checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SINHA20

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: SINHA20

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Bond precision:  C-C = 0.0128 A          Wavelength=0.71075

Cell:          a=7.8158(3)       b=10.6904(6)     c=11.1768(6)
               alpha=69.742(5)   beta=69.700(4)   gamma=70.830(4)
Temperature:   93 K
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	Calculated	Reported
Volume	798.34(8)	798.34(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Bi I4, C7 H11 N2	C7 H11 Bi I4 N2
Sum formula	C7 H11 Bi I4 N2	C7 H11 Bi I4 N2
Mr	839.76	839.78
Dx,g cm-3	3.493	3.493
Z	2	2
Mu (mm-1)	18.751	18.734
F000	724.0	724.0
F000’	712.81	
h,k,lmax	11,15,16	10,15,16
Nref	5436	4899
Tmin,Tmax	0.011,0.570	0.161,0.570
Tmin’	0.005	

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Correction method= # Reported T Limits: Tmin=0.161 Tmax=0.570
AbsCorr = MULTI-SCAN

Data completeness= 0.901          Theta(max)= 31.740

R(reflections)= 0.0522( 4367)     wR2(reflections)= 0.1445( 4899)

S = 1.038                 Npar= 131
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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 A

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.82A From Bi1 5.66 eA-3
PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.82A From Bi1 5.65 eA-3
PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.83A From Bi1 -6.03 eA-3
PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.72A From Bi1 -5.70 eA-3
PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.63A From Bi1 -3.88 eA-3
PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.64A From Bi1 -3.60 eA-3

Alert level B

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.82A From I5 3.31 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.92A From I4 3.24 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.87A From I3 3.00 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.84A From I5 2.99 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.83A From I3 2.89 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.88A From Bi1 2.86 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.79A From I4 2.58 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.79A From I4 -3.40 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.75A From I4 -3.35 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.79A From I5 -3.27 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.79A From I5 -3.13 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.74A From I3 -3.03 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.80A From I2 -2.99 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.76A From Bi1 -2.97 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.86A From I3 -2.92 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.29A From Bi1 -2.83 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.30A From Bi1 -2.55 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.58A From I4 -2.54 eA-3

Alert level C

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01275 Ang.
PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N6 - H6 . 1.03 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 46 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 16 Note
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.85A From Bi1 2.50 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.80A From I2 2.46 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.37A From Bi1 2.45 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.85A From I2 2.30 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.27A From I4 2.19 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.10A From Bi1 2.14 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.27A From I5 2.05 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.93A From I3 2.00 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.12A From Bi1 1.96 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.28A From I4 1.94 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.86A From I2 1.87 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.28A From I2 1.81 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.80A From Bi1 1.81 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.79A From I4 1.79 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.96A From I3 1.76 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.67A From Bi1 1.73 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.81A From I2 -2.40 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.73A From I5 -2.33 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.14A From Bi1 -2.24 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.75A From Bi1 -2.24 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.56A From I2 -2.22 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.52A From I3 -2.21 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.56A From I5 -2.03 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.77A From I4 -1.89 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.23A From I4 -1.88 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.40A From Bi1 -1.75 eA-3

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PLAT977_ALERT_2_C Check Negative Difference Density on H8              -0.53 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10             -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H13B            -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H13C            -0.59 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H14A            -0.66 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
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Alert level G

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CHEMS02_ALERT_1_G  Please check that you have entered the correct
           _publ_requested_category classification of your compound;
           FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
           FO or CO or EO for organic.
           From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or A
           From the CIF: _chemical_formula_sum :C7 H11 Bi1 I4 N2
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Bi1      --I4_a     .       7.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Bi1      --I5_b     .       6.3 s.u.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C13 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C14 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.13 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Bi1       (III)     .      3.04 Info
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......    Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       420 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         1 Note
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6 **ALERT level A** = Most likely a serious problem - resolve or explain
18 **ALERT level B** = A potentially serious problem, consider carefully
36 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
59 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
4 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 22/12/2019; check.def file version of 13/12/2019

Datablock SINHA20 - ellipsoid plot