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: b_120k

Bond precision: C-C = 0.0070 A Wavelength=0.71073

Cell: a=7.0858(3) b=7.6608(3) c=8.2660(4)
alpha=68.185(4) beta=84.185(4) gamma=89.502(4)
Temperature: 120 K

	Calculated	Reported
Volume	414.22(3)	414.22(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C4 H16 I2 N4 Pt, 2(I), 2(H2O)	C4 H16 I2 N4 Pt, 2(I), 2(H2O)
Sum formula	C4 H20 I4 N4 O2 Pt	C4 H20 I4 N4 O2 Pt
Mr	858.92	858.93
Dx,g cm-3	3.443	3.443
Z	1	1
Mu (mm-1)	15.915	15.915
F000	378.0	378.0
F000'	374.72	
h,k,lmax	10,11,12	10,10,12
Nref	2838	2354
Tmin,Tmax	0.058,0.204	0.307,1.000
Tmin'	0.030	

Correction method= # Reported T Limits: Tmin=0.307 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.829 Theta(max)= 31.823

R(reflections)= 0.0330(2341) wR2(reflections)= 0.0868(2354)

S = 1.129 Npar= 73

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.975 Why?
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 6 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.004 Degree
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # I 2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.8 Low

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

1 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
2 ALERT type 3 Indicator that the structure quality may be low
2 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 06/07/2023; check.def file version of 30/06/2023

Datablock b_120k - ellipsoid plot