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: Mo- O = 0.0070 A Wavelength=0.71073

Cell: a=20.0720(8) b=7.7549(3) c=11.4644(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1784.51(12)	1784.51(12)
Space group	P m n 21	P m n 21
Hall group	P 2ac -2	P 2ac -2
Moiety formula	F14 Mo4 O8, F7 Mo2 O4, 2.0(I), 10(K)	F14 Mo4 O8, F7 Mo2 O4, 2.0(I), 10(K)
Sum formula	F21 I2 K10 Mo6 O12	F21 I2 K10 Mo6 O12
Mr	1811.31	1811.31
Dx,g cm-3	3.371	3.371
Z	2	2
Mu (mm-1)	5.091	5.092
F000	1665.9	1665.9
F000’	1648.34	
h,k,lmax	28,10,16	28,10,16
Nref	5357[2802]	5358
Tmin,Tmax	0.659,0.858	0.347,0.883
Tmin’	0.263	

Correction method= MULTI-SCAN

Data completeness= 1.91/1.00 Theta(max)= 30.030

R(reflections)= 0.0427(4916) wR2(reflections)= 0.1186(5358)

S = 1.067 Npar= 255

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

```
DIFMX01_ALERT_2_B  The maximum difference density is > 0.1*ZMAX*1.00
           _refine_diff_density_max given =      5.545
           Test value =      5.300
           Crystal system given = orthorhombic
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       5.55 eA-3
```

Alert level C

```
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 ....       2.62
```

Alert level G

```
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          2
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ? Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       5.58
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................         56 %
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................         25 %
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I2D    --  K3      ..       3.72 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I2D    --  K3      ..       3.72 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I2D    --  K4      ..       3.78 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I2D    --  K4      ..       3.78 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I2D    --  K5      ..       3.89 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I2D    --  K6      ..       3.61 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I6D    --  K4      ..       3.52 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I6D    --  K4      ..       3.52 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I6D    --  K6      ..       3.57 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I4D    --  K3      ..       3.58 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I4D    --  K3      ..       3.58 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I5D    --  K3      ..       4.00 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I5D    --  K3      ..       4.00 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I5D    --  K4      ..       3.89 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I5D    --  K4      ..       3.89 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I5D    --  K5      ..       3.76 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   I5D    --  K6      ..       4.05 Ang.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su ..       0.08
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          2
```

---

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

  18 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check

---

checkCIF publication errors

Alert level A

```
PUBL002_ALERT_1_A  The contact author’s address is missing,
            _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
            _publ_contact_author_phone are all missing.
            At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. ’Acta Crystallographica Section C’
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

Alert level G

```
PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
            missing. This is required for a full paper submission (but is
            optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

7 **ALERT level A** = Data missing that is essential or data in wrong format
2 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL002_GLOBAL
;
PROBLEM: The contact author’s address is missing,
```

```
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 01/06/2013; check.def file version of 24/05/2013

Datablock I - ellipsoid plot

