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: Fe-TMPP

Bond precision: C-C = 0.0141 A Wavelength=0.71073

Cell: a=9.5980(6) b=11.0408(7) c=14.4682(10)
alpha=70.702(3) beta=86.792(3) gamma=75.171(2)
Temperature: 213 K

	Calculated	Reported
Volume	1398.16(16)	1398.16(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H34 Cl Fe N8, 2(Cl4 Fe) [+ solvent]	C44 H34 Cl Fe N8, 2(Cl4 Fe) [+ solvent]
Sum formula	C44 H34 Cl9 Fe3 N8 [+ solvent]	C44 H34 Cl9 Fe3 N8
Mr	1161.39	1161.39
Dx,g cm-3	1.379	1.379
Z	1	1
Mu (mm-1)	1.234	1.234
F000	585.0	585.0
F000'	587.48	
h,k,lmax	10,12,16	10,12,16
Nref	4014	4006
Tmin,Tmax	0.929,0.940	0.929,0.940
Tmin'	0.691	

Correction method= # Reported T Limits: Tmin=0.929 Tmax=0.940
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 23.255

R(reflections)= 0.1007(2844)

wR2(reflections)= 0.3123(4006)

S = 1.057 Npar= 339

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

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5555

Author Response: The crystal exhibits nearly no diffraction at the high-resolution (low angle) region. This is likely due to the quick evaporation of crystalline solvate during the experiment though low temperature is used. Refinement with the inclusion of these weak data leads to a very high R-value of around 20%. Therefore, a resolution cutoff of 0.90 is applied to obtain a reasonable R factor.

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density .... 6.18 Report

Author Response: A residual density (3.02 e\%A^-3^) is identified and such density is 1.812 \%A from Cl1 and 2.850 \%A from the disordered Cl2A. Our refinement of this residual density using a disordered solvate model failed to result in any meaningful results. The presence of this residual density might be due to the low-quality of the crystal.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 3.02 eA-3

Author Response: This alert describes the same issue as that for PLAT094. A residual density (3.02 e\%A^-3^) is identified and such density is 1.812 \%A from Cl1 and 2.850 \%A from the disordered Cl2A. Our refinement of this residual density using a disordered solvate model failed to result in any meaningful results. The presence of this residual density might be due to the low-quality of the crystal.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.31 Report
PLAT213_ALERT_2_C Atom C1 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C3 has ADP max/min Ratio ..... 3.3 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.5 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3 Check

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)        2.6 Note
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01409 Ang.
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C44 H34 Cl9 Fe3 N8
           Atom count from _chemical_formula_moiety:C44 H34 Cl1 Fe1 N8
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         10 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
             H1
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.72 Why ?
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
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         4% 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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       3.64 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)       1.36 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C1 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C7 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl1      ..C3       .       3.06 Ang.
                                               -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl1      ..C2       .       3.15 Ang.
                                               -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl2      ..C3       .       3.23 Ang.
                                            2-x,-y,1-z  =      2_756 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        104 A**3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       26.92 Deg.
             FE1  -N3   -FE1     1_555   1_555   2_655 ......     #   37 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       27.38 Deg.
             FE1  -N4   -FE1     2_655   1_555   1_555 ......     #   43 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         56 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          9 Note
               1  0  0,   1  3  5,   0  0  6,  -2  2  0,   1  4  5,   1  3  6,
               2  0  2,   3  3  1,  -2 -1  2,
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  28 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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 16 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
 15 ALERT type 4 Improvement, methodology, query or suggestion
  1 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 Fe-TMPP - ellipsoid plot