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 = 0.0060 A Wavelength=0.71073

Cell: a=12.7351(10) b=12.7351(10) c=18.0797(14)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2932.2(5)	2932.2(4)
Space group	P -4 n 2	P -4 n 2
Hall group	P -4 -2n	P -4;-2n
Moiety formula	Mo O40 Si W11, 30(O)	?
Sum formula	Mo O70 Si W11	H64 Mo1 O70 Si1 W11
Mr	3266.31	3330.82
Dx,g cm-3	3.700	3.773
Z	2	2
Mu (mm-1)	21.840	21.842
F000	2860.0	2860.0
F000’	2842.54	
h,k,lmax	15,15,22	15,15,22
Nref	3025[1662]	3013
Tmin,Tmax	0.084,0.174	0.500,0.800
Tmin’	0.033	

Correction method= # Reported T Limits: Tmin=0.500 Tmax=0.800
AbsCorr = MULTI-SCAN

Data completeness= 1.81/1.00 Theta(max)= 26.420

R(reflections)= 0.0229(2677) wR2(reflections)= wR= 0.0276(3013)

S = 0.430 Npar= 175

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.
WEIGH01_ALERT_1_A Unit weights are not acceptable for submissions to Acta Crystallographica Section C.
n.b. unit is however a legal CIF keyword.

PLAT211_ALERT_2_A	ADP of Atom O6 is N.P.D. or (nearly) 2D ...	Please Check
PLAT213_ALERT_2_A	Atom O1 has ADP max/min Ratio	9.4 prolat
PLAT213_ALERT_2_A	Atom O5 has ADP max/min Ratio	5.6 prolat

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Alert level B

GOODF01_ALERT_2_B The least squares goodness of fit parameter lies outside the range 0.60 <> 4.00
Goodness of fit given = 0.430

PLAT043_ALERT_1_B	Calculated and Reported Mol. Weight Differ by ..	64.51 Check
PLAT214_ALERT_2_B	Atom Ow2 (Anion/Solvent) ADP max/min Ratio	5.7 prolat
PLAT220_ALERT_2_B	Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range	6.7 Ratio
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	O5 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

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Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.
Absorption correction given as multi-scan
CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.99 <> 1.01
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 3330.82
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
H	1.01	0.00	0.00
Mo	95.94	1.00	95.90
O	16.00	70.00	1119.93
Si	28.09	1.00	28.09
W	183.85	11.00	2022.42

Calculated formula weight 3266.34
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.500
From the CIF: _refine_ls_abs_structure_Flack_su 0.030

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	Please Check
PLAT127_ALERT_1_C	Implicit Hall Symbol Inconsistent with Explicit	P -4;-2n
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	1 Check
PLAT214_ALERT_2_C	Atom Ow5 (Anion/Solvent) ADP max/min Ratio	4.9 prolat

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O6 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:H64 Mo1 O70 Si1 W11
           Atom count from the _atom_site data:  Mo1.0046 O70 Si1 W11.
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  H64 Mo1 O70 Si1 W11
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          H        128.00      0.00  128.00
          Mo         2.00      2.00    0.00
          O        140.00    140.00    0.00
          Si         2.00      2.00    0.00
          W         22.00     22.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
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
PLAT300_ALERT_4_G Atom Site Occupancy of >W1     is Constrained at     0.9167 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >W2     is Constrained at     0.9167 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >W3     is Constrained at     0.9167 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Mo1    is Constrained at     0.0833 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Mo2    is Constrained at     0.0833 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Mo3    is Constrained at     0.0833 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =         21 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          8 Note
PLAT792_ALERT_1_G The Model has Chirality at Si1     (Polar  SPGR)          R Verify
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
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   6 ALERT level A = Most likely a serious problem - resolve or explain
  13 ALERT level B = A potentially serious problem, consider carefully
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  17 ALERT level G = General information/check it is not something unexpected

  12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  21 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
   8 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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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