

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: sad

Bond precision: Fe- O = 0.0049 A Wavelength=0.71073

Cell: a=5.155(5) b=5.155(5) c=6.902(13)
 alpha=90 beta=90 gamma=120
Temperature: 296 K

	Calculated	Reported
Volume	158.8(5)	158.9(4)
Space group	P -3 1 m	P-31m
Hall group	-P 3 2	?
Moiety formula	Fe4 O7, K0.48, 12(K0.13)	Fe4 K2 O7
Sum formula	Fe4 K1.98 O7	Fe4 K2 O7
Mr	412.82	413.60
Dx,g cm-3	4.317	4.323
Z	1	1
Mu (mm-1)	10.243	10.252
F000	197.6	198.0
F000'	199.47	
h,k,lmax	7,7,9	7,7,9
Nref	202	198
Tmin,Tmax	0.238,0.324	0.236,0.332
Tmin'	0.207	

Correction method= EMPIRICAL

Data completeness= 0.980 Theta(max)= 30.850

R(reflections)= 0.0327(194) wR2(reflections)= 0.1214(198)

S = 1.125 Npar= 21

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

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full Low	0.971
PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	? Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	? Check
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.62
PLAT148_ALERT_3_C	su on the c - Axis is (Too) Large	0.013 Ang.

● 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: Fe4 K2 O7
Atom count from the _atom_site data: Fe4 K1.98 O7

PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension . 3

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ? Do !

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ ? Check

PLAT301_ALERT_3_G Note: Main Residue Disorder 1 %

PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: FE1 -- K1' .. 3.51 Ang.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 274
K1' -O1 -K1' 8.565 1.555 2.655 37.40 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 279
K1' -O1 -K1 2.655 1.555 1.555 12.50 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 283
K1' -O1 -K1 8.565 1.555 7.665 12.50 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 290
K1' -O1 -K1' 2.655 1.555 3.665 22.40 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 291
K1 -O1 -K1' 1.555 1.555 3.665 12.80 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 296
K1' -O1 -K1' 8.565 1.555 7.665 22.40 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 299
K1 -O1 -K1' 7.665 1.555 7.665 12.80 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 304
K1' -O1 -K1' 8.565 1.555 9.555 18.50 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 307
K1 -O1 -K1' 7.665 1.555 9.555 10.15 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 309
K1' -O1 -K1' 7.665 1.555 9.555 20.50 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 314
K1' -O1 -K1' 2.655 1.555 1.555 18.50 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 315
K1 -O1 -K1' 1.555 1.555 1.555 10.15 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 317
K1' -O1 -K1' 3.665 1.555 1.555 20.50 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 351
K1' -O2 -K1' 2.545 1.555 8.455 35.70 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 352
K1' -O2 -K1' 9.445 1.555 8.455 24.30 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 358
K1' -O2 -K1' 8.565 1.555 2.655 35.70 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 361
K1' -O2 -K1' 3.665 1.555 2.655 24.30 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 368
K1' -O2 -K1' 2.545 1.555 1.445 24.30 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 371
K1' -O2 -K1' 7.655 1.555 1.445 35.70 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 377
K1' -O2 -K1' 8.565 1.555 7.665 24.30 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 382
K1' -O2 -K1' 1.455 1.555 7.665 35.70 Deg.

PLAT794_ALERT_5_G Note: Tentative Bond Valency for Fe1 (III) 2.98

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
21 ALERT type 4 Improvement, methodology, query or suggestion
5 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*, 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.

