## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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.

## Datablock: Cd2H2O4WCN8.2H2O

Bond precision:	W- C = 0.0001 A	Wavelength=0.71073	
Cell:		b=12.1877(5)	
Temperature:	alpha=90 300 K	beta=91.81(3)	gamma=90
Sum formula Mr Dx,g cm-3 Z Mu (mm-1) F000 F000'	I -2ya C16 Cd4 N16 O8 W2, C16 Cd4 N16 O12 W2 1425.64 2.462 2 8.197 1288.0 1278.83		
h,k,lmax Nref Tmin,Tmax Tmin'	21,22,24 11911[ 5961]		
Correction method= Not given			
Data completeness= 0.00/0.00		Theta(max)=	
R(reflections) = S =	Npar=		wR2(reflections)=

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.

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🖊 Alert level B
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .....
                                                                            06 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ......
                                                                            07 Check
Alert level C
{\tt PLAT601\_ALERT\_2\_C~Unit~Cell~Contains~Solvent~Accessible~VOIDS~of~.}
                                                                            37 Ang**3
Alert level G
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension
                                                                             3 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..
                                                                        Please Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...
                                                                           -55 Units
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data
                                                                        Please Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1
                                                       (II)
                                                                        2.32 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd2
                                                       (II)
                                                                         2.29 Info
PLAT982_ALERT_1_G The C-f'= 0.0170 Deviates from IT-value =
                                                                       0.0033 Check
PLAT982_ALERT_1_G The Cd-f'=
                              -0.0790 Deviates from IT-value =
                                                                      -0.8075 Check
                                                                       0.0061 Check
PLAT982_ALERT_1_G The N-f'=
                              0.0290 Deviates from IT-value =
                               0.0470 Deviates from IT-value = -6.0480 Deviates from IT-value = 0.0090 Deviates from IT-Value = 4.6530 Deviates from IT-Value =
PLAT982_ALERT_1_G The O-f'=
                                                                        0.0106 Check
PLAT982_ALERT_1_G The W-f'=
                                                                       -0.8490 Check
PLAT983_ALERT_1_G The C-f"=
                                                                        0.0016 Check
PLAT983_ALERT_1_G The Cd-f"=
                                                                       1.2024 Check
PLAT983_ALERT_1_G The N-f"= 0.0180 Deviates from IT-Value =
                                                                       0.0033 Check
PLAT983_ALERT_1_G The O-f"= 0.0320 Deviates from IT-Value =
                                                                       0.0060 Check
PLAT983_ALERT_1_G The W-f"= 5.5770 Deviates from IT-Value =
                                                                       6.8722 Check
   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected
  12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   O ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   3 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

