checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: Si- O = 0.0088 A Wavelength=0.71073

Cell: a=4.7587(3) b=7.6796(4) c=9.9669(6)
alpha=90 beta=90.263(6) gamma=90
Temperature: 696 K

	Calculated	Reported
Volume	364.24(4)	364.24(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Bi0.40 Mn0.47 O20 Si4.48 Y3.60, 3.52(Be)	?
Sum formula	Be3.52 Bi0.40 Mn0.47 O20 Si4.48 Y3.60	Be3.52 Bi0.40 Ca0 Mn0.48 O20 Si4.48 Y3.60
Mr	907.14	907.60
Dx,g cm-3	4.136	4.138
Z	1	1
Mu (mm-1)	19.898	19.905
F000	422.2	422.0
F000'	411.47	
h,k,lmax	6,10,13	6,10,13
Nref	975	873
Tmin,Tmax	0.678,0.672	
Tmin'	0.665	

Correction method= Not given

Data completeness= 0.895 Theta(max)= 29.083

R(reflections)= 0.0627(767) wR2(reflections)= 0.1347(873)

S = 1.211 Npar= 77

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

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      7.477 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.111 Check
```

Alert level G

```
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    1
          From the CIF: _chemical_formula_sum  Be3.52 Bi0.40 Ca0 Mn0.48 O20 Si4.4
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          Be         3.52      3.52    0.00
          Bi         0.40      0.40    0.00
          Ca         1.00      0.00    1.00
          Mn         0.48      0.47    0.01
          O         20.00     20.00    0.00
          Si         4.48      4.48    0.00
          Y          3.60      3.60    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      11.94 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Bi1        Constrained at        0.1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Y1         Constrained at        0.9 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mn1        Constrained at     0.2358 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Si2        Constrained at       0.12 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Be2        Constrained at       0.88 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        18% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% 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        103 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.0 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
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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
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
18 **ALERT level G** = General information/check it is not something unexpected

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

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  2 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
 10 ALERT type 4 Improvement, methodology, query or suggestion
  1 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 28/11/2022; check.def file version of 28/11/2022

Datablock shelx - ellipsoid plot