checkCIF/PLATON report

Structure factors have been supplied for datablock(s) COMPOUND1

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: COMPOUND1

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Bond precision:  C-C = 0.0115 A          Wavelength=1.54178

Cell:            a=6.4893(1)    b=14.9997(3)       c=14.2753(3)
                 alpha=90       beta=90.637(1)     gamma=90
Temperature:     160 K

                Calculated                Reported
Volume          1389.44(5)                1389.44(5)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C12 H8 Cl2 N4 O2 Zn       ?
Sum formula     C12 H8 Cl2 N4 O2 Zn       C12 H8 Cl2 N4 O2 Zn
Mr              376.51                    376.49
Dx,g cm-3       1.800                     1.800
Z               4                         4
Mu (mm-1)       6.090                     6.090
F000            752.0                     752.0
F000'           750.35
h,k,lmax        7,17,16                   7,17,16
Nref            2368                      2338
Tmin,Tmax       0.506,0.578               0.522,1.000
Tmin'           0.120

Correction method= # Reported T Limits: Tmin=0.522 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.987          Theta(max)= 64.987

R(reflections)= 0.0705( 1890)     wR2(reflections)= 0.1654( 2338)

S = 1.124                 Npar= 191
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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

PLAT230_ALERT_2_B Hirshfeld Test Diff for N3 --C7 . 8.7 s.u.

Author Response: As the data and model do not suffer from unresolved effects such as twinning, absorption correction errors or disorder, this difference is usually caused by wrong atom assignment. The wrong atom assignment can clearly be excluded in the present compound, the identity of which has been confirmed by detailed NMR (1H, 13C, 15N) studies and accurate elemental (C, H, N) analyses. Moreover, advanced theoretical calculations (DFT) and literature reports on published complexes with the same ligand, fully support the proposed assignments. This Alert is probably caused by the adequate use of the rigid bond assumption of the Hirshfeld test and the charge deformation due to chemical bonding, as it is considered in our case, giving this difference in the values of anisotropic displacement parameters along this chemical bond. This case is often met in structure analysis studies.

Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5878
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check
PLAT230_ALERT_2_C Hirshfeld Test Diff for O2 --N3 . 6.0 s.u.

Author Response: As the data and model do not suffer from unresolved effects such as twinning, absorption correction errors or disorder, this difference is usually caused by wrong atom assignment. The wrong atom assignment can clearly be excluded in the present compound, the identity of which has been confirmed by detailed NMR (1H, 13C, 15N) studies and accurate elemental (C, H, N) analyses. Moreover, advanced theoretical calculations (DFT) and literature reports on published complexes with the same ligand, fully support the proposed assignments. This Alert is probably caused by the adequate use of the rigid bond assumption of the Hirshfeld test and the charge deformation due to chemical bonding, as it is considered in our case, giving this difference in the values of anisotropic displacement parameters along this chemical bond. This case is often met in structure analysis studies.

PLAT234_ALERT_4_C Large Hirshfeld Difference O1 --N4 . 0.17 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01145 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H11 ..CL2 . 2.92 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H12 ..CL1 . 2.99 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.422 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.588 28 Report

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Alert level G

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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.45 Why ?
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       1.97 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        57% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          2 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_THETM01_COMPOUND1
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.590
RESPONSE: ...
;
_vrf_PLAT018_COMPOUND1
;
PROBLEM: _diffrn_measured_fraction_theta_max .NE. *_full           ! Check
RESPONSE: ...
;
_vrf_PLAT234_COMPOUND1
;
PROBLEM: Large Hirshfeld Difference O1       --N4       .       0.17 Ang.
RESPONSE: ...
;
_vrf_PLAT341_COMPOUND1
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.01145 Ang.
RESPONSE: ...
;
_vrf_PLAT480_COMPOUND1
;
PROBLEM: Long H...A H-Bond Reported H11      ..CL2      .       2.92 Ang.
RESPONSE: ...
;
_vrf_PLAT906_COMPOUND1
;
PROBLEM: Large K Value in the Analysis of Variance ......      3.422 Check
RESPONSE: ...
;
_vrf_PLAT911_COMPOUND1
;
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PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.588         28 Report
RESPONSE: ...
;
# end Validation Reply Form
```

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 10/08/2020; check.def file version of 06/08/2020

Datablock COMPOUND1 - ellipsoid plot