

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: a

Bond precision: O- B = 0.0091 A Wavelength=0.71073

Cell: a=11.574(4) b=11.574(4) c=12.361(4)
 alpha=90 beta=90 gamma=120
Temperature: 296 K

	Calculated	Reported
Volume	1434.0(13)	1433.9(9)
Space group	P 63/m	P6(3)/m
Hall group	-P 6c	-P 6c
Moiety formula	6(B3 Cu O12 P2), 3(Na0.67 O0.67), 2(K), 10(Na0.50)	?
Sum formula	B18 Cu6 K2 Na10 O74 P12	B9 Cu3 H5 K Na5 O37 P6
Mr	2439.62	1224.78
Dx,g cm-3	2.825	2.825
Z	1	2
Mu (mm-1)	2.914	2.914
F000	1184.0	1184.0
F000'	1188.52	
h,k,lmax	14,14,15	14,14,15
Nref	1045	1040
Tmin,Tmax	0.538,0.627	0.518,0.653
Tmin'	0.464	

Correction method= MULTI-SCAN

Data completeness= 0.995 Theta(max)= 26.440

R(reflections)= 0.0525(741) wR2(reflections)= 0.1402(1040)

S = 1.051 Npar= 104

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 C

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	?
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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: H5 B9 Cu3 K1 Na5 O37 P6
Atom count from the _atom_site data: B9 Cu3 K1 Na5 O37 P6
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 2
From the CIF: _chemical_formula_sum B9 Cu3 H5 K Na5 O37 P6
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
B	18.00	18.00	0.00
Cu	6.00	6.00	0.00
H	10.00	0.00	10.00
K	2.00	2.00	0.00
Na	10.00	10.00	0.00
O	74.00	74.00	0.00
P	12.00	12.00	0.00

PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension .	1
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	?
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by	0.50 Ratio
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	12.06
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.l. Differ by ...	4 Units
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder	33 Perc.
PLAT793_ALERT_4_G	The Model has Chirality at P1 (Verify)	S

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 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*, 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.

