

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: libbyite

Bond precision:	S- O = 0.0267 A	Wavelength=0.71075	
Cell:	a=10.7037(11)	b=10.7037(11)	c=31.824(2)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	3646.1(8)	3646.0(8)	
Space group	P 41 21 2	P 41 21 2	
Hall group	P 4abw 2nw	P 4abw 2nw	
Moiety formula	O68 S12 U8, 14(O), 3.52(N), 0.48(K), 5.6(Na)	?	
Sum formula	K0.48 N3.52 Na5.60 O82 S12 U8	H4.50 K0.25 N1.75 Na2.81 O41 S6 U4	
Mr	3797.79	1903.78	
Dx, g cm ⁻³	3.459	3.468	
Z	2	4	
Mu (mm ⁻¹)	18.248	18.249	
F000	3358.7	3377.0	
F000'	3212.49		
h, k, lmax	12, 12, 37	11, 12, 37	
Nref	3218[1944]	2829	
Tmin, Tmax	0.251, 0.694	0.589, 1.000	
Tmin'	0.052		

Correction method= # Reported T Limits: Tmin=0.589 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.46/0.88

Theta(max)= 25.018

R(reflections)= 0.0576(2421)

wR2(reflections)=
0.1676(2829)

S = 1.120

Npar= 236

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

PLAT029_ALERT_3_A	_diffrn_measured_fraction_theta_full value Low .	0.927	Why?
PLAT213_ALERT_2_A	Atom O10 has ADP max/min Ratio	5.5	prolat

Alert level B

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

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 ..	9.77	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
PLAT213_ALERT_2_C	Atom O7 has ADP max/min Ratio	3.7	oblate
PLAT214_ALERT_2_C	Atom Ow5 (Anion/Solvent) ADP max/min Ratio	4.2	oblate
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S3	Check

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:H4.5 K0.25 N1.75 Na2.81 O41 S6 U
Atom count from the _atom_site data: K0.24 N1.76 Na2.8 O41 S6 U4
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 H4.50 K0.25 N1.75 Na2.81 O41 S6 U4
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
H	18.00	0.00	18.00
K	1.00	0.96	0.04
N	7.00	7.04	-0.04
Na	11.24	11.20	0.04
O	164.00	164.00	0.00
S	24.00	24.00	0.00
U	16.00	16.00	0.00

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
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	169.72	Why ?
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	1	Report

PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
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 9)	100%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	5	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for U2 (VI) .	6.06	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	2	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

2 **ALERT level A** = Most likely a serious problem - resolve or explain
 4 **ALERT level B** = A potentially serious problem, consider carefully
 7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 18 **ALERT level G** = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 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
 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.

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

Datablock libbyte - ellipsoid plot

