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: kalyuzhnyite-Ce

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Bond precision:    Si- O = 0.0098 A          Wavelength=0.71073

Cell:              a=18.647(4)      b=11.214(2)          c=14.642(3)
                   alpha=90         beta=129.55(3)       gamma=90
Temperature:       293 K

                   Calculated                Reported
Volume             2360.8(13)                2360.9(11)
Space group        P 2/c                     P 2/c
Hall group         -P 2yc                    -P 2yc
                   F4 K0.45 Nd3.80 O88 Pb1.46
Moiety formula     Si32 Ti4, Cs1.14 H8 O4,   ?
                   0.254(Ca2),
                   Ca Cs1.14 F4 H8 K1.15     Ba0.24 H25.68 Ca1.48 Cs1.20
Sum formula        Na3.03 Nd3.80 O100.38     F3.60 K1.48 Na4.28 Nb0.16
                   Pb1.46 Si32 Sr4.03        Nd4.10 O1
Mr                 4290.37                   4436.47
Dx,g cm-3          3.018                     3.120
Z                  1                         1
Mu (mm-1)          8.328                     8.233
F000               2021.7                    2101.0
F000'              2014.97
h,k,lmax           24,14,19                  24,14,19
Nref               5426                      5562
Tmin,Tmax          0.568,0.814               0.765,0.901
Tmin'              0.556

Correction method= # Reported T Limits: Tmin=0.765 Tmax=0.901
AbsCorr = EMPIRICAL

Data completeness= 1.025              Theta(max)= 27.499
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R(reflections)= 0.0274(3907)   wR2(reflections)=
                                                 0.0809(5562)

S = 1.033   Npar= 409

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 =   4.797
           Value of mu given   =   8.233
CHEMW01_ALERT_1_A The ratio of given/expected molecular weight as calculated
           from the _chemical_formula_sum lies outside
           the range 0.90 <> 1.10
           Calculated formula weight = 2920.8442
           Formula weight given   = 4436.4702
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   2.814
           Additional refinement cycles may be required.
PLAT031_ALERT_4_A Refined Extinction Parameter Within Range of ...   0.000 Sigma
PLAT075_ALERT_1_A Occupancy   1.008 Greater Than 1.0 for ......   SR
PLAT080_ALERT_2_A Maximum Shift/Error ....   2.81 Why ?
PLAT214_ALERT_2_A Atom Ca1   (Anion/Solvent) ADP max/min Ratio   6.9 oblate
PLAT430_ALERT_2_A Short Inter D...A Contact W7   ..W7   .   2.41 Ang.
                                         -x,y,1/2-z =   2_555 Check
PLAT430_ALERT_2_A Short Inter D...A Contact W8   ..W8   .   2.33 Ang.
                                         -x,y,1/2-z =   2_555 Check

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🟠 Alert level B
PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by ..   146.10 Check
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group   P2/m Check
           Check Model Parameter Symmetry for Reflection Data Support
PLAT213_ALERT_2_B Atom O3   has ADP max/min Ratio .....   4.2 oblate
PLAT430_ALERT_2_B Short Inter D...A Contact O6   ..W7   .   2.79 Ang.
                                         x,1-y,-1/2+z =   4_565 Check
PLAT430_ALERT_2_B Short Inter D...A Contact W3   ..W3   .   2.67 Ang.
                                         -x,y,1/2-z =   2_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact W4   ..W4   .   2.57 Ang.
                                         -x,y,1/2-z =   2_555 Check

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🟡 Alert level C
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .   1.15 %
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
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.10 Report
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   F Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor W1   --H2   .   Please Check
PLAT430_ALERT_2_C Short Inter D...A Contact O4   ..W9   .   2.86 Ang.
                                         1-x,y,1/2-z =   2_655 Check

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:H25.68 Ba0.24 Ca1.48 Cs1.2 F3.6
               Atom count from the _atom_site data:  H8 Ca1. Cs1.14 F4 K1.146 Na3.028
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    1
              From the CIF: _chemical_formula_sum  Ba0.24 H25.68 Ca1.48 Cs1.20 F3.60
              TEST: Compare cell contents of formula and atom_site data
              WARNING: Unexpected atom type is in site list: Sr
              WARNING: Unexpected atom type is in site list: Ti
              WARNING: Formula and atom_type_symbol element names mismatch.

              atom    Z*formula  cif sites diff
              Ba        0.24       0.00    0.24
              H        25.68       8.00   17.68
              Ca        1.48       1.00    0.48
              Cs        1.20       1.14    0.06
              F         3.60       4.00   -0.40
              K         1.48       1.15    0.33
              Na        4.28       3.03    1.25
              Nb        0.16       0.00    0.16
              Nd        4.10       3.80    0.30
              O       100.84     100.37    0.47
              Pb        0.96       1.46   -0.50
              Si        3.00      32.00  -29.00
               WARNING: Site labels do not match formula elements
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          5 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          8 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of X          as         F
PLAT017_ALERT_1_G Check Scattering Type Consistency of W1         as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W2         as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W3         as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W4         as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W5         as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W6         as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W7         as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W8         as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W9         as         O
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       9.36 Why ?
PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Translation ...        ? Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem       c/2      100 %Fit
PLAT116_ALERT_2_G ADDSYM Included (Pseudo) Lattice Translation ... Please Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...        2 Units
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        5 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 Ca1        Constrained at   0.1272 Check
PLAT300_ALERT_4_G Atom Site Occupancy of W2         Constrained at   0.4176 Check
PLAT300_ALERT_4_G Atom Site Occupancy of W3         Constrained at   0.2759 Check
PLAT300_ALERT_4_G Atom Site Occupancy of W4         Constrained at   0.3219 Check
PLAT300_ALERT_4_G Atom Site Occupancy of W5         Constrained at   0.3933 Check
PLAT300_ALERT_4_G Atom Site Occupancy of W6         Constrained at   0.1374 Check
PLAT300_ALERT_4_G Atom Site Occupancy of W7         Constrained at   0.2565 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of W8         Constrained at      0.241 Check
PLAT300_ALERT_4_G Atom Site Occupancy of W9         Constrained at     0.2468 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca2        Constrained at     0.1217 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )          8% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2 )         36% 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5 )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6 )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7 )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8 )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9 )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10 )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11 )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 13 )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 14 )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 15 )        100% Note
PLAT303_ALERT_2_G Full Occupancy Atom H1      with # Connections        1.75 Check
PLAT303_ALERT_2_G Full Occupancy Atom H2      with # Connections        1.39 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         W2 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         W3 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         W4 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         W5 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         W6 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         W7 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         W8 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         W9 Check
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O4        .    135.1 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O6        .    124.4 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O7        .    134.6 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O8        .    139.1 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O13       .    139.3 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O17       .    125.1 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        10 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         5 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 !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.9 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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 9 ALERT level A = Most likely a serious problem - resolve or explain
 6 ALERT level B = A potentially serious problem, consider carefully
 7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
71 ALERT level G = General information/check it is not something unexpected

22 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
38 ALERT type 2 Indicator that the structure model may be wrong or deficient
 3 ALERT type 3 Indicator that the structure quality may be low
28 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_kalyuzhnyite-Ce
;
PROBLEM: The ratio of given/expected absorption coefficient lies
RESPONSE: ...
;
_vrf_CHEMW01_kalyuzhnyite-Ce
;
PROBLEM: The ratio of given/expected molecular weight as calculated
RESPONSE: ...
;
_vrf_SHFSU01_kalyuzhnyite-Ce
;
PROBLEM: The absolute value of parameter shift to su ratio > 0.20
RESPONSE: ...
;
_vrf_PLAT031_kalyuzhnyite-Ce
;
PROBLEM: Refined Extinction Parameter Within Range of ...      0.000 Sigma
RESPONSE: ...
;
_vrf_PLAT075_kalyuzhnyite-Ce
```

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;
PROBLEM: Occupancy      1.008 Greater Than 1.0 for ......           SR
RESPONSE: ...
;
_vrf_PLAT080_kalyuzhnyite-Ce
;
PROBLEM: Maximum Shift/Error ...........................     2.81 Why ?
RESPONSE: ...
;
_vrf_PLAT214_kalyuzhnyite-Ce
;
PROBLEM: Atom Ca1       (Anion/Solvent) ADP max/min Ratio      6.9 oblate
RESPONSE: ...
;
_vrf_PLAT430_kalyuzhnyite-Ce
;
PROBLEM: Short Inter D...A Contact  W7        ..W7       .      2.41 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 10/05/2023; check.def file version of 10/05/2023

Datablock kalyuzhnyite-Ce - ellipsoid plot