checkCIF/PLATON report

Structure factors have been supplied for datablock(s) y

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: y

Bond precision: C-C = 0.0032 A   Wavelength=0.71073

Cell: a=17.0971(3)   b=17.0971(3)   c=13.6304(5)
                  alpha=90   beta=90   gamma=120
Temperature: 293 K

	Calculated	Reported
Volume	3450.5(2)	3450.51(15)
Space group	P -3	P-3
Hall group	-P 3	?
Moiety formula	C24 H12 Cd2 N3 O15, C24 H12 Cd N3 O9, 0.99(O)	?
Sum formula	C48 H24 Cd3 N6 O25	C48 H24 Cd3 N6 O25
Mr	1421.80	1421.93
Dx,g cm-3	1.368	1.369
Z	2	2
Mu (mm-1)	0.987	0.988
F000	1395.8	1396.0
F000'	1391.76	
h,k,lmax	21,21,16	21,21,16
Nref	4568	4566
Tmin,Tmax	0.821,0.837	0.827,0.842
Tmin'	0.821	

Correction method= MULTI-SCAN

Data completeness= 1.000   Theta(max)= 26.060

R(reflections)= 0.0886(4296)   wR2(reflections)= 0.2591(4566)

S = 1.038   Npar= 226

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 A
PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of .   315 A**3

Alert level B

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PLAT220_ALERT_2_B Large Non-Solvent    O     Ueq(max)/Ueq(min) ...        4.5 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O8    -- C9      ..        9.0 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O8    -- C16     ..       10.1 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    N2    -- C16     ..        9.7 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    N2    -- C16_f   ..       31.2 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C7    -- C8      ..       11.0 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C12   -- C15     ..       11.3 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O7    -- C3      ..        9.5 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O7    -- C14     ..       15.1 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cd2   -- O4      ..       30.0 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cd3   -- O5      ..       29.5 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cd3   -- O6      ..       28.8 su
PLAT241_ALERT_2_B Check High     Ueq as Compared to Neighbors for      O4
PLAT241_ALERT_2_B Check High     Ueq as Compared to Neighbors for      O1
PLAT242_ALERT_2_B Check Low      Ueq as Compared to Neighbors for      Cd2
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Alert level C

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RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
          Weighted R factor given   0.259
SHFSU01_ALERT_2_C  The absolute value of parameter shift to su ratio > 0.05
          Absolute value of the parameter shift to su ratio given   0.065
          Additional refinement cycles may be required.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...        ?
PLAT080_ALERT_2_C Maximum Shift/Error ...........................       0.06
PLAT084_ALERT_2_C High wR2 Value ................................       0.26
PLAT213_ALERT_2_C Atom C16           has ADP max/min Ratio .....       4.0 prola
PLAT220_ALERT_2_C Large Non-Solvent   Cd    Ueq(max)/Ueq(min) ...       3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C7    -- C12     ..        6.0 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O2    -- C13     ..        6.3 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C3    -- C4      ..        7.0 su
PLAT241_ALERT_2_C Check High     Ueq as Compared to Neighbors for      C7
PLAT241_ALERT_2_C Check High     Ueq as Compared to Neighbors for      C15
PLAT241_ALERT_2_C Check High     Ueq as Compared to Neighbors for      O2
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for      C12
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for      Cd1
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for      C13
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) .....       2
PLAT918_ALERT_3_C Reflection(s) # with I(obs) much smaller I(calc)       2
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Alert level G

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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:C48 H24 Cd3 N6 O25
          Atom count from the _atom_site data:  C48 H24 Cd3 N6 O24.99
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       9
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....      12
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .       2
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .       2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF       ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.     0.17
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.     8.63
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .    mixed
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.1. Differ by ...       5 Units
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature     293 K
PLAT200_ALERT_1_G Check the Reported  _diffrn_ambient_temperature      293 K
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cd1    -- O2       ..       6.0 su
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..................      100 Perc.
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O1W
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PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.11 Ratio
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        79
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         !
PLAT931_ALERT_5_G Check Twin Law ( 0 0  1)[         ] Estimated BASF      0.50
PLAT931_ALERT_5_G Check Twin Law ( 1-1  0)[         ] Estimated BASF      0.50
PLAT931_ALERT_5_G Check Twin Law ( 1-2  0)[         ] Estimated BASF      0.50
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  1 ALERT level A = Most likely a serious problem - resolve or explain
 15 ALERT level B = A potentially serious problem, consider carefully
 18 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 21 ALERT level G = General information/check it is not something unexpected

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 37 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
  3 ALERT type 4 Improvement, methodology, query or suggestion
  6 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*, 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 05/11/2012; check.def file version of 05/11/2012