checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C__Crystal_VRAC_131hot_asym_trsep14s

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: C__Crystal_VRAC_131hot_asym_trsep14s

```
Bond precision:  Zn- N = 0.0062 A        Wavelength=0.71073

Cell:             a=5.7715(4)     b=10.2359(4)     c=6.5456(6)
                  alpha=90        beta=90          gamma=90
Temperature:      298 K
```

	Calculated	Reported
Volume	386.69(5)	386.69(5)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	H24 N10 Zn4, 2(Cl)	?
Sum formula	Cl2 H24 N10 Zn4	H24 Cl2 N10 Zn4
Mr	496.75	496.75
Dx,g cm-3	2.133	2.133
Z	1	1
Mu (mm-1)	6.467	6.467
F000	248.0	248.0
F000’	249.45	
h,k,lmax	7,13,8	7,12,8
Nref	844[522]	844
Tmin,Tmax		
Tmin’		

```
Correction method= Not given

Data completeness= 1.62/1.00      Theta(max)= 26.972

R(reflections)= 0.0380( 744)      wR2(reflections)= 0.0983( 844)

S = 1.021                 Npar= 58
```

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

```
EXPT005_ALERT_1_A  _exptl_crystal_description is missing
            Crystal habit description.
            The following tests will not be performed.
            CRYSR_01
DIFF003_ALERT_1_A  _diffrn_measurement_device_type is missing
            Diffractometer make and type. Replaces _diffrn_measurement_type.
PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used value ....     Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min value ......     Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max value ......     Please Do !
```

Alert level B

```
CHEMS01_ALERT_1_B  The sum formula contains elements in the wrong order.
            H  precedes Cl
            Sequence must be alphabetical for inorganic structures.
PLAT927_ALERT_1_B Reported and Calculated  wR2 Differ by .........     0.0060 Check
PLAT987_ALERT_1_B The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
```

Alert level C

```
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   0.055
            Additional refinement cycles may be required.
STRVA01_ALERT_4_C           Flack test results are ambiguous.
           From the CIF: _refine_ls_abs_structure_Flack    0.490
           From the CIF: _refine_ls_abs_structure_Flack_su    0.030
PLAT031_ALERT_4_C Refined Extinction Parameter within Range ......      2.833 Sigma
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.20 Report
PLAT420_ALERT_2_C D-H Without Acceptor       N1     --  H1A    ...     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N1     --  H1B    ...     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N3     --  H3A    ...     Please Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
              H24 N10 Zn4
PLAT926_ALERT_1_C Reported and Calculated   R1 Differ by .........     0.0015 Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          9 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.490 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          6 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          6 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
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   5 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   6 ALERT level G = General information/check it is not something unexpected

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

PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock C__Crystal_VRAC_131hot_asym_trsep14s - ellipsoid plot