checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0047 A Wavelength=0.71073

Cell: a=16.7871(4) b=26.5431(5) c=18.7034(5)
alpha=90 beta=111.915(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	7731.7(4)	7731.7(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C86 H64 Cd2 N8 O10, 2(C H4 O)	Cd (C H4 O) (C12 H10 N4) (C15 H9 O2)2, 0.5(H2 O) (C H4 O)
Sum formula	C88 H72 Cd2 N8 O12	C44 H37 Cd N4 O6.5
Mr	1658.36	838.17
Dx,g cm-3	1.425	1.440
Z	4	8
Mu (mm-1)	0.619	0.621
F000	3392.0	3432.0
F000’	3386.92	
h,k,lmax	21,34,24	21,34,24
Nref	17939	17868
Tmin,Tmax	0.830,0.911	0.864,0.936
Tmin’	0.805	

Correction method= GAUSSIAN

Data completeness= 0.996 Theta(max)= 27.604

R(reflections)= 0.0387(14196) wR2(reflections)= 0.0975(17868)

S = 1.019 Npar= 1002

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

PLAT015_ALERT_5_A No _shelx_hkl_file record in SHELXL20xy CIF ... Please Do !

Author Response: File is too large.

Alert level B

Crystal system given = monoclinic
PLAT910_ALERT_3_B Missing # of FCF Reflections Below Th(Min) ..... 24 Report

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Alert level C

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.99 <> 1.01
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_weight 838.17
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	44.00	528.48
H	1.01	36.00	36.29
N	14.01	4.00	56.03
O	16.00	6.00	95.99
Cd	112.41	1.00	112.41

Calculated formula weight 829.20

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.4 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 5.4 Ratio
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C67 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... O9 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X H11 .. H87A .. 1.99 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 4 Report
PLAT975_ALERT_2_C Check Calcd Residual Density 0.81A From O6 0.54 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 0.41A From O11 -0.65 eA-3

Alert level G

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 H37 Cd1 N4 O6.5
Atom count from _chemical_formula_moiety:
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 H37 Cd1 N4 O6.5
Atom count from the _atom_site data: C44 H36 Cd1 N4 O6
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_sum C44 H37 Cd N4 O6.5
TEST: Compare cell contents of formula and atom_site data

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           atom    Z*formula  cif sites diff
           C        352.00    352.00    0.00
           H        296.00    288.00    8.00
           Cd         8.00      8.00    0.00
           N         32.00     32.00    0.00
           O         52.00     48.00    4.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         14 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         11 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension .......          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT044_ALERT_1_G Calculated and Reported Density Dx  Differ by ..     0.0153 Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ............       0.50 Ratio
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      12.12 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd1    --  O2      ..        7.5 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd1    --  O4      ..        5.5 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd2    --  O6      ..        5.6 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd2    --  O8      ..        6.7 su
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          2 Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  C87    ..  N2'     ..       2.51 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C87    ..  N3'     ..       3.05 Ang.
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .         36 A**3
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          13 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         73 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         43 Note
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
27 **ALERT level G** = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
17 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
6 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 24/07/2014; check.def file version of 24/07/2014

Datablock I - ellipsoid plot