checkCIF/PLATON report

Structure factors have been supplied for datablock(s) d437

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: d437

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Bond precision:   C-C = 0.0073 A            Wavelength=0.71073

Cell:          a=9.067(1)        b=11.7201(13)     c=12.4367(14)
               alpha=91.649(9)   beta=108.557(10)  gamma=104.506(10)
Temperature:   228 K

                  Calculated                 Reported
Volume            1204.4(3)                  1204.4(2)
Space group       P -1                       P -1
Hall group        -P 1                       -P 1
Moiety formula    C42 H46 Cl2 N4 O16 Zn4     C42 H46 Cl2 N4 O16 Zn4
Sum formula       C42 H46 Cl2 N4 O16 Zn4     C42 H46 Cl2 N4 O16 Zn4
Mr                1195.29                    1195.21
Dx,g cm-3         1.648                      1.648
Z                 1                          1
Mu (mm-1)         2.151                      2.151
F000              608.0                      608.0
F000'             609.67
h,k,lmax          11,14,15                   11,14,15
Nref              4748                       4729
Tmin,Tmax         0.603,0.665                0.892,1.000
Tmin'             0.591

Correction method= MULTI-SCAN

Data completeness= 0.996          Theta(max)= 26.020

R(reflections)= 0.0441( 3459)     wR2(reflections)= 0.1167( 4729)

S = 1.044                   Npar= 312
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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.

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.

Datablock **d437** - ellipsoid plot