0  0,   0  0  2,   0  1  2,   0  0  6,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.57Ang From Bi2             1.75 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.57Ang From Bi2            -1.75 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.49Ang From Bi2            -1.68 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.77Ang From Bi1            -1.65 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.71Ang From Bi3            -1.61 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6B      .       -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H12B     .       -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15A     .       -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H21A     .       -0.64 eA-3
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⚪ Alert level G

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       4 Note
            C00R     H00A     H00B     H00C
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       1 Note
              1  1  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600       41 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....       2 Note
              1  1  0,   2  0  0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     3.5 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......   Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........    1.62 Note
            Predicted wR2: Based on SigI**2  3.53 or SHELX Weight  5.46
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
 11 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

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 10 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
  2 ALERT type 4 Improvement, methodology, query or suggestion
  2 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 06/01/2024; check.def file version of 05/01/2024