checkCIF/PLATON report

Structure factors have been supplied for datablock(s) c20yb71_0m_aa_ca

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: c20yb71_0m_aa_ca

Bond precision: C-C = 0.0037 A   Wavelength=0.71073

Cell: a=11.6745(12)   b=13.2064(13)   c=15.5353(16)
               alpha=67.641(3)   beta=85.612(4)   gamma=73.680(4)
Temperature: 100 K

	Calculated	Reported
Volume	2124.6(4)	2124.6(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C88 H78 Ca N8 O18 Zn2, 2(C2 H6 O)	C88 H78 Ca N8 O18 Zn2, C2 H6 O
Sum formula	C92 H90 Ca N8 O20 Zn2	C92 H90 Ca N8 O20 Zn2
Mr	1798.58	1798.53
Dx,g cm-3	1.406	1.406
Z	1	1
Mu (mm-1)	0.703	0.703
F000	938.0	938.0
F000'	939.20	
h,k,lmax	16,18,22	16,18,22
Nref	13093	13031
Tmin,Tmax	0.908,0.967	0.657,0.746
Tmin'	0.843	

Correction method= # Reported T Limits: Tmin=0.657 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.995   Theta(max)= 30.593

R(reflections)= 0.0429(8339)   wR2(reflections)= 0.1406(13031)

S = 1.046   Npar= 563

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

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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      3.60 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -1.960 Report
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         6 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         1 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .     45.26 Check
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⚪ Alert level G

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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:   C92 H90 Ca1 N8 O20 Zn2
                   Atom count from _chemical_formula_moiety:C90 H84 Ca1 N8 O19 Zn2
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         5 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn1       --O1        .      5.2 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O1W       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1W       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2W       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1WO      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1WA      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1WB      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2WA      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2WB      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2WC      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2W       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3W       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4W       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2WO      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3WA      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3WB      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4WA      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4WB      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4WC      Constrained at       0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )     100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )     100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )     4.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )     4.50 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H8       ..H3WA      .     2.07 Ang.
                                              x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       12 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #       18 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       50 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        6 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........      1.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        2 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  35 ALERT level G = General information/check it is not something unexpected
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 3 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
26 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check
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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 18/09/2020; check.def file version of 20/08/2020