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: a_120k

```
Bond precision:   C-C = 0.0060 A          Wavelength=0.71073

Cell:             a=21.6964(5)     b=9.5333(2)          c=13.5282(4)
                  alpha=90         beta=101.775(2)      gamma=90
Temperature:      120 K

                 Calculated                Reported
Volume           2739.27(12)               2739.27(12)
Space group      C 2/c                     C 1 2/c 1
Hall group       -C 2yc                    -C 2yc
Moiety formula   C8 H32 I3 N8 Pt2, 3(I)    C8 H32 I3 N8 Pt2, 3(I)
Sum formula      C8 H32 I6 N8 Pt2          C8 H32 I6 N8 Pt2
Mr               1391.98                   1391.99
Dx,g cm-3        3.375                     3.375
Z                4                         4
Mu (mm-1)        16.975                    16.975
F000             2440.0                    2440.0
F000'            2417.28
h,k,lmax         32,14,20                  31,13,19
Nref             4693                      4177
Tmin,Tmax        0.548,0.712               0.484,0.728
Tmin'            0.424

Correction method= # Reported T Limits: Tmin=0.484 Tmax=0.728
AbsCorr = EMPIRICAL

Data completeness= 0.890           Theta(max)= 31.837

R(reflections)= 0.0254( 3996)                wR2(reflections)=
                                             0.0624( 4177)
S = 1.047                  Npar= 111
```

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field. Absorption correction given as empirical

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	8	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	18.84	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pt1 --I2 .	15.2	s.u.
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3)	0.50	Check
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	4	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.4	Low

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 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 a_120k - ellipsoid plot