checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mof-508-no2

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: mof-508-no2

Bond precision: C-C = 0.0094 A   Wavelength=0.41270

Cell: a=8.0536(13)   b=10.1473(17)   c=10.2709(17)
               alpha=63.945(4)   beta=83.150(6)   gamma=71.754(5)
Temperature: 195 K

	Calculated	Reported
Volume	716.0(2)	716.0(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C13 H6 N2 O6 Zn	C26 H12 N4 O12 Zn2
Sum formula	C13 H6 N2 O6 Zn	C26 H12 N4 O12 Zn2
Mr	351.59	703.14
Dx,g cm-3	1.631	1.631
Z	2	1
Mu (mm-1)	0.404	0.404
F000	352.0	352.0
F000'	352.46	
h,k,lmax	14,18,18	13,18,18
Nref	8612	7111
Tmin,Tmax		0.500,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.500 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.826   Theta(max)= 21.678

R(reflections)= 0.0881(3537)   wR2(reflections)= 0.2585(7111)

S = 1.017   Npar= 169

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           yellowish
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ....   0.26 Report
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   C11 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.1 Note
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C7   -C9_c   1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C11   -C13   1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00937 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   35.485 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.156 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   6.281 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   3.020 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.91A   From O7   0.40 eA-3

Alert level G

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   11 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   2.00 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.11 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka   0.41270 Ang.
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records   1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O3   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2   Constrained at   0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   41% Note
PLAT395_ALERT_2_G Deviating X-O-Y   Angle From 120 for O9   141.0 Degree
PLAT395_ALERT_2_G Deviating X-O-Y   Angle From 120 for O10   95.3 Degree
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C3B   --C3B   1.70 Ang.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....   ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   22 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   1449 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   2 Info
PLAT984_ALERT_1_G The Zn-f'=   0.2616 Deviates from the B&C-Value   0.2601 Check
PLAT985_ALERT_1_G The Zn-f"=   0.5384 Deviates from the B&C-Value   0.5357 Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by   1 Check

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

    8 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
 8 ALERT type 3 Indicator that the structure quality may be low
 9 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.

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