checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C16H18N3S3FeCN6x12p36H2O

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: C16H18N3S3FeCN6x12p36H2O

Bond precision: C-C = 0.0061 A Wavelength=0.70000

Cell: a=9.7710(19) b=12.201(2) c=13.651(3)
alpha=84.18(3) beta=72.06(3) gamma=89.45(3)
Temperature: 100 K

	Calculated	Reported
Volume	1539.9(6)	1539.9(6)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	3(C16 H18 N3 S), C6 Fe N6, 12.361(H2 O)	C6 Fe N6, 3(C16 H18 N3 S), 12.361(H2 O)
Sum formula	C54 H78.72 Fe N15 O12.36 S3	C54 H78.72 Fe N15 O12.36 S3
Mr	1287.85	1287.83
Dx,g cm-3	1.389	1.389
Z	1	1
Mu (mm-1)	0.399	0.404
F000	680.6	681.0
F000’	681.56	
h,k,lmax	12,15,17	12,15,17
Nref	12612[6306]	10607
Tmin,Tmax		0.321,1.000
Tmin’		

Correction method= # Reported T Limits: Tmin=0.321 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.68/0.84 Theta(max)= 25.944

R(reflections)= 0.0439(10495) wR2(reflections)= 0.1202(10607)

S = 1.053 Npar= 849

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

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.376
From the CIF: _refine_ls_abs_structure_Flack_su 0.014

Author Response: The presence of merohedral twinning is the reason for the ambiguities with the Flack parameter.

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.971 Why?

Author Response: The synchrotron measurement conducted consisted in the only full 360 degrees rotation around the spindle axis, thus resulting in a fraction of the reciprocal space left uncollected.

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

Author Response: The presence of substitutional disorder involving the presence of alternatively 1 and 2 water molecules results in a non-integer final stoichiometry. This is caused by the fact that both parts were refined so that their sum resulted in occupancy 1.

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.21 Note

Author Response: The synchrotron measurement conducted consisted in the only full 360 degrees rotation around the spindle axis, thus resulting in a fraction of the reciprocal space left uncollected.

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00606 Ang.

Author Response: The synchrotron measurement conducted consisted in the only full 360 degrees rotation around the spindle axis, thus resulting in a fraction of the reciprocal space left uncollected.

PLAT412_ALERT_2_C Short Intra XH3 .. XHn H44 ..H48B . 1.86 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen atoms positions were refined after locating them as electron density maxima and therefore fixing their positions. As many H atoms were disordered in more than two locations for each water molecules, the final model contain some short H-H contacts, when these are not recognised as belonging to different disordered parts.

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PLAT417_ALERT_2_C Short Inter D-H..H-D       H8B      ..H9B      .       2.12 Ang.
                                                    x,y,z  =      1_555 Check
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Author Response: Hydrogen atoms positions were refined after locating them as electron density maxima and therefore fixing their positions. As many H atoms were disordered in more than two locations for each water molecules, the final model contain some short H-H contacts, when these are not recognised as belonging to different disordered parts.

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PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
              C16 H18 N3 S
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        159 Report
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Author Response: The synchrotron measurement conducted consisted in the only full 360 degrees rotation around the spindle axis, thus resulting in a fraction of the reciprocal space left uncollected.

Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         10 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         26 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.376 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.70000 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.03 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          6 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          3 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          7 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 16  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 17  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 18  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 16  )       1.92 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 17  )       1.08 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 18  )       1.08 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C33 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H31B     ..H12A     .       2.03 Ang.
                                               -1+x,y,1+z  =      1_456 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H40      ..H2CC     .       1.70 Ang.
                                              -1+x,-1+y,z  =      1_445 Check
PLAT417_ALERT_2_G Short Inter D-H..H-D       H11B     ..H12A     .       2.10 Ang.
                                                    x,y,z  =      1_555 Check
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Author Response: Hydrogen atoms positions were refined after locating them as electron density maxima and therefore fixing their positions. As many H atoms were disordered in more than two locations for each water molecules, the final model contain some short H-H contacts, when these are not recognised as belonging to different disordered parts.

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          4 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C16 H18 N3 S
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
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             H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
             H2 O
PLAT794_ALERT_5_G Tentative Bond Valency for Fe01      (III)     .       3.05 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        22 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         23 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.1 Low
PLAT984_ALERT_1_G The Fe-f'=    0.3555 Deviates from the B&C-Value     0.3456 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  32 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
  21 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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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_PLAT790_C16H18N3S3FeCN6x12p36H2O
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd.  #          1 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.

PLATON version of 22/04/2020; check.def file version of 09/03/2020

Datablock C16H18N3S3FeCN6x12p36H2O - ellipsoid plot