

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: P- O = 0.0133 A Wavelength=0.71090

Cell: a=5.198 (4) b=16.905 (6) c=7.510 (12)
 alpha=90 beta=110.02 (3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	620.0 (11)	620.0 (11)
Space group	P 21/m	P 1 21/m 1
Hall group	-P 2yb	-P 2yb
Moiety formula	Fe _{9.48} O ₃₄ P ₆	?
Sum formula	Fe _{9.48} O ₃₄ P ₆	O ₁₇ H ₆ P ₃ Mn ₂ Fe ₃
Mr	1259.50	648.40
Dx, g cm ⁻³	3.373	3.473
Z	1	2
Mu (mm ⁻¹)	5.914	5.902
F000	608.6	609.0
F000'	612.79	
h, k, lmax	7, 24, 11	5, 22, 10
Nref	2134	1069
Tmin, Tmax	0.899, 0.971	0.519, 0.746
Tmin'	0.554	

Correction method= # Reported T Limits: Tmin=0.519 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.501 Theta (max)= 31.590

R(reflections)= 0.0759 (1008) wR2(reflections)=
S = 3.060 Npar= 57 wR= 0.1032 (1069)

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

ATOM007_ALERT_1_A _atom_site_aniso_label is missing

Unique label identifying the atom site.

PLAT027_ALERT_3_A _diffrn_refl_theta_full value (too) Low 20.39 Degree

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.930 Why?

Fe1 Mn2 Fe3 P1 P2 etc.

Alert level B

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 37.30 Check

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

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00

Goodness of fit given = 3.060

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large 0.012 Ang.

PLAT799_ALERT_4_C Numeric Label on Displacement Par. Record ? Check

Alert level G

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: H6 Fe3 Mn2 O17 P3

Atom count from the _atom_site data: Fe4.742 O17 P3

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 2

From the CIF: _chemical_formula_sum O17 H6 P3 Mn2 Fe3

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
O	34.00	34.00	0.00
H	12.00	0.00	12.00
P	6.00	6.00	0.00
Mn	4.00	0.00	4.00
Fe	6.00	9.48	-3.48

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !

PLAT017_ALERT_1_G Check Scattering Type Consistency of MN2 as FE

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check

PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	14% Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe3 (III) .	2.95 Info
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2 Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2 Units
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0 Sig(I)

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- 3 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
6 **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
- 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
7 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.

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_ATOM007_I
;
PROBLEM: _atom_site_aniso_label is missing
RESPONSE: ...
;
_vrf_PLAT027_I
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ..... 20.39 Degree
RESPONSE: ...
;
_vrf_PLAT029_I
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low . 0.930 Why?
RESPONSE: ...
;
_vrf_PLAT043_I
;
PROBLEM: Calculated and Reported Mol. Weight Differ by .. 37.30 Check
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock I - ellipsoid plot

