checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: BiI3-hs3112030

Bond precision: Bi- I = 0.0167 A Wavelength=0.41312

Cell: a=4.044(2) b=12.796(7) c=9.493(4)
alpha=90 beta=90 gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	491.2(4)	491.3(6)
Space group	C m c m	C m c m
Hall group	-C 2c 2	?
Moiety formula	Bi I3	?
Sum formula	Bi I3	BiI3
Mr	589.68	589.67
Dx,g cm-3	7.974	7.971
Z	4	4
Mu (mm-1)	13.129	14.920
F000	968.0	968.0
F000’	943.02	
h,k,lmax	4,12,9	
Nref	166	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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

```
POWD002_ALERT_1_B _refine_ls_goodness_of_fit_all is missing (this is chi, i.e.
              the square root of 'chi squared'). This should be
              present for a powder diffraction study.
POWD004_ALERT_1_B No 'Bragg' R factor has been given. Please supply a value
              for _refine_ls_R_factor_all [R(F)], _refine_ls_R_Fsqd_factor
              [R(F^2)] or _refine_ls_R_I_factor [R(I)].
```

Alert level C

```
REFI015_ALERT_1_C  _refine_ls_shift/su_max is missing
            Maximum shift/s.u. ratio after final refinement cycle.
            The following tests will not be performed
            SHFSU_01
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT702_ALERT_1_C Angle   Calc     79.3(3), Rep    79.61(4), Dev..       1.03 Sigma
              I2      -BI      -I2        11.564  1.555 11.464     #   20 Check
PLAT702_ALERT_1_C Angle   Calc     79.3(3), Rep    79.61(4), Dev..       1.03 Sigma
              I2      -BI      -I2        13.566  1.555 13.466     #   35 Check
PLAT702_ALERT_1_C Angle   Calc     95.4(4), Rep    95.93(4), Dev..       1.32 Sigma
              BI      -I2      -I2        11.565  1.555 13.466     #  170 Check
PLAT702_ALERT_1_C Angle   Calc     95.4(4), Rep    95.93(4), Dev..       1.32 Sigma
              BI      -I2      -I2        11.465  1.555 13.566     #  181 Check
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Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.41312 Ang.
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         -2 Units
PLAT434_ALERT_2_G Short Inter HL..HL Contact I2       ..I2              3.55 Ang.
                                                 -x,y,3/2-z  =      7_556 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact I2       ..I2              3.58 Ang.
                                                  x,1-y,1-z  =      6_566 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Bi        (III)     .       3.26 Info
PLAT985_ALERT_1_G The Bi-f"=    4.4290 Deviates from the B&C-Value     4.4264 Check
PLAT986_ALERT_1_G No non-zero f' Anomalous Scattering Values Found     Please Check
```

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

  13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   1 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 07/08/2019; check.def file version of 30/07/2019

Datablock BiI3-hs3112030 - ellipsoid plot