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: I

Bond precision: Si- O = 0.0072 A Wavelength=0.71073

Cell: a=10.1951(2) b=14.4697(2) c=14.8556(2)
alpha=90 beta=100.3961(8) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2155.52(6)	2155.52(6)
Space group	P 21/m	P 1 21/m 1
Hall group	-P 2yb	-P 2yb
Moiety formula	Mo3 O40 Si W9, 10(O)	?
Sum formula	Mo3 O50 Si W9	H24 Mo3 O50 Si1 W9
Mr	2770.47	2794.70
Dx,g cm-3	4.269	4.306
Z	2	2
Mu (mm-1)	24.897	24.899
F000	2412.0	2412.0
F000’	2390.11	
h,k,lmax	13,19,20	13,19,20
Nref	5740	5729
Tmin,Tmax	0.026,0.019	0.500,0.950
Tmin’	0.013	

Correction method= # Reported T Limits: Tmin=0.500 Tmax=0.950
AbsCorr = ?

Data completeness= 0.998 Theta(max)= 28.620

R(reflections)= 0.0284(4506) wR2(reflections)= wR= 0.0448(5729)

S = 1.920 Npar= 176

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

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

Alert level B

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 ?) ..... O20 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 .. 24.23 Check
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 7 Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 58 Ang3

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:H24 Mo3 O50 Si1 W9
Atom count from the _atom_site data: Mo3 O50 Si1 W9
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 H24 Mo3 O50 Si1 W9
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
H	48.00	0.00	48.00
Mo	6.00	6.00	0.00
O	100.00	100.00	0.00
Si	2.00	2.00	0.00
W	18.00	18.00	0.00

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.50) in Resd. # 2 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.50) in Resd. # 5 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.50) in Resd. # 6 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.50) in Resd. # 8 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 6 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 7 Note
O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 8 Note
O

PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found Please Check

---

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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
8 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 08/07/2016; check.def file version of 05/07/2016

Datablock I - ellipsoid plot