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: Crystal

```
Bond precision:    C-C = 0.0050 A            Wavelength=1.79725

Cell:              a=5.8207(3)      b=11.2873(5)        c=6.3126(4)
                   alpha=90         beta=90             gamma=90
Temperature:       298 K

                   Calculated                Reported
Volume             414.74(4)                 414.74(4)
Space group        P n m a                   P n m a
Hall group         -P 2ac 2n                 -P 2ac 2n
Moiety formula     C2 H0.06 D0.94 O5 Sb      ?
Sum formula        C2 H0.06 D0.94 O5 Sb      C2 D0.936 H0.064 O5 Sb
Mr                 227.73                    227.70
Dx,g cm-3          3.647                     0.000
Z                  4                         4
Mu (mm-1)          0.000                     0.000
F000               215.6                     0.0
F000'              415.97
h,k,lmax           6,11,6
Nref               266
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 A
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value ....   Please Do !
powder!

🟠 Alert level B
PLAT430_ALERT_2_B Short Inter D...A Contact O3   ..O3   .   2.59 Ang.
typical values for oxalates   x,3/2-y,z =   7_565 Check

🟡 Alert level C
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check

⚪ Alert level G
RADNT01_ALERT_1_G Extra text has been found in the _diffrn_radiation_type field.
            Radiation given as Constant Wavelength Neutron Diffraction
            Radiation identified as neutron
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info

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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 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
   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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT699_Crystal
;
PROBLEM: Missing _exptl_crystal_description Value .......    Please Do !
RESPONSE: ...
;
_vrf_PLAT430_Crystal
;
PROBLEM: Short Inter D...A Contact  O3       ..O3      .       2.59 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 22/12/2019; check.def file version of 13/12/2019