

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: 114-11

Bond precision: C-C = 0.0035 Å Wavelength=0.71073

Cell: a=22.930(5) b=11.750(2) c=9.6800(19)
 alpha=90 beta=98.82(3) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	2577.2(9)	2577.2(9)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C26 H20 Cd Cl2 N2 O6	?
Sum formula	C26 H20 Cd Cl2 N2 O6	C26 H20 Cd Cl2 N2 O6
Mr	639.75	639.74
Dx,g cm-3	1.649	1.649
Z	4	4
Mu (mm-1)	1.099	1.099
F000	1280.0	1280.0
F000'	1278.48	
h,k,lmax	29,15,12	29,15,12
Nref	2975	2940
Tmin,Tmax	0.821,0.876	0.821,0.876
Tmin'	0.803	

Correction method= # Reported T Limits: Tmin=0.821 Tmax=0.876
AbsCorr = PSI-SCANS

Data completeness= 0.988 Theta(max)= 27.520

R(reflections)= 0.0268(2894) wR2(reflections)= 0.0677(2940)

S = 1.088 Npar= 170

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 C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as PSI-Scans

PLAT193_ALERT_1_C Cell and Diffraction Temperatures Differ by 5 Degree
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 03 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C8 Check

● Alert level G

ABSTY01_ALERT_1_G Extra text has been found in the _exptl_absorpt_correction_type
field, which should be only a single keyword. A literature
citation should be included in the _exptl_absorpt_process_details
field.

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.11 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1 (II) . 2.12 Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2018 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
3 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.

