checkCIF/PLATON report

Structure factors have been supplied for datablock(s) za86

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: za86

Bond precision: C-C = 0.0072 A Wavelength=0.71073

Cell: a=14.2774(8) b=16.5172(8) c=32.5398(17)
alpha=90 beta=91.241(2) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	7671.8(7)	7671.8(7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C28 H16 I2 N2 O8 Zn2 [+ solvent]	C28 H16 I2 N2 O8 Zn2, 1.5[C3H7NO]
Sum formula	C28 H16 I2 N2 O8 Zn2 [+ solvent]	C28 H16 I2 N2 O8 Zn2
Mr	892.98	892.97
Dx,g cm-3	1.546	1.546
Z	8	8
Mu (mm-1)	2.900	2.900
F000	3423.9	3424.0
F000'	3422.26	
h,k,lmax	21,25,50	21,25,50
Nref	14647	14617
Tmin,Tmax	0.713,0.793	0.619,0.747
Tmin'	0.605	

Correction method= # Reported T Limits: Tmin=0.619 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 33.156

R(reflections)= 0.0800(10567)

wR2(reflections)= 0.2342(14617)

S = 1.030 Npar= 423

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

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3       ..O8       .       2.79 Ang.
                                                   1+x,y,z  =      1_655 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O4       ..O7       .       2.82 Ang.
                                                   1+x,y,z  =      1_655 Check
PLAT972_ALERT_2_B Check Calcd Resid. Dens.  1.05Ang From I4             -2.77 eA-3
```

Alert level C

```
PLAT213_ALERT_2_C Atom I4              has ADP max/min Ratio .....        3.8 prolat
PLAT213_ALERT_2_C Atom I1              has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom O8              has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C22             has ADP max/min Ratio .....        3.4 prolat
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Zn1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)         2.6 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.398 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          8 Report
                1  1  1,   1  3  1,  -1  1  2,   0  2  2,   0  4  2,   0  2  3,
               -2  0 14,   0  0 22,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          2 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.17Ang From I4              2.48 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.95Ang From I5              2.28 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.27Ang From I4             -2.30 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.75Ang From I1             -1.92 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.64Ang From I1             -1.84 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.83Ang From I2             -1.77 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.48Ang From I3             -1.54 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.47Ang From I2             -1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.73Ang From I5             -1.52 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:   C28 H16 I2 N2 O8 Zn2
           Atom count from _chemical_formula_moiety:C32.5 H26.5 I2 N3.5 O9.5 Zn2
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          7 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C28 H16 I2 N2 O8 Zn2
```

```
             Rep.: C28 H16 I2 N2 O8 Zn2, 1.5[C3H7NO]
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      76.21 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        14% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        835 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2       (II)      .       2.04 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         43 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                  1  1  0,   0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         21 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          6 Note
                 -2  0 14,   0  2  2,   0  2  3,   0  4  2,   1  1  1,   1  3  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       4.69 Note
             Predicted wR2: Based on SigI**2  5.00 or SHELX Weight 23.07
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

---

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
5 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.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock za86 - ellipsoid plot