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: 1

Bond precision: Mn- O = 0.0030 A Wavelength=0.71073

Cell: a=12.132(3) b=12.290(3) c=13.130(4)
alpha=73.394(10) beta=67.727(10) gamma=73.205(11)
Temperature: 150 K

	Calculated	Reported
Volume	1699.7(8)	1699.7(8)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	H6 Mn O24 W6, 14(O), K, 2(Na)	?
Sum formula	H6 K Mn Na2 O38 W6	H62 K2 Mn2 Na4 O76 W12
Mr	1857.11	3764.74
Dx,g cm-3	3.629	3.678
Z	2	1
Mu (mm-1)	20.844	20.846
F000	1640.0	1690.0
F000’	1633.38	
h,k,lmax	17,17,18	17,17,18
Nref	9985	9922
Tmin,Tmax	0.094,0.434	0.091,0.489
Tmin’	0.009	

Correction method= MULTI-SCAN

Data completeness= 0.994 Theta(max)= 30.070

R(reflections)= 0.0340(9472) wR2(reflections)= 0.0981(9922)

S = 1.174 Npar= 460

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 B

PLAT222_ALERT_3_B Large Non-Solvent H Uiso(max)/Uiso(min) .. 8.2 Ratio
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) O1W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) O2W

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PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O3W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O4W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O5W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O6W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O7W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O8W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O9W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O10W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O11W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O12W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O13W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O14W
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Alert level C

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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                   1
          From the CIF: _chemical_formula_weight          3764.74
          TEST: Calculate formula weight from _atom_site_*
          atom     mass    num     sum
          O        16.00   76.00 1215.92
          H         1.01   12.00   12.10
          Mn       54.94    2.00  109.88
          W       183.85   12.00 2206.20
          Na       22.99    4.00   91.96
          K        39.10    2.00   78.20
          Calculated formula weight             3714.25
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT043_ALERT_1_C Check Reported Molecular Weight ................    3764.74
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
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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:H62 K2 Mn2 Na4 O76 W12
           Atom count from the _atom_site data:  H12 K2 Mn2 Na4 O76 W12
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    1
          From the CIF: _chemical_formula_sum  H62 K2 Mn2 Na4 O76 W12
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          H         62.00     12.00   50.00
          K          2.00      2.00    0.00
          Mn         2.00      2.00    0.00
          Na         4.00      4.00    0.00
          O         76.00     76.00    0.00
          W         12.00     12.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6
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 ............       2.00 Ratio
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      13.12
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  W2     --  O7      ..        5.2 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  W6     --  O20     ..        5.4 su
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   W6     --  K1      ..       3.69 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   K1     --  NA3     ..       3.89 Ang.
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PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   K1     --  NA2     ..       3.95 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   K1     --  NA4     ..       4.20 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   NA2    --  K1      ..       3.95 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   NA4    --  K1      ..       4.20 Ang.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         4
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   0 ALERT level A = Most likely a serious problem - resolve or explain
  15 ALERT level B = A potentially serious problem, consider carefully
   4 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
  20 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
   0 ALERT type 4 Improvement, methodology, query or suggestion
   2 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*, 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 24/04/2013; check.def file version of 23/04/2013

Datablock 1 - ellipsoid plot