checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MIP-203

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.

Datablock: MIP-203

Bond precision:	C-C = 0.0300	<i>I</i> A	Wavelength=0.82660		
Cell:	a=10.000(2) alpha=90	b=11.94 beta=90		c=19.829(11) gamma=90	
Temperature:	100 K	Deca-30		gamma-90	
1	Calculated		Reported		
Volume	2367.6(15)		2367.6(1	-5)	
Space group			I m m m		
Hall group		F (0.0 F 0)	-I 2 2		
Moiety formula		5(00.50)	?	040 7 6	
Sum formula	C9 H5 O20 Zr3		C18 H10	040 Zr6	
Mr	706.79 1.983		1413.58 1.983		
Dx,g cm-3 Z	1.963		2		
Mu (mm-1)	2.047		2.047		
F000	1356.0		1356.0		
F000'	1339.58		1330.0		
h,k,lmax	11,14,23		11,12,23	}	
Nref	1232		1022		
Tmin,Tmax	0.884,0.903				
Tmin'	0.664				
Correction method= Not given					
Data completeness= 0.830		Theta(max) = 29.717			
R(reflections)=	wR2(ref	wR2(reflections)= 0.3548(1022)			
S = 1.170	Npar= 93				

Click on the hyperlinks for more details of the test.

Alert level A

RINTA01_ALERT_3_A The value of Rint is greater than 0.25 Rint given 0.259

Author Response: The crystal is very small (20*5 microns) and weakly diffracting, so the ssentially "unobserved" reflections are being used in the refinement

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PLAT058_ALERT_1_A Maximum Transmission Factor Missing?

Author Response: XDS package doesn't provide transmission factor

PLAT059_ALERT_1_A Minimum Transmission Factor Missing ?

Author Response: XDS package doesn't provide transmission factor

PLAT183 ALERT 1 A Missing cell measurement reflns used Value Please Do !

Author Response: XDS package doesn't provide this information

PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value Please Do !

Author Response: XDS package doesn't provide this information

PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value Please Do!

Author Response: XDS package doesn't provide this information

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Zr1 3.77 eA-3

Author Response: The residual density on all heavy atoms is likely related to the quality of the data as indicated by the high wR2 value of 35.5%

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Zr2 2.90 eA-3

Author Response: The residual density on all heavy atoms is likely related to the quality of the data as indicated by the high wR2 value of 35.5%

🖳 Alert level B PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 01W Check Author Response: This oxygen corresponds to a water molecule in the pore of the MOF. PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 02W Check Author Response: This oxygen corresponds to a water molecule in the pore of the MOF. PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.03 Ang. Author Response: The overall quality of the data is related to the small crystal size. PLAT430_ALERT_2_B Short Inter D...A Contact O2W ..O3W 2.62 Ang. x, y, z =1_555 Check Author Response: Water molecules in the pores interacting by H bond PLAT430_ALERT_2_B Short Inter D...A Contact O2W 2.62 Ang. ..O3W 2_565 Check -x, 1-y, z =Author Response: Water molecules in the pores interacting by H bond PLAT430_ALERT_2_B Short Inter D...A Contact O3W 2.68 Ang. ..O3W -x, 1-y, z =2_565 Check Author Response: Water molecules in the pores interacting by H bond PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of . 124 Ang**3 Author Response: This is expected in this porous MOF PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 179 Report

Author Response: Missing data due to rotation about one axis

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PLAT082_ALERT_2_C High R1 Value .....
                                                                                                     0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ......
                                                                                                     0.35 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference Zrl --03 .
                                                                                                     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Zr1 --O3 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Zr1 --O4 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1 --C1 . 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Zr1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Zr2 Check
                                                                                                     Zr2 Check
2.3 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....
                                                                                                  0.140 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including 01W
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O2W PLAT260_ALERT_2_C Large Average Ueq of Residue Including O3W
                                                                                                   0.171 Check
                                                                                                   0.150 Check
PLAT430_ALERT_2_C Short Inter D...A Contact O2W ...O6 .
                                                                                                     2.88 Ang.
                                                           1/2-x,1/2+y,1/2-z = 8_555 Check
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Author Response: Water molecules in the pores interacting by H bond

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PLAT430_ALERT_2_C Short Inter D...A Contact O2W ..06 . 2.88 Ang. 1/2-x,1/2-y,1/2+z = 6_555 Check
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Author Response: Water molecules in the pores interacting by H bond

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PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by . 1.49 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.42A From C3 1.85 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.42A From C3 1.64 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.97A From Zr2 -2.16 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.94A From Zr1 -1.93 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.98A From Zr2 -1.84 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.29A From O3 -1.78 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.04A From Zr2 -1.78 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.04A From Zr2 -1.78 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.95A From Zr1 -1.69 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.75A From O3W 1.05 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.07A From C3 0.58 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.07A From C3 0.58 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.71A From O4 0.57 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.78A From O1W -0.75 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.85A From O1 -0.62 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.70A From O1 -0.62 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.70A From O1 -0.62 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.70A From O1 -0.62 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.54A From O2W -0.59 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.54A From O2W -0.59 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.
                                                                              1 Note
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension
                                                                                 3 Info
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
                                                                             0.18 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 15.42 Why?
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.82660 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C3 Constrained at PLAT300_ALERT_4_G Atom Site Occupancy of H3 Constrained at PLAT300_ALERT_4_G Atom Site Occupancy of O3W Constrained at
                                                                              0.5 Check
                                                                              0.5 Check
                                                                              0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ......(Resd 1 )
                                                                            6% Note
100% Note
                                                                               6% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4 )
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....
                                                                              03W Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 141 Check
               C3 -O5 -C3 10.555 1.555 1.555 36.00 Deg.
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PLAT794_ALERT_5_G Tentative Bond Valency for Zr1
                                                                    4.06 Info
                                                   (IV) .
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters
                                                                       4 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
                                                                       1 Note
                                                                 Please Do !
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still
                                                                   33% Note
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ
                                                                       2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ
                                                                       2 Units
PLAT984_ALERT_1_G The Zr-f'= -1.4547 Deviates from the B&C-Value
                                                                -1.4492 Check
PLAT985_ALERT_1_G The Zr-f"= 0.7529 Deviates from the B&C-Value 0.7414 Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by
                                                                       1 Check
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9 ALERT level A = Most likely a serious problem - resolve or explain
8 ALERT level B = A potentially serious problem, consider carefully
32 ALERT level C = Check. Ensure it is not caused by an omission or oversight
25 ALERT level G = General information/check it is not something unexpected

13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
38 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
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.

