checkCIF/PLATON report

Structure factors have been supplied for datablock(s) xgph2n2_zn_0m_5

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: xgph2n2_zn_0m_5

Bond precision: C-C = 0.0041 A Wavelength=1.54178

Cell: a=10.9759(13) b=11.303(3) c=19.281(4)
alpha=100.700(13) beta=91.091(9) gamma=108.195(15)
Temperature: 100 K

	Calculated	Reported
Volume	2225.3(8)	2225.4(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C47 H55 B N4 O2 Zn, 0.5(C6 H14)	C47 H55 B N4 O2 Zn, C3 H7
Sum formula	C50 H62 B N4 O2 Zn	C50 H62 B N4 O2 Zn
Mr	827.24	827.21
Dx,g cm-3	1.235	1.234
Z	2	2
Mu (mm-1)	1.094	1.093
F000	882.0	882.0
F000'	881.02	
h,k,lmax	13,13,23	13,13,23
Nref	8164	7964
Tmin,Tmax	0.937,0.957	0.411,0.652
Tmin'	0.858	

Correction method= # Reported T Limits: Tmin=0.411 Tmax=0.652
AbsCorr = MULTI-SCAN

Data completeness= 0.976 Theta(max)= 68.283

R(reflections)= 0.0403(7434) wR2(reflections)= 0.1001(7964)

S = 1.071 Npar= 535

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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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.978 Why?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C47 H55 B N4 O2 Zn, 0.5(C6 H14)
             Rep.: C47 H55 B N4 O2 Zn, C3 H7
PLAT766_ALERT_4_C INS Embedded LIST 8 Instruction Should be LIST 4     Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        180 Report
               -1   3   0, -12   9   0, -11   9   0, -11 10   0,   -2 13   0,   11-10   1,
               12  -9   1, -13   3   1, -13   6   1, -12   8   1, -11 10   1,   11-10   2,
               11  -9   2,   12 -9   2,   -1   0   2, -13   3   2, -13   4   2, -13   5   2,
              -12   8   2, -11 10   2,   11-10   3,   12 -9   3, -13   3   3, -13   4   3,
              -13   5   3, -12   6   3, -12   8   3, -11 10   3,   -5 10   3, -12   1   4,
              -12   2   4, -12   3   4, -13   4   4, -12   6   4, -12   8   4,    4 10   4,
              -12  -1   5, -12   0   5, -12   1   5, -12   2   5, -12   4   5, -12   6   5,
                5   9   5,   12 -1   6, -12   0   6, -12   1   6, -11   1   6, -12   2   6,
              -11   2   6, -12   3   6, -11   3   6, -12   4   6, -12   5   6, -12   6   6,
              -12   7   6,    6   8   6,   -1 -4   7, -11 -3   7, -11 -2   7, -11 -1   7,
               -8  -1   7, -12   0   7, -11   0   7, -10   0   7, -12   1   7, -11   1   7,
              -10   1   7, -12   2   7, -11   2   7, -12   3   7, -11   3   7, -12   4   7,
              -11   4   7, -12   5   7, -12   6   7,   -9   8   7, -10 -4   8, -10 -3   8,
              -11  -2   8, -10 -2   8,   -9 -2   8, -11 -1   8, -10 -1   8,   -9 -1   8,
              -12   0   8, -11   0   8, -10   0   8, -12   1   8, -11   1   8, -10   1   8,
              -12   2   8, -11   2   8, -12   3   8, -11   3   8, -12   4   8, -12   5   8,
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Alert level G

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PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn1      --O2       .        5.6 s.u.
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O1       .      105.2 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       1.85 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
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         29 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
               -1   3   0,   -1   0   2,
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 0 1)         Est.d BASF       0.15 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          5 Note
              -10  -2   8, -10   0   7,   -9 -2   8,   -9 -1   8,   -5 10   3,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      1.630 Note
              Predicted wR2: Based on SigI**2  6.14 or SHELX Weight  9.35
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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
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

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

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  3 ALERT type 2 Indicator that the structure model may be wrong or deficient
  4 ALERT type 3 Indicator that the structure quality may be low
  3 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 22/08/2024; check.def file version of 21/08/2024

Datablock xgph2n2_zn_0m_5 - ellipsoid plot