checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CdO12N4C22H30

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: CdO12N4C22H30

Bond precision: C-C = 0.0055 A Wavelength=0.71073

Cell: a=10.329(3) b=11.424(2) c=14.067(3)
alpha=98.266(17) beta=106.557(19) gamma=115.422(18)
Temperature: 223 K

	Calculated	Reported
Volume	1367.4(7)	1367.5(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H20 Cd N4 O7, 5(H2 O)	C22 H20 Cd N4 O7, 5(H2 O)
Sum formula	C22 H30 Cd N4 O12	C22 H30 Cd N4 O12
Mr	654.91	654.90
Dx,g cm-3	1.591	1.591
Z	2	2
Mu (mm-1)	0.866	0.866
F000	668.0	668.0
F000'	666.74	
h,k,lmax	12,14,17	12,14,17
Nref	5659	5647
Tmin,Tmax	0.690,0.878	0.718,0.902
Tmin'	0.642	

Correction method= # Reported T Limits: Tmin=0.718 Tmax=0.902
AbsCorr = NUMERICAL

Data completeness= 0.998 Theta(max)= 26.499

R(reflections)= 0.0358(4837) wR2(reflections)= 0.0807(5647)

S = 1.054 Npar= 394

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

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PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  Cd1      --O5       .       12.5 s.u.
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O10      --H10B     .     Please Check
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Alert level C

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PLAT213_ALERT_2_C Atom O4              has ADP max/min Ratio .....        3.1 prolat
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Cd1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C22 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O11      0.103 Check
PLAT417_ALERT_2_C Short Inter D-H..H-D       H7A      ..H12B     .       2.10 Ang.
                                                      x,y,z  =      1_555 Check
PLAT417_ALERT_2_C Short Inter D-H..H-D       H10B     ..H11A     .       2.11 Ang.
                                                      x,y,z  =      1_555 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H10B     ..O4       .       2.66 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H10      ..O7       .       2.66 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.034 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         10 Report
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         15 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         11 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd1      --O2       .        7.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd1      --O7       .        5.5 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1       (II)      .       2.06 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         11 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.2 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
   2 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 13/07/2021; check.def file version of 13/07/2021

Datablock CdO12N4C22H30 - ellipsoid plot

