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: Fe2-3-PhenylPropylPyridine2FeCN5NO

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Bond precision:   C-C = 0.0101 A          Wavelength=0.71073

Cell:               a=14.633(2)      b=14.626(5)      c=15.789(5)
                    alpha=90         beta=90          gamma=90
Temperature:        0 K

                 Calculated                 Reported
Volume           3379.2(16)                 3379.4(2)
Space group      P 21 21 2                  P 21 21 2
Hall group       P 2 2ab                    P 2 2ab
Moiety formula   C38 Fe4 N14 O2, 2(C14 N)   ?
Sum formula      C66 Fe4 N16 O2             Fe4 C66 N16 O2
Mr               1272.22                    0.00
Dx,g cm-3        1.250                      0.000
Z                2                          2
Mu (mm-1)        0.894                      0.000
F000             1256.0                     0.0
F000'            1259.11
h,k,lmax         20,20,22
Nref             9850[ 5439]
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 0.00/0.00        Theta(max)=

R(reflections)=                                  wR2(reflections)=
S =                      Npar=
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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

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.
GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.
GEOM002_ALERT_1_A _geom_bond_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM003_ALERT_1_A _geom_bond_distance is missing
Distance between atom sites 1 and 2.
GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.
PLAT043_ALERT_1_A Calculated and Reported Mol. Weight Differ by .. 1272.22 Check
PLAT044_ALERT_1_A Calculated and Reported Density Dx Differ by .. 1.2504 Check
PLAT198_ALERT_1_A Missing _diffrn_ambient_temperature Datum .... Please Add

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Alert level B

POWD002_ALERT_1_B _refine_ls_goodness_of_fit_all is missing (this is chi, i.e.
the square root of 'chi squared'). This should be
present for a powder diffraction study.
PLAT601_ALERT_2_B Unit Cell Contains Solvent Accessible VOIDS of . 148 Ang**3

Alert level C

REFI015_ALERT_1_C _refine_ls_shift/su_max is missing
Maximum shift/s.u. ratio after final refinement cycle.
The following tests will not be performed
SHFSU_01
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01014 Ang.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 14 Units
PLAT432_ALERT_2_G Short Inter X...Y Contact N3 ..C101 . 2.95 Ang.
1/2+x,1/2-y,1-z = 2_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact N5 ..C113 . 1.80 Ang.
1/2+x,1/2-y,-z = 2_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact N5 ..C112 . 2.13 Ang.
1/2+x,1/2-y,-z = 2_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C5 ..C113 . 2.92 Ang.
1/2+x,1/2-y,-z = 2_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C5 ..C112 . 3.02 Ang.
1/2+x,1/2-y,-z = 2_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C107 ..C208 . 1.94 Ang.
x,y,-1+z = 1_554 Check

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PLAT432_ALERT_2_G Short Inter X...Y Contact  C107     ..C207     .       2.69 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C107     ..C209     .       2.80 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C107     ..C214     .       2.91 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C107     ..C206     .       3.14 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C108     ..C208     .       1.89 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C108     ..C209     .       2.56 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C108     ..C214     .       2.64 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C109     ..C208     .       2.24 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C110     ..C208     .       2.97 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C113     ..C211     .       2.84 Ang.
                                             -1/2+x,1/2-y,1-z  =      2_456 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C113     ..C212     .       2.86 Ang.
                                             -1/2+x,1/2-y,1-z  =      2_456 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C114     ..C211     .       2.60 Ang.
                                             -1/2+x,1/2-y,1-z  =      2_456 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C114     ..C206     .       2.87 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C114     ..C208     .       2.92 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C114     ..C210     .       3.06 Ang.
                                             -1/2+x,1/2-y,1-z  =      2_456 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          2 Note
PLAT769_ALERT_4_G CIF Embedded explicitly supplied scattering data     Please Note
PLAT794_ALERT_5_G Tentative Bond Valency for FeE       (II)      .       1.52 Info
PLAT982_ALERT_1_G The  C-f'=    0.0170 Deviates from  IT-value =       0.0033 Check
PLAT982_ALERT_1_G The Fe-f'=   -1.1790 Deviates from  IT-value =       0.3463 Check
PLAT982_ALERT_1_G The  N-f'=    0.0290 Deviates from  IT-value =       0.0061 Check
PLAT982_ALERT_1_G The  O-f'=    0.0470 Deviates from  IT-value =       0.0106 Check
PLAT983_ALERT_1_G The  C-f"=    0.0090 Deviates from  IT-Value =       0.0016 Check
PLAT983_ALERT_1_G The Fe-f"=    3.2040 Deviates from  IT-Value =       0.8444 Check
PLAT983_ALERT_1_G The  N-f"=    0.0180 Deviates from  IT-Value =       0.0033 Check
PLAT983_ALERT_1_G The  O-f"=    0.0320 Deviates from  IT-Value =       0.0060 Check
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9 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
35 **ALERT level G** = General information/check it is not something unexpected

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

PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock Fe2-3-PhenylPropylPyridine2FeCN5NO - ellipsoid plot