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: nacareniobsite-Y

Bond precision: Si- O = 0.0043 A Wavelength=0.71073

Cell: a=7.4069(15) b=5.6540(11) c=18.787(4)
alpha=90 beta=101.36(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	771.4(3)	771.3(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Nb1.67 O28 Si8 Y3.37, 7.776(F), 2.888(Sr), 4(Na0.55), 4(Na1.09)	?
Sum formula	F7.78 Na6.54 Nb1.67 O28 Si8 Sr2.89 Y3.37	Ca3.06 Ce0.15 Dy0.08 F3 Ho0.02 La0.04 Na2.82 Nb0.64 Nd0.16 O15
Mr	1678.33	793.65
Dx,g cm-3	3.613	3.417
Z	1	2
Mu (mm-1)	12.365	5.813
F000	787.4	760.0
F000'	771.51	
h,k,lmax	9,7,24	9,7,24
Nref	1774	1863
Tmin,Tmax	0.755,0.890	0.549,0.746
Tmin'	0.740	

Correction method= # Reported T Limits: Tmin=0.549 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 1.050 Theta(max)= 27.494

R(reflections)= 0.0350(1788)

wR2(reflections)= 0.0972(1863)

S = 1.081 Npar= 145

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

ABSMU01_ALERT_1_A The ratio of given/expected absorption coefficient lies outside the range 0.90 <> 1.10
Calculated value of mu = 3.768
Value of mu given = 5.813
SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 0.868
Additional refinement cycles may be required.
PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 112.72 %
PLAT075_ALERT_1_A Occupancy 1.099 Greater Than 1.0 for MO2
PLAT075_ALERT_1_A Occupancy 1.086 Greater Than 1.0 for MO3
PLAT080_ALERT_2_A Maximum Shift/Error ..... 0.87 Why ?

Alert level B

CHEMW01_ALERT_1_B The ratio of given/expected molecular weight as calculated from the _chemical_formula_sum lies outside the range 0.95 <> 1.05
Calculated formula weight = 755.6865
Formula weight given = 793.6500
PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 91.03 Check

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Alert level C

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT213_ALERT_2_C Atom Mo1 has ADP max/min Ratio ..... 3.3 prolat

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Alert level G

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:Ca3.06 Ce0.15 Dy.08 F3 Ho.02 La.
Atom count from the _atom_site data: F3.8878 Na3.271 Nb0.834 O14 Si4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum Ca3.06 Ce0.15 Dy0.08 F3 Ho0.02 La0
TEST: Compare cell contents of formula and atom_site data
WARNING: Unexpected atom type is in site list: Y
WARNING: Unexpected atom type is in site list: Sr
WARNING: Formula and atom_type_symbol element names mismatch.

atom Z*formula cif sites diff

```
            Ca          6.12      0.00    6.12
            Ce          0.30      0.00    0.30
            Dy          0.16      0.00    0.16
            F           6.00      7.78   -1.78
            Ho          0.04      0.00    0.04
            La          0.08      0.00    0.08
            Na          5.64      6.54   -0.90
            Nb          1.28      1.67   -0.39
            Nd          0.32      0.00    0.32
            O          30.00     28.00    2.00
            Pr          0.02      0.00    0.02
            Si          8.00      8.00    0.00
            Sm          2.00      0.00    2.00
             WARNING: Site labels do not match formula elements
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of MH       as          Y
PLAT017_ALERT_1_G Check Scattering Type Consistency of AP       as          SR
PLAT017_ALERT_1_G Check Scattering Type Consistency of MO1      as          NB
PLAT017_ALERT_1_G Check Scattering Type Consistency of       MO2as          NA
PLAT017_ALERT_1_G Check Scattering Type Consistency of       MO3as          NA
PLAT017_ALERT_1_G Check Scattering Type Consistency of XM       as          F
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Xm         Constrained at     0.9439 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        16% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          6 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.8 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       55.0 Degree
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6 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

19 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
6 ALERT type 4 Improvement, methodology, query or suggestion
2 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_ABSMU01_nacareniobsite-Y
;
PROBLEM: The ratio of given/expected absorption coefficient lies
RESPONSE: ...
;
_vrf_SHFSU01_nacareniobsite-Y
;
PROBLEM: The absolute value of parameter shift to su ratio > 0.20
RESPONSE: ...
;
_vrf_PLAT051_nacareniobsite-Y
;
PROBLEM: Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .     112.72 %
RESPONSE: ...
;
_vrf_PLAT075_nacareniobsite-Y
;
PROBLEM: Occupancy      1.099 Greater Than 1.0 for ......          MO2
RESPONSE: ...
;
_vrf_PLAT080_nacareniobsite-Y
```

```
;
PROBLEM: Maximum Shift/Error ..........................       0.87 Why ?
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock nacareniobsite-Y - ellipsoid plot