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: em1-6-3c

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Bond precision:  Si- O = 0.0126 A        Wavelength=0.71073

Cell:          a=12.560(2)       b=19.013(3)      c=20.359(4)
               alpha=92.925(3)   beta=98.002(3)   gamma=93.086(3)
Temperature:   100 K
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	Calculated	Reported
Volume	4799.1(14)	4799.1(15)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	2(Fe4 O72 Si2 W18), 55(O), 8(K)	?
Sum formula	Fe8 K8 O199 Si4 W36	Fe4 K4 O99.50 Si2 W18
Mr	10674.20	5337.28
Dx,g cm-3	3.693	3.694
Z	1	2
Mu (mm-1)	22.371	22.371
F000	4672.0	4672.0
F000’	4653.44	
h,k,lmax	16,24,26	16,24,26
Nref	22044	20941
Tmin,Tmax	0.134,0.209	0.192,0.303
Tmin’	0.074	

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Correction method= # Reported T Limits: Tmin=0.192 Tmax=0.303
AbsCorr = EMPIRICAL

Data completeness= 0.950          Theta(max)= 27.500

R(reflections)= 0.0605( 16625)    wR2(reflections)= 0.1642( 20941)

S = 1.032                 Npar= 1010
```

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

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 0.268
Additional refinement cycles may be required.

PLAT080_ALERT_2_A	Maximum Shift/Error	0.27	Why ?
PLAT213_ALERT_2_A	Atom O2 has ADP max/min Ratio	10.6	prolat
PLAT213_ALERT_2_A	Atom O9 has ADP max/min Ratio	5.4	prolat
PLAT213_ALERT_2_A	Atom O21 has ADP max/min Ratio	9.2	prolat
PLAT213_ALERT_2_A	Atom O23 has ADP max/min Ratio	6.7	prolat
PLAT213_ALERT_2_A	Atom O44 has ADP max/min Ratio	8.0	prolat
PLAT213_ALERT_2_A	Atom O49 has ADP max/min Ratio	10.5	prolat
PLAT213_ALERT_2_A	Atom O62 has ADP max/min Ratio	6.2	prolat

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Alert level B

DIFMX01_ALERT_2_B The maximum difference density is > 0.1*ZMAX*1.00
_refine_diff_density_max given = 12.713
Test value = 7.400

PLAT029_ALERT_3_B	_diffrn_measured_fraction_theta_full Low	0.950	Note
PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	12.71	eA-3
PLAT213_ALERT_2_B	Atom O37 has ADP max/min Ratio	4.4	prolat
PLAT250_ALERT_2_B	Large U3/U1 Ratio for Average U(i,j) Tensor	4.5	Note
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O73	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O74	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O75	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O76	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O77	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O78	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O79	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O80	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O81	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O82	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O83	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O84	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O85	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O86	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O87	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O88	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O89	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O90	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O91	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O92	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O93	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O94	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O95	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O96	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O97	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O98	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O99	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O100	Check
PLAT601_ALERT_2_B	Structure Contains Solvent Accessible VOIDS of .	132	Ang3

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

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           _exptl_absorpt_process_details field.
           Absorption correction given as empirical
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.51 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........        28 Check
PLAT213_ALERT_2_C Atom W2              has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom W6              has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom W12             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom O3              has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom O4              has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom O6              has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom O8              has ADP max/min Ratio .....       4.0 prolat
PLAT213_ALERT_2_C Atom O11             has ADP max/min Ratio .....       3.7 prolat
PLAT213_ALERT_2_C Atom O12             has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom O15             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom O16             has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom O31             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom O32             has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom O51             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom O53             has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom O55             has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom O61             has ADP max/min Ratio .....       3.3 prolat
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          7 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     214.85 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.003 Degree
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.50) in Resd. #         28 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         24 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         30 Note
             K
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        42 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
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   9 ALERT level A = Most likely a serious problem - resolve or explain
  34 ALERT level B = A potentially serious problem, consider carefully
  21 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

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  62 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 07/03/2016; check.def file version of 02/03/2016

Datablock em1-6-3c - ellipsoid plot