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: njy1

Bond precision: O- O = 0.0120 A Wavelength=0.71073

Cell: a=17.680(5) b=13.346(4) c=26.399(8)
alpha=90 beta=90 gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	6229(3)	6229(3)
Space group	P n m a	Pnma
Hall group	-P 2ac 2n	?
Moiety formula	As8 Cs2 Nb16 O88, 2(Cs O4), 36(O), 6(Cs), 8(Na)	?
Sum formula	As8 Cs10 Na8 Nb16 O132	As4 Cs5 H25 Na4 Nb8 O66
Mr	5710.94	2880.67
Dx,g cm-3	3.045	3.072
Z	2	4
Mu (mm-1)	6.565	6.566
F000	5228.0	5328.0
F000'	5157.31	
h,k,lmax	21,15,31	21,15,31
Nref	5742	5707
Tmin,Tmax	0.373,0.455	0.420,0.506
Tmin'	0.336	

Correction method= MULTI-SCAN

Data completeness= 0.994 Theta(max)= 25.000

R(reflections)= 0.0513(4647) wR2(reflections)= 0.1740(5707)

S = 1.073 Npar= Npar = 457

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 B

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O1W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O2W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O3W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O4W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O5W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O6W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O7W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O8W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O9W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O10W Check
```

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..      50.40 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
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Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:H25 As4 Cs5 Na4 Nb8 O66
            Atom count from the _atom_site data:  As4 Cs5 Na4 Nb8 O66
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  As4 Cs5 H25 Na4 Nb8 O66
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           As        16.00     16.00    0.00
           Cs        20.00     20.00    0.00
           H        100.00      0.00  100.00
           Na        16.00     16.00    0.00
           Nb        32.00     32.00    0.00
           O        264.00    264.00    0.00
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by .............      0.50 Ratio
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.11 Why ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      56.31 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cs5    --  O1      ..       10.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cs5    --  O23_a   ..       13.2 su
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          2 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =         12 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         11 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         14 Note
            Cs
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         15 Note
            Cs
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         17 Note
            Na
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
10 **ALERT level B** = A potentially serious problem, consider carefully

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  3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 17 ALERT level G = General information/check it is not something unexpected

  6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 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
  7 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
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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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock njy1 - ellipsoid plot