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

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Bond precision:    Si- O = 0.0090 A           Wavelength=0.71073

Cell:              a=4.7560(4)      b=7.6721(5)           c=9.9678(7)
                   alpha=90         beta=90.265(7)        gamma=90
Temperature:       293 K
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	Calculated	Reported
Volume	363.71(5)	363.71(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Bi0.40 H4 Mn0.47 O20 Si4.48 Y3.60, 3.52(Be)	?
Sum formula	Be3.52 Bi0.40 H4 Mn0.47 O20 Si4.48 Y3.60	Be3.52 H4 Bi0.40 Ca0 Mn0.48 O20 Si4.48 Y3.60
Mr	911.17	911.63
Dx,g cm-3	4.160	4.162
Z	1	1
Mu (mm-1)	19.928	19.935
F000	426.2	426.0
F000'	415.46	
h,k,lmax	6,10,13	6,10,13
Nref	1014	872
Tmin,Tmax	0.555,0.550	
Tmin'	0.544	

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Correction method= Not given

Data completeness= 0.860           Theta(max)= 29.416


R(reflections)= 0.0630( 752)                      wR2(reflections)=
                                                  0.1388( 872)
S = 1.222                    Npar= 81
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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

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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
PLAT245_ALERT_2_C U(iso) H1       Smaller than U(eq) O5       by       0.015 Ang**2
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      6.716 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.063 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.80Ang From O4      .      -0.83 eA-3
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⚪ Alert level G

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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 Mn0.48 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       4.00    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
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         2 Note
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
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)       293 Check
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
PLAT303_ALERT_2_G Full Occupancy Atom H1        with # Connections      1.59 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         1 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       139 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.1 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
   8 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

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 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
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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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