checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 420-17Cd

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: 420-17Cd

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Bond precision:   C-C = 0.0073 A            Wavelength=0.71073

Cell:           a=11.5673(3)     b=18.4564(4)        c=11.9067(3)
                alpha=90         beta=93.468(3)      gamma=90
Temperature:    293 K

                Calculated                  Reported
Volume          2537.32(11)                 2537.31(11)
Space group     P 21/c                      P 21/c
Hall group      -P 2ybc                     -P 2ybc
Moiety formula  C26 H16 Cd2 N2 O10          ?
Sum formula     C26 H16 Cd2 N2 O10          C52 H32 Cd4 N4 O20
Mr              741.23                      1482.41
Dx,g cm-3       1.940                       1.940
Z               4                           2
Mu (mm-1)       1.739                       1.739
F000            1448.0                      1448.0
F000'           1442.23
h,k,lmax        13,21,14                    13,21,14
Nref            4488                        4479
Tmin,Tmax       0.677,0.706                 0.690,0.722
Tmin'           0.664

Correction method= # Reported T Limits: Tmin=0.690 Tmax=0.722
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 25.050

R(reflections)= 0.0370( 3550)     wR2(reflections)= 0.0715( 4479)

S = 1.068                 Npar= 361
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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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PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range       3.9 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cd1       --O3_d     .       7.4 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cd1       --O4_d     .       6.3 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cd1       --O8_e     .       6.5 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C24 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).        9 Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....        1 Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.        0 Info
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        2 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     2.00 Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)       293 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .     1.19 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1        (II)     .     2.01 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd2        (II)     .     2.09 Info
PLAT883_ALERT_1_G No Info for _atom_sites_solution_primary .......   Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still      64% Note
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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
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 18/02/2019; check.def file version of 18/02/2019