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: wang1

```
Bond precision:    C-C = 0.0138 A              Wavelength=0.71073

Cell:              a=14.631(4)      b=18.462(5)          c=15.946(4)
                   alpha=90         beta=98.955(4)       gamma=90
Temperature:       293 K

                   Calculated                   Reported
Volume             4255(2)                      4255(2)
Space group        P 21/c                       P 1 21/c 1
Hall group         -P 2ybc                      -P 2ybc
Moiety formula     C44 H34 Cd2 N8 O10, 2(H2     C44 H34 Cd2 N8 O10, 2(H2
                   O)                           O)
Sum formula        C44 H38 Cd2 N8 O12           C44 H40 Cd2 N8 O12
Mr                 1095.65                      1097.66
Dx,g cm-3          1.710                        1.714
Z                  4                            4
Mu (mm-1)          1.075                        1.075
F000               2200.0                       2208.0
F000'              2194.49
h,k,lmax           17,21,18                     17,21,18
Nref               7478                         7423
Tmin,Tmax          0.716,0.764
Tmin'              0.702

Correction method= Not given

Data completeness= 0.993            Theta(max)= 24.998

R(reflections)= 0.0634( 5229)       wR2(reflections)= 0.1916( 7423)

S = 1.060                   Npar= 605
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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

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PLAT220_ALERT_2_B Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range      8.4 Ratio
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of      C32 Check
PLAT415_ALERT_2_B Short Inter D-H..H-X       H1A      ..H33          1.96 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor       O1       --H1A       Please Check
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Alert level C

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PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full          ! Check
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ   Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..    2.01 Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given   Please Do !
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT213_ALERT_2_C Atom C42           has ADP max/min Ratio .....     3.6 prolat
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range    5.8 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      N7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C13 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C41 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C42 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      N6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C35 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C40 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C35     -C40          1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.01377 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D       H1A      ..H2B          2.11 Ang.
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C44 H40 Cd2 N8 O12
            Atom count from _chemical_formula_moiety:C44 H38 Cd2 N8 O12
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C44 H40 Cd2 N8 O12
            Atom count from the _atom_site data:  C44 H38 Cd2 N8 O12
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
        From the CIF: _cell_formula_units_Z    4
        From the CIF: _chemical_formula_sum  C44 H40 Cd2 N8 O12
        TEST: Compare cell contents of formula and atom_site data

        atom    Z*formula  cif sites diff
        C        176.00    176.00   0.00
        H        160.00    152.00   8.00
        Cd         8.00      8.00   0.00
        N         32.00     32.00   0.00
        O         48.00     48.00   0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...     2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension     2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............     6 Report
PLAT012_ALERT_1_G N.O.K.  _shelx_res_checksum Found in CIF ......   Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large   0.10 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large  10.90 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records     2 Report
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PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)      293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       2% Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C31 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.12 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1        (II)     .       2.06 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd2        (II)     .       2.16 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       12 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        6 Note
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  4 ALERT level B = A potentially serious problem, consider carefully
 22 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 20 ALERT level G = General information/check it is not something unexpected

 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 25 ALERT type 2 Indicator that the structure model may be wrong or deficient
  4 ALERT type 3 Indicator that the structure quality may be low
  2 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 23/04/2018; check.def file version of 23/04/2018