checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 200602_mof-508-no2__sq

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: 200602_mof-508-no2__sq

Bond precision: O- C = 0.0035 A Wavelength=0.41270

Cell: a=10.9023(3) b=10.9089(3) c=14.0384(3)
alpha=95.951(2) beta=91.201(2) gamma=100.414(2)
Temperature: 100 K

	Calculated	Reported
Volume	1631.92(7)	1631.92(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H12.32 N3 O10 Zn2, 0.072(N2 O4), 0.854(N O2) [+ solvent]	C26 H12.322 N3.999 O11.998 Zn2
Sum formula	C26 H12.32 N4 O12 Zn2 [+ solvent]	C26 H14 N4 O12 Zn2
Mr	703.41	705.15
Dx,g cm-3	1.431	1.435
Z	2	2
Mu (mm-1)	0.354	1.472
F000	704.6	708.0
F000’	705.48	
h,k,lmax	18,18,23	17,18,23
Nref	15818	14912
Tmin,Tmax		0.795,1.000
Tmin’		

Correction method= # Reported T Limits: Tmin=0.795 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.943 Theta(max)= 20.116

R(reflections)= 0.0752(12782) wR2(reflections)= 0.2074(14912)

S = 1.093 Npar= 342

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

```
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       3.19 eA-3
PLAT430_ALERT_2_B Short Inter D...A Contact  O8       ..N5B      .       2.60 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O8       ..N5A      .       2.72 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O8       ..O13B     .       2.84 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O10      ..N6B      .       2.67 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O10      ..O15B     .       2.79 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O11      ..N6A      .       2.59 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O11      ..N7B      .       2.66 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O11      ..O15A     .       2.78 Ang.
                                                     x,y,z  =      1_555 Check
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on       Zn2       1.66 eA-3
```

Alert level C

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..     Please Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O8 Check
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        Zn2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT430_ALERT_2_C Short Inter D...A Contact  O8       ..O13A     .       2.88 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  O11      ..O16B     .       2.87 Ang.
                                                     x,y,z  =      1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     4.067 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          8 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          9 Report
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Zn1       1.48 eA-3
```

Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C26 H14 N4 O12 Zn2
           Atom count from _chemical_formula_moiety:C26 H12.322 N4.004 O12.003 Zn
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C26 H14 N4 O12 Zn2
           Atom count from the _atom_site data:  C26 H12.32199 N4.003 O12.001 Zn2
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    2
```

From the CIF: _chemical_formula_sum C26 H14 N4 O12 Zn2
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	52.00	52.00	0.00
H	28.00	24.64	3.36
N	8.00	8.00	0.00
O	24.00	23.99	0.01
Zn	4.00	4.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 14 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.41270 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 66% Note
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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O15A 152.3 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact C19 ..N5B 2.99 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C19 ..N5A 3.00 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C26 ..N6B 2.94 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C26 ..N6A 2.96 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C26 ..N7B 2.97 Ang.
x,y,z = 1_555 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 38 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks 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= 0.600 863 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note
PLAT984_ALERT_1_G The Zn-f'= 0.2839 Deviates from the B&C-Value 0.2601 Check
PLAT985_ALERT_1_G The Zn-f"= 1.4301 Deviates from the B&C-Value 0.5357 Check

---

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
27 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
12 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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 04/06/2020; check.def file version of 02/06/2020

Datablock 200602_mof-508-no2__sq - ellipsoid plot