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.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Cd2H2O4MoCN8.2H2O

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Bond precision:   Cd- N = 0.0009 A          Wavelength=0.71073

Cell:              a=11.8123(6)      b=12.2011(5)       c=13.372(5)
                   alpha=90          beta=91.91(3)      gamma=90
Temperature:       300 K

                 Calculated                    Reported
Volume           1926.1(7)                     1926.1(3)
Space group      I a                           I a
Hall group       I -2ya                        I -2ya
Moiety formula   C16 Cd4 Mo2 N16 O8, 4(O)      C16 Cd4 Mo2 N16 O8, 4(O)
Sum formula      C16 Cd4 Mo2 N16 O12           C16 Cd4 Mo2 N16 O12
Mr               1249.84                       1249.84
Dx,g cm-3        2.155                         2.155
Z                2                             2
Mu (mm-1)        2.867                         0.000
F000             1160.0                        1160.0
F000'            1147.04
h,k,lmax         21,22,24
Nref             11933[ 5972]
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 0.00/0.00        Theta(max)=

R(reflections)=                                      wR2(reflections)=
S =                        Npar=
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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 B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O6 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O7 Check

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Alert level C

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 ... 4 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
PLAT982_ALERT_1_G The Mo-f'= -0.1910 Deviates from IT-value = -1.6832 Check
PLAT982_ALERT_1_G The N-f'= 0.0290 Deviates from IT-value = 0.0061 Check
PLAT982_ALERT_1_G The O-f'= 0.0470 Deviates from IT-value = 0.0106 Check
PLAT983_ALERT_1_G The C-f"= 0.0090 Deviates from IT-Value = 0.0016 Check
PLAT983_ALERT_1_G The Cd-f"= 4.6530 Deviates from IT-Value = 1.2024 Check
PLAT983_ALERT_1_G The Mo-f"= 2.7350 Deviates from IT-Value = 0.6857 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

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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
0 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

Datablock Cd2H2O4MoCN8.2H2O - ellipsoid plot