checkCIF/PLATON report

Structure factors have been supplied for datablock(s) xg_phcho_zn_new_0m_a

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: xg_phcho_zn_new_0m_a

Bond precision: C-C = 0.0027 A   Wavelength=1.54178

Cell: a=13.3489(2)   b=14.1103(2)   c=18.9440(3)
                   alpha=90   beta=91.461(1)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3567.08(9)	3567.08(9)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C70 H90 B2 N4 O4 Zn2, C6 H14	C70 H90 B2 N4 O4 Zn2, C6 H14
Sum formula	C76 H104 B2 N4 O4 Zn2	C76 H104 B2 N4 O4 Zn2
Mr	1290.03	1289.99
Dx,g cm-3	1.201	1.201
Z	2	2
Mu (mm-1)	1.204	1.204
F000	1380.0	1380.0
F000'	1377.00	
h,k,lmax	16,17,23	15,17,23
Nref	6771	6712
Tmin,Tmax	0.917,0.953	0.672,0.753
Tmin'	0.908	

Correction method= # Reported T Limits: Tmin=0.672 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.991   Theta(max)= 70.019

R(reflections)= 0.0336(6115)   wR2(reflections)= 0.0909(6712)

S = 1.057   Npar= 437

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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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600       35 Report
              14  0  0,  14  1  0,  15  1  0,  13  2  0, -15  0  1,  15  0  1,
             -15  1  1, -14  1  1, -13  1  1, -15  2  1, -14  2  1, -14  0  2,
             -15  1  2, -14  1  2, -13  1  2, -15  2  2, -13  2  2, -15  0  3,
             -13  0  3, -15  1  3, -14  1  3, -13  1  3, -15  2  3, -14  0  4,
             -15  1  4, -14  1  4, -15  2  4, -14  2  4, -15  0  5, -15  1  5,
             -15  1  6, -15  0  7, -15  1  7, -15  1  8, -13  0  9,
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        6 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms         6 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0400 Report
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)    10.70 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)     9.30 Check
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O003    .    107.6 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       98 Note
          Zn01    O002    O003    N004    N005    C006    C007    C008
          C009    C00A    C00B    H00B    C00C    C00D    H00D    C00E
          C00F    H00F    C00G    H00A    H00C    H00E    C00H    H00H
          C00I    H00I    C00J    C00K    C00L    H00G    H00J    H00K
          C00M    H00M    C00N    H00N    C00O    H00O    C00P    C00Q
          H00Q    C00R    H00R    C00S    H00L    H00P    H00S    C00T
          H00T    C00U    H00U    C00V    H00V    C00W    H00W    C00X
          H00X    B00Y    C00Z    H00Y    Ha      C010    H01A    H01B
          H01C    C011    H01D    H01E    H01F    C012    H01G    H01H
          H01I    C013    H01J    H01K    H01L    C014    H01M    H01N
          H01O    C015    H01P    H01Q    H01R    C016    H01S    H01T
          H01U    C017    H01V    H01W    C018    H01X    H01Y    C0
          H0A     H0B
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C1        --C1          1.75 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       64 Note
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        4 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        6 Note
             -14  0  4, -14  1  1, -14  1  2, -14  1  3, -13  0  3,  14  0  0,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........    3.861 Note
          Predicted wR2: Based on SigI**2  2.36 or SHELX Weight  8.60
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       11 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
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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  20 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
   9 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 22/08/2024; check.def file version of 21/08/2024

NOMOVE FORCED

Prob = 50
Temp = 100

53 Y

PLATON-Sep 25 0:12:09 2024 - (220824)

Z -88   xg_phcho_zn_new_OP 1 21/n 1   R = 0.03   RES= 0   85 X