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 = 0.0190 A Wavelength=0.71073

Cell: a=4.7513(10) b=7.6230(18) c=10.0282(18)
alpha=90 beta=90.276(18) gamma=90
Temperature: ?

	Calculated	Reported
Volume	363.21(13)	363.21(13)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Bi0.40 Mn0.86 O20 Si4.48 Y3.60, 1.76(Be2)	?
Sum formula	Be3.52 Bi0.40 Mn0.86 O20 Si4.48 Y3.60	Be3.52 H4 Bi0.40 Ca0 Mn0.86 O20 Si4.48 Y3.60
Mr	928.52	932.51
Dx,g cm-3	4.245	4.263
Z	1	1
Mu (mm-1)	20.278	20.278
F000	431.9	436.0
F000'	421.33	
h,k,lmax	6,10,13	6,10,13
Nref	967	874
Tmin,Tmax	0.673,0.667	
Tmin'	0.660	

Correction method= Not given

Data completeness= 0.904 Theta(max)= 29.015

R(reflections)= 0.1022(432) wR2(reflections)= 0.2706(874)

S = 1.054 Npar= 72

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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.211

Author Response: The quality of the crystal is not good due to decomposition process

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.211 Report

Author Response: The quality of the crystal is not good due to decomposition process

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.55Ang From O5 3.17 eA-3

Author Response: The quality of the crystal is not good due to decomposition process

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Alert level C

PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ... 2.889 Sigma
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.99 Check
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.27 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.21 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 1 Check
Be2
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 10.237 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.476 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.083 Check
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.99Ang From O4 . -1.03 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From O1 . -0.83 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 1.06Ang From O5 . -0.83 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.72Ang From O1 . -0.81 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.62Ang From O4 . -0.81 eA-3

Alert level G

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:H4 Be3.52 Bi0.4 Mn0.86 O20 Si4.4
Atom count from the _atom_site data: Be3.52 Bi0.4 Mn0.8608 O20 Si4.48
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 H4 Bi0.40 Ca0 Mn0.86 O20 Si
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Be	3.52	3.52	0.00
H	4.00	0.00	4.00
Bi	0.40	0.40	0.00
Ca	1.00	0.00	1.00
Mn	0.86	0.86	-0.00
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
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	0.4304	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)	21%	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	93	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.9	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
3 **ALERT level B** = A potentially serious problem, consider carefully
17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
17 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
11 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