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: paramarkeyite

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Bond precision:   O- C = 0.0220 A          Wavelength=0.71075

Cell:             a=17.9507(7)     b=18.1030(8)         c=18.3688(13)
                  alpha=90         beta=108.029(8)      gamma=90
Temperature:      293 K
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	Calculated	Reported
Volume	5676.1(6)	5676.1(6)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C6 O22 U2, C6 O22 U2, C6 O22 U2, 2(C3 O11 U), 36.42(O), 0.24(Sr	?
Sum formula	C24 Ca14.08 Na1.68 O124.42 Sr0.24 U8	C3 H9.11 Ca1.76 Na0.21 O15.55 Sr0.03 U
Mr	4807.18	610.07
Dx,g cm-3	2.813	2.856
Z	2	16
Mu (mm-1)	12.271	12.272
F000	4369.1	4515.0
F000'	4225.42	
h,k,lmax	21,21,21	21,21,21
Nref	10028	9933
Tmin,Tmax	0.276,0.375	0.631,1.000
Tmin'	0.249	

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Correction method= # Reported T Limits: Tmin=0.631 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991           Theta(max)= 25.028
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R(reflections)= 0.0647(6657)

wR2(reflections)= 0.1472(9933)

S = 1.030 Npar= 788

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

PLAT213_ALERT_2_A Atom C8 has ADP max/min Ratio ..... 5.7 prolat
PLAT214_ALERT_2_A Atom O18 (Anion/Solvent) ADP max/min Ratio 6.8 prolat
PLAT214_ALERT_2_A Atom C5 (Anion/Solvent) ADP max/min Ratio 18.6 prolat

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Alert level B

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 73.38 Check
PLAT213_ALERT_2_B Atom O23 has ADP max/min Ratio ..... 4.4 prolat
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O18 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow2 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow3 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow4 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow5 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow6 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow7 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow8 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow9 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow10 Check

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Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please 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
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 8 Check
Ow11 Ow12 Ow13 Ow14 Ow16 Ow19 etc.
PLAT213_ALERT_2_C Atom O25 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom O27 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom O34 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom O35 has ADP max/min Ratio ..... 4.0 prolat
PLAT213_ALERT_2_C Atom O36 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C12 has ADP max/min Ratio ..... 3.3 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O27 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O35 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O15 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of U3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.5 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.6 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.7 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Ow6 0.104 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Ca8 0.105 Check
PLAT732_ALERT_1_C Angle Calc 179.65(17), Rep 179.7(5) ..... 2.94 s.u.-R

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            C12     -U4      -CA4        1_555  1_555  1_555     #  263 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:C3 H9.11 Ca1.76 Na0.21 O15.55 Sr
           Atom count from the _atom_site data:  C3 Ca1.76 Na0.21 O15.55249 Sr.03
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   16
          From the CIF: _chemical_formula_sum  C3 H9.11 Ca1.76 Na0.21 O15.55 Sr0.
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         48.00     48.00    0.00
          H        145.76      0.00  145.76
          Ca        28.16     28.16    0.00
          Na         3.36      3.36    0.00
          O        248.80    248.84   -0.04
          Sr         0.48      0.48    0.00
          U         16.00     16.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.12 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     176.60 Why ?
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 Ow11       Constrained at      0.945 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow12       Constrained at      0.655 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow13       Constrained at      0.737 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow14       Constrained at      0.773 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow16       Constrained at      0.592 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow19       Constrained at      0.582 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow21       Constrained at      0.697 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow22       Constrained at      0.547 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow15       Constrained at       0.47 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow17       Constrained at      0.482 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow18       Constrained at      0.437 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow20       Constrained at      0.431 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow23       Constrained at      0.486 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow24       Constrained at      0.376 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca8        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na8        Constrained at       0.38 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 15  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 16  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 17  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 18  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 19  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 20  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 21  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 22  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 23  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 24  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 25  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 26  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 27  )       100% Note
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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 28  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 29  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 36  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 37  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 38  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 39  )       100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow11 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow12 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow13 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow14 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow16 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow19 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow21 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow22 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow15 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow17 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow18 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow20 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow23 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow24 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Ow12     ..C10             2.88 Ang.
                                                    x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        24 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      2.66 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for U1        (VI)      .      6.25 Info
PLAT794_ALERT_5_G Tentative Bond Valency for U3        (VI)      .      6.40 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.9 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged    Please Check
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3 **ALERT level A** = Most likely a serious problem - resolve or explain
13 **ALERT level B** = A potentially serious problem, consider carefully
22 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
67 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
51 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
38 ALERT type 4 Improvement, methodology, query or suggestion
3 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 paramarkeyite - ellipsoid plot