checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 202210171_a

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: 202210171_a

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Bond precision:   Al-Al = 0.0030 A         Wavelength=0.71073

Cell:               a=7.635(3)      b=6.392(2)      c=4.2007(14)
                    alpha=90        beta=90         gamma=90
Temperature:        300 K

                 Calculated                  Reported
Volume           205.01(12)                  205.01(12)
Space group      C m c m                     C m c m
Hall group       -C 2c 2                     -C 2c 2
Moiety formula   Al11.44 Fe4                 ?
Sum formula      Al11.44 Fe4                 Al2.86 Fe
Mr               532.05                      132.98
Dx,g cm-3        4.310                       4.308
Z                1                           4
Mu (mm-1)        8.087                       8.087
F000             252.7                       253.0
F000'            254.76
h,k,lmax         9,7,4                       9,7,4
Nref             112                         100
Tmin,Tmax        0.564,0.785                 0.514,0.746
Tmin'            0.518

Correction method= # Reported T Limits: Tmin=0.514 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.893            Theta(max)= 24.997

R(reflections)= 0.0363( 76)                    wR2(reflections)=
                                               0.0844( 100)
S = 1.017                  Npar= 19
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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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.893 Why?
Response: The high angle diffraction data are not very good since the structure is highly disordered.

PLAT088_ALERT_3_A Poor Data / Parameter Ratio ..... 5.26 Note
Response: As the structure is highly disordered thus it requires more parameters to refine the model thus leads to a poor data/parameter ratio.

Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.595 12 Report
1 7 0, 3 7 0, 4 4 0, 8 0 0, 0 6 3, 1 5 3,
2 4 3, 3 5 3, 0 4 4, 1 3 4, 2 4 4, 3 3 4,

Response: The missing FCF Refl(ections) Between Thmin & STh/L = 0.595 12 are caused by the poor high angle diffraction data, actually it has been checked manually that the above listed 12 reflection are too weak to be integrated and included in the solving and refining the structural model.

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
CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
drak
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT213_ALERT_2_C Atom Al2 has ADP max/min Ratio ..... 3.5 prolat
PLAT215_ALERT_3_C Disordered Al1 has ADP max/min Ratio ..... 3.5 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.257 Check

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
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
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 43% Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 13 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 80% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.8 Low
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameter Values Zero ..... Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 0.92 Note
Predicted wR2: Based on SigI**2 9.21 or SHELX Weight 9.21

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

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  6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  3 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
  4 ALERT type 4 Improvement, methodology, query or suggestion
  3 ALERT type 5 Informative message, check
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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.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock 202210171_a - ellipsoid plot