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-Ce

Bond precision: Si- O = 0.0097 A Wavelength=0.71073

Cell: a=7.4684(15) b=5.6891(11) c=18.891(4)
alpha=90 beta=101.37(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	786.9(3)	786.9(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	F4 Nb1.78 O28 Si8 Y7.23, 3.778(F), 3.525(Ca)	?
Sum formula	Ca3.53 F7.78 Nb1.78 O28 Si8 Y7.23	Ca3.01 Ce0.55 F2.76 Gd0.02 La0.23 Na2.77 Nb0.77 Nd0.22 O15.24 P
Mr	1769.47	838.50
Dx,g cm-3	3.734	3.539
Z	1	2
Mu (mm-1)	14.809	5.650
F000	831.2	794.9
F000'	809.43	
h,k,lmax	8,6,22	8,6,22
Nref	1380	1456
Tmin,Tmax	0.307,0.919	
Tmin'	0.262	

Correction method= Not given

Data completeness= 1.055 Theta(max)= 24.996

R(reflections)= 0.0680(1421)

wR2(reflections)= 0.1735(1456)

S = 1.510 Npar= 124

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

PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 162.11 %
PLAT058_ALERT_1_A Maximum Transmission Factor Missing ..... ?
PLAT059_ALERT_1_A Minimum Transmission Factor Missing ..... ?
PLAT213_ALERT_2_A Atom O4 has ADP max/min Ratio ..... 8.0 oblate

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Alert level B

ABSMU01_ALERT_1_B The ratio of given/expected absorption coefficient lies
outside the range 0.95 <> 1.05
Calculated value of mu = 5.215
Value of mu given = 5.650
PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 92.47 Check
PLAT213_ALERT_2_B Atom Mo1 has ADP max/min Ratio ..... 4.8 prolat
PLAT213_ALERT_2_B Atom Mh has ADP max/min Ratio ..... 4.1 oblate
PLAT213_ALERT_2_B Atom MhA has ADP max/min Ratio ..... 4.1 oblate

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Alert level C

CHEMW01_ALERT_1_C The ratio of given/expected molecular weight as calculated
from the _chemical_formula_sum lies outside
the range 0.99 <> 1.01
Calculated formula weight = 817.0982
Formula weight given = 838.5000
SHFSU01_ALERT_2_C The absolute value of parameter shift to su ratio > 0.05
Absolute value of the parameter shift to su ratio given 0.060
Additional refinement cycles may be required.
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check
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
PLAT080_ALERT_2_C Maximum Shift/Error ..... 0.06 Why ?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.94 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 3.31 eA-3
PLAT213_ALERT_2_C Atom Si1 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom Si2 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom O2 has ADP max/min Ratio ..... 3.5 prolat
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O7 Check

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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:Ca3.01 Ce0.55 F2.76 Gd.02 La0.23
Atom count from the _atom_site data: Ca1.7625 F3.888800 Nb0.8888 O14
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

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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  Ca3.01 Ce0.55 F2.76 Gd0.02 La0.23
          TEST: Compare cell contents of formula and atom_site data
          WARNING: Unexpected atom type is in site list: Y
          WARNING: Formula and atom_type_symbol element names mismatch.

          atom    Z*formula  cif sites diff
          Ca         6.02      3.53    2.49
          Ce         1.10      0.00    1.10
          F          5.52      7.78   -2.26
          Gd         0.04      0.00    0.04
          La         0.46      0.00    0.46
          Na         5.54      0.00    5.54
          Nb         1.54      1.78   -0.24
          Nd         0.44      0.00    0.44
          O         30.48     28.00    2.48
          Pr         0.12      0.00    0.12
          Si         8.02      8.00    0.02
          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         Y
PLAT017_ALERT_1_G Check Scattering Type Consistency of MO1      as         NB
PLAT017_ALERT_1_G Check Scattering Type Consistency of       MO2as         CA
PLAT017_ALERT_1_G Check Scattering Type Consistency of       MO3as         CA
PLAT017_ALERT_1_G Check Scattering Type Consistency of XM       as         F
PLAT017_ALERT_1_G Check Scattering Type Consistency of APA      as         Y
PLAT017_ALERT_1_G Check Scattering Type Consistency of MHA      as         Y
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       9.00 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          6 Report
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 Mo1        Constrained at     0.8888 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mh         Constrained at     0.8519 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ap         Constrained at     0.7338 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Xm         Constrained at     0.9444 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo2        Constrained at     0.5905 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo3        Constrained at      0.586 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        21% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% 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 ..........          8 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
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 !
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 ..       50.0 Degree
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4 **ALERT level A** = Most likely a serious problem - resolve or explain
5 **ALERT level B** = A potentially serious problem, consider carefully

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

 22 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
  2 ALERT type 3 Indicator that the structure quality may be low
 13 ALERT type 4 Improvement, methodology, query or suggestion
  3 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* 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_PLAT051_nacareniobsite-Ce
;
PROBLEM: Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .     162.11 %
RESPONSE: ...
;
_vrf_PLAT058_nacareniobsite-Ce
;
PROBLEM: Maximum Transmission Factor Missing .............          ?
RESPONSE: ...
;
_vrf_PLAT059_nacareniobsite-Ce
```

```
;
PROBLEM: Minimum Transmission Factor Missing .....          ?
RESPONSE: ...
;
_vrf_PLAT213_nacareniobsite-Ce
;
PROBLEM: Atom O4              has ADP max/min Ratio .....        8.0 oblate
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock nacareniobsite-Ce - ellipsoid plot