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:  C-C = 0.0077 A          Wavelength=1.54184

Cell:         a=13.5805(2)       b=18.4093(3)      c=19.7628(4)
              alpha=64.7970(18)  beta=78.3502(16)  gamma=68.6517(16)
Temperature:  123 K
```

	Calculated	Reported
Volume	4157.30(14)	4157.29(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 Al F46 O3, C20 H30 Ag As10 Fe2, 0.5(C5 H12), 1.5(C H2 Cl2)	2(C10 H15 Ag0.5 As5 Fe), Al C36 F46 O3, 0.5(C5 H12), 1.5(C H2 C
Sum formula	C60 H39 Ag Al As10 Cl3 F46 Fe2 O3	C60 H39 Ag Al As10 Cl3 F46 Fe2 O3
Mr	2784.01	2784.01
Dx,g cm-3	2.224	2.224
Z	2	2
Mu (mm-1)	11.415	11.415
F000	2660.0	2660.0
F000’	2648.84	
h,k,lmax	16,22,24	16,22,24
Nref	16797	16069
Tmin,Tmax	0.432,0.584	0.444,0.666
Tmin’	0.248	

```
Correction method= # Reported T Limits: Tmin=0.444 Tmax=0.666
AbsCorr = GAUSSIAN

Data completeness= 0.957          Theta(max)= 73.731

R(reflections)= 0.0460( 13047)    wR2(reflections)= 0.1296( 16069)

S = 1.088                 Npar= 1192
```

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 C

```
DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
           _refine_diff_density_max given =      4.072
           Test value =      3.525
```

Author Response: The final model involves only one position of Ag1 in an anisotropic \ aproximation. There is a very large residual density peak close to Ag1. Ag1 shows very large displacement parameters and an oblate elipsoid geometry. The \ reason for this is either movement of the Ag atom or a positional disorder. During our investigation we performed the X-ray analysis of this compound at temperatures as low as 90K and also with Mo radiation to minimize absorption. Please check full publication for further information.

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
```

Author Response: The final model involves only one position of Ag1 in an anisotropic \ aproximation. There is a very large residual density peak close to Ag1. Ag1 shows very large displacement parameters and an oblate elipsoid geometry. The \ reason for this is either movement of the Ag atom or a positional disorder. During our investigation we performed the X-ray analysis of this compound at temperatures as low as 90K and also with Mo radiation to minimize absorption. Please check full publication for further information.

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.30 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       4.07 eA-3
```

Author Response: The final model involves only one position of Ag1 in an anisotropic \ aproximation. There is a very large residual density peak close to Ag1. Ag1 shows very large displacement parameters and an oblate elipsoid geometry. The \ reason for this is either movement of the Ag atom or a positional disorder. During our investigation we performed the X-ray analysis of this compound at temperatures as low as 90K and also with Mo radiation to minimize absorption. Please check full publication for further information.

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    As4    --  As5     ..        6.0 su
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       As8 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       Fe1 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       Fe2 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of       C906 Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         1 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       5.53 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1    --  As1     ..       27.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1    --  As4     ..       19.5 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1    --  As5     ..       25.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1    --  As4_a   ..        6.8 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  As1    --  Fe1     ..        6.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  As2    --  Fe1     ..        7.8 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  As3    --  Fe1     ..        5.8 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag2    --  As6_b   ..       19.8 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag2    --  As7_b   ..        7.7 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag2    --  As8_b   ..       39.2 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag2    --  As9_b   ..       52.1 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  As8    --  Fe2     ..        5.2 su
PLAT300_ALERT_4_G Atom Site Occupancy of *Ag1    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Ag1_a  is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Ag2    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Ag2_b  is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C900   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C901   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C902   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C903   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C904   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Cl3    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Cl4    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C800   is Constrained at      0.500 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          1 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =         57 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   8.50) in Resd. #          4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   2.50) in Resd. #          6 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F16    ..  C8      ..       2.93 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F16    ..  C3      ..       2.94 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         22 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....          7 Note
```

---

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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  24 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
  18 ALERT type 4 Improvement, methodology, query or suggestion
   0 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.
```

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   0 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 a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# 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 29/01/2015; check.def file version of 29/01/2015

Datablock I - ellipsoid plot