checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ysb2o4cl

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: ysb2o4cl

```
Bond precision:   Sb- O = 0.0080 A          Wavelength=0.71069

Cell:               a=7.7356(4)      b=7.7356(4)      c=8.7891(6)
                    alpha=90         beta=90          gamma=90
Temperature:        293 K

                 Calculated                  Reported
Volume           525.94(7)                   525.94(5)
Space group      P 4 21 2                    P4212
Hall group       P 4ab 2ab                   ?
Moiety formula   Cl O4 Sb2 Y                 ?
Sum formula      Cl O4 Sb2 Y                 Cl O4 Sb2 Y
Mr               431.88                      431.86
Dx,g cm-3        5.454                       5.454
Z                4                           4
Mu (mm-1)        21.560                      21.560
F000             760.0                       760.0
F000'            745.26
h,k,lmax         10,10,11                    10,10,11
Nref             605[ 396]                   606
Tmin,Tmax        0.529,0.824                 0.372,0.857
Tmin'            0.409

Correction method= # Reported T Limits: Tmin=0.372 Tmax=0.857
AbsCorr = NUMERICAL

Data completeness= 1.53/1.00        Theta(max)= 27.400

R(reflections)= 0.0399( 548)                wR2(reflections)=
                                            0.0848( 606)
S = 1.090                  Npar= 41
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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 C

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STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.450
          From the CIF: _refine_ls_abs_structure_Flack_su    0.060
PLAT199_ALERT_1_C Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_C Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.79A   From Sb             1.77 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.75A   From Sb            -1.67 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.96A   From O2             0.79 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.85A   From O1            -0.72 eA-3
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.450 Note
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         m         85 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         a         85 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         m         85 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         a         85 %Fit
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         2 Units
PLAT794_ALERT_5_G Tentative Bond Valency for Sb        (III)     .       2.79 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y1        (III)     .       3.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y2        (III)     .       3.00 Info
PLAT899_ALERT_4_G SHELXL97  is Deprecated and Succeeded by SHELXL/       2018 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  12 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   5 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 13/07/2021; check.def file version of 13/07/2021

Datablock ysb2o4cl - ellipsoid plot