checkCIF/PLATON report

Structure factors have been supplied for datablock(s) p78bkten_a2

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: p78bkten_a2

```
Bond precision:  S- O = 0.0018 A         Wavelength=0.71073

Cell:            a=5.5990(11)     b=6.0840(12)      c=23.676(5)
                 alpha=90         beta=95.22(3)     gamma=90
Temperature:     100 K
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	Calculated	Reported
Volume	803.2(3)	803.2(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	?
Moiety formula	Cu7.60 H12 O28 S4 Zn0.40, Co1.24 H24 Ni0.64 O12 Zn0.12	Cu7.60 H12 O28 S4 Zn0.40, Co1.24 H24 Ni0.64 O12 Zn0.12
Sum formula	Co1.24 Cu7.60 H36 Ni0.64 O40 S4 Zn0.52	Co1.24 Cu7.60 H36 Ni0.64 O40 S4 Zn0.52
Mr	1432.15	1432.15
Dx,g cm-3	2.961	2.961
Z	1	1
Mu (mm-1)	6.694	6.694
F000	707.4	707.0
F000’	711.51	
h,k,lmax	8,9,35	8,8,33
Nref	2848	2419
Tmin,Tmax	0.935,0.987	0.936,0.987
Tmin’	0.935	

```
Correction method= # Reported T Limits: Tmin=0.936 Tmax=0.987
AbsCorr = MULTI-SCAN

Data completeness= 0.849          Theta(max)= 32.250

R(reflections)= 0.0310( 2387)     wR2(reflections)= 0.0831( 2419)

S = 1.066                  Npar= 152
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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

```
PLAT420_ALERT_2_B D-H Without Acceptor       O3       --H3       .     Please Check
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on       Zn2       1.53 eA-3
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on       Cu2       1.53 eA-3
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Alert level C

```
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..     Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          7 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.14A   From Zn              1.52 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Cu1       1.45 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Zn1       1.45 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.81A   From O6              0.48 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.81A   From O9             -0.52 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.03A   From O4             -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2               -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H91              -0.42 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                 not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         13 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cu1        Constrained at       0.95 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cu2        Constrained at       0.95 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Zn1        Constrained at       0.05 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Zn2        Constrained at       0.05 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Zn         Constrained at       0.06 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Co         Constrained at       0.62 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ni         Constrained at       0.32 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        20% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        25% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          8 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2018 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        391 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ           2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ           2 Units
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          1 Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
23 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
  4 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 22/12/2019; check.def file version of 13/12/2019

Datablock p78bkten_a2 - ellipsoid plot