

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 = 0.0030 A Wavelength=0.71075

Cell: a=13.983 (3) b=5.207 (1) c=12.200 (2)
 alpha=90 beta=98.84 (3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	877.7 (3)	877.7 (3)
Space group	P 2/a	P 1 2/a 1
Hall group	-P 2ya	-P 2ya
Moiety formula	Fe7.86 Mn6 O44 P8, 4(O)	?
Sum formula	Fe7.86 Mn6 O48 P8	Fe2 Mn1.5 O12 P2
Mr	1784.60	453.10
Dx, g cm ⁻³	3.376	3.429
Z	1	4
Mu (mm ⁻¹)	5.743	5.798
F000	858.5	858.0
F000'	864.46	
h, k, lmax	20, 7, 18	18, 7, 17
Nref	3047	1812
Tmin, Tmax	0.757, 0.891	0.700, 0.900
Tmin'	0.528	

Correction method= # Reported T Limits: Tmin=0.700 Tmax=0.900
AbsCorr = MULTI-SCAN

Data completeness= 0.595 Theta(max)= 31.980

R(reflections)= 0.0425 (1269) wR2(reflections)=
S = 1.660 Npar= 168 wR= 0.0526 (1812)

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

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 27.80 Check

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group C2/m Check

Note: (Pseudo) Lattice Translation Implemented



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

CHEMW01_ALERT_1_C The ratio of given/expected molecular weight as calculated
from the _chemical_formula_sum lies outside
the range 0.99 <> 1.01

Calculated formula weight = 448.0413

Formula weight given = 453.1000

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

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1 Check
O12A

PLAT213_ALERT_2_C Atom O5 has ADP max/min Ratio 3.5 prolat

PLAT213_ALERT_2_C Atom O7 has ADP max/min Ratio 3.1 prolat

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.5 Note



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: Fe2 Mn1.5 O12 P2

Atom count from the _atom_site data: Fe1.966 Mn1.5 O12 P2

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: check formula stoichiometry or atom site occupancies.

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_sum Fe2 Mn1.5 O12 P2

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Fe	8.00	7.86	0.14
Mn	6.00	6.00	0.00
O	48.00	48.00	0.00
P	8.00	8.00	0.00

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 !

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check

PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Translation ... ? Check

PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem C 100 %Fit

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 11% Note

PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100% Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	012A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	012B Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III) .	3.08 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1 (II) .	2.19 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn2 (II) .	2.11 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
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0 Sig(I)

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

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 9 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
 3 ALERT type 4 Improvement, methodology, query or suggestion
 8 ALERT type 5 Informative message, check

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_ABSTY02_I
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_CHEMW01_I
;
PROBLEM: The ratio of given/expected molecular weight as calculated
RESPONSE: ...
;
_vrf_PLAT043_I
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..      27.80 Check
RESPONSE: ...
;
_vrf_PLAT113_I
;
PROBLEM: ADDSYM Suggests Possible Pseudo/New Space Group      C2/m Check
RESPONSE: ...
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula Strings Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT077_I
;
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PROBLEM: Unitcell Contains Non-integer Number of Atoms ..      Please Check
RESPONSE: ...
;
_vrf_PLAT202_I
;
PROBLEM: Isotropic non-H Atoms in Anion/Solvent .....      1 Check
RESPONSE: ...
;
_vrf_PLAT213_I
;
PROBLEM: Atom O5          has ADP max/min Ratio .....      3.5 prolat
RESPONSE: ...
;
_vrf_PLAT250_I
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.5 Note
RESPONSE: ...
;
# end Validation Reply Form

```

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.

Datablock I - ellipsoid plot

