

CCDC_2469368

1.2MeOH

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Fe_ppt4cf3_120k

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: Fe_ppt4cf3_120k

Bond precision:	C-C = 0.0037 Å	Wavelength=0.71073	
Cell:	a=12.7730 (3)	b=9.9855 (3)	c=28.7032 (8)
	alpha=90	beta=90	gamma=90
Temperature:	120 K		
	Calculated	Reported	
Volume	3660.94 (17)	3660.94 (17)	
Space group	P b c n	P b c n	
Hall group	-P 2n 2ab	-P 2n 2ab	
Moiety formula	C34 H20 F6 Fe N12, 2 (C H4 O)	C34 H20 F6 Fe N12, 2 (C H4 O)	
Sum formula	C36 H28 F6 Fe N12 O2	C36 H28 F6 Fe N12 O2	
Mr	830.55	830.55	
Dx, g cm ⁻³	1.507	1.507	
Z	4	4	
Mu (mm ⁻¹)	0.495	0.495	
F000	1696.0	1696.0	
F000'	1698.21		
h, k, lmax	16, 12, 36	16, 12, 36	
Nref	4005	4002	
Tmin, Tmax	0.977, 0.985	0.810, 1.000	
Tmin'	0.976		

Correction method= # Reported T Limits: Tmin=0.810 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.000

R(reflections)= 0.0436 (3227)

wR2(reflections)=
0.1133 (4002)

S = 1.136

Npar= 287

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

PLAT213_ALERT_2_C Atom F3	has ADP max/min Ratio	3.4	prolat
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)		2.1	Note



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	8	Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms	8	Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	1	Report
H1A		
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF	Please	Check
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fel --N1 .	5.7	s.u.
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of	C17	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1 Constrained at	0.75	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2 Constrained at	0.75	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3 Constrained at	0.75	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1B Constrained at	0.25	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2B Constrained at	0.25	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3B Constrained at	0.25	Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1)	11%	Note
PLAT794_ALERT_5_G Tentative Bond Valency for Fel (II) .	2.02	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	93	Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]= 0 0 2, 1 0 2,	2.59	Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 0 2 6,	1	Note
PLAT960_ALERT_3_G Number of Intensities with I < - 2*Sigma(I)	3	Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..	54.0	Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value	3.749	Note
Predicted wR2: Based on SigI**2 3.02 or SHELX Weight	9.98	
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	9	Info

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

- 1 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
6 ALERT type 3 Indicator that the structure quality may be low
8 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check
-
-

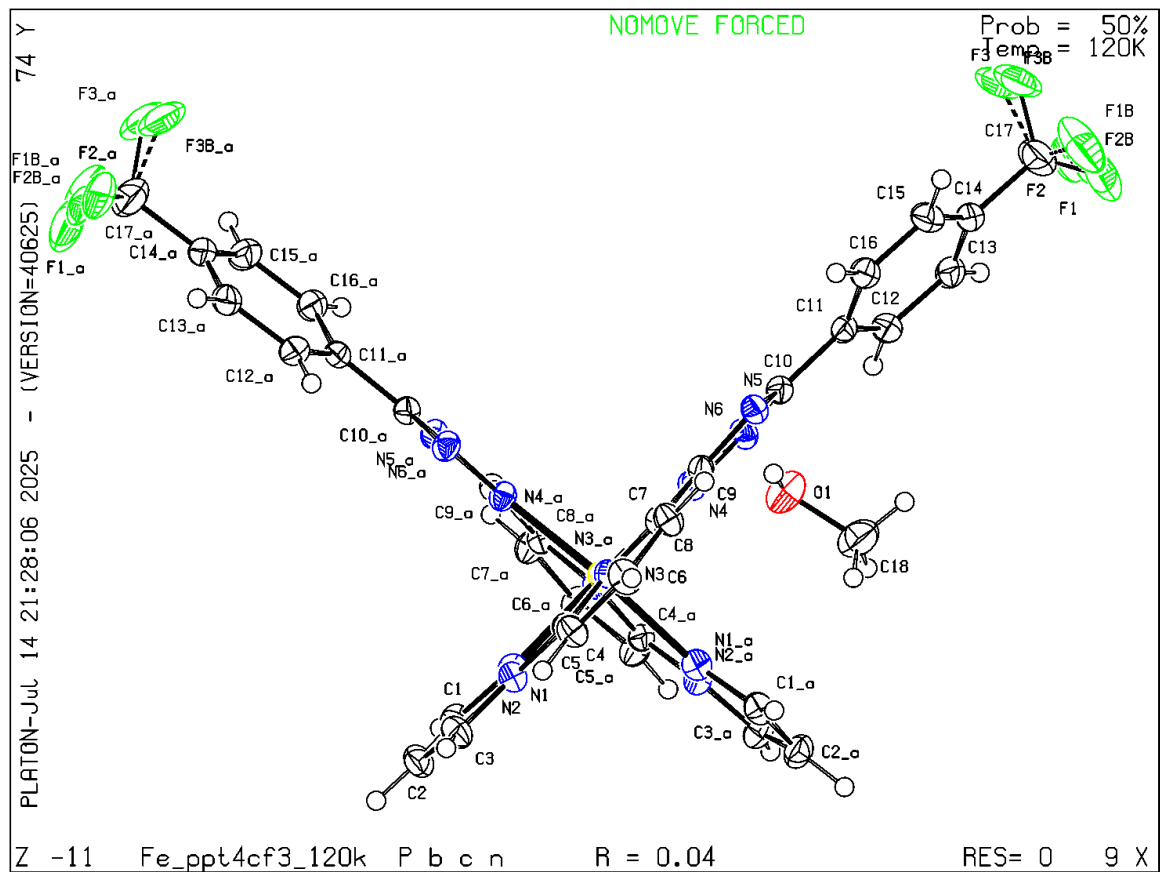
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



CCDC_2468400

1 (LS)

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 4CF3-LS

Bond precision: C-C = 0.0700 Å Wavelength=0.72979

Cell: a=12.6766(1) b=10.21388(13) c=25.1175(3)
 alpha=90 beta=90 gamma=90

Temperature: 220 K

	Calculated	Reported
Volume	3252.15(6)	3252.15(6)
Space group	P b c n	Pbcn
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C34 H20 F6 Fe N12	C34 H20 F6 Fe N12
Sum formula	C34 H20 F6 Fe N12	C34 H20 F6 Fe N12
Mr	766.47	766.47
Dx, g cm ⁻³	1.565	1.565
Z	4	4
Mu (mm ⁻¹)	0.582	0.000
F000	1552.0	0.0
F000'	1554.20	
h, k, lmax		
Nref		
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= Theta (max)=

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

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

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.07 Ang.

Author Response: The structure was solved and refined from powder X-ray diffraction data by the Rietveld method. The lower precision of bond lengths is typical for powder data and is considered acceptable for the present discussion.

 Alert level C

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Fe1 Check

 Alert level G

PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.72979 Ang.
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 10 Note
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at 0.5 Check
F1 F1B F2 F2B F3 F3B
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 11% Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 37.00 Deg.
F1 -C17 -F3B 1_555 1_555 1_555 # 76 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 37.00 Deg.
F1B -C17 -F2 1_555 1_555 1_555 # 78 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 37.00 Deg.
F2B -C17 -F3 1_555 1_555 1_555 # 87 Check

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0 ALERT type 5 Informative message, check
-

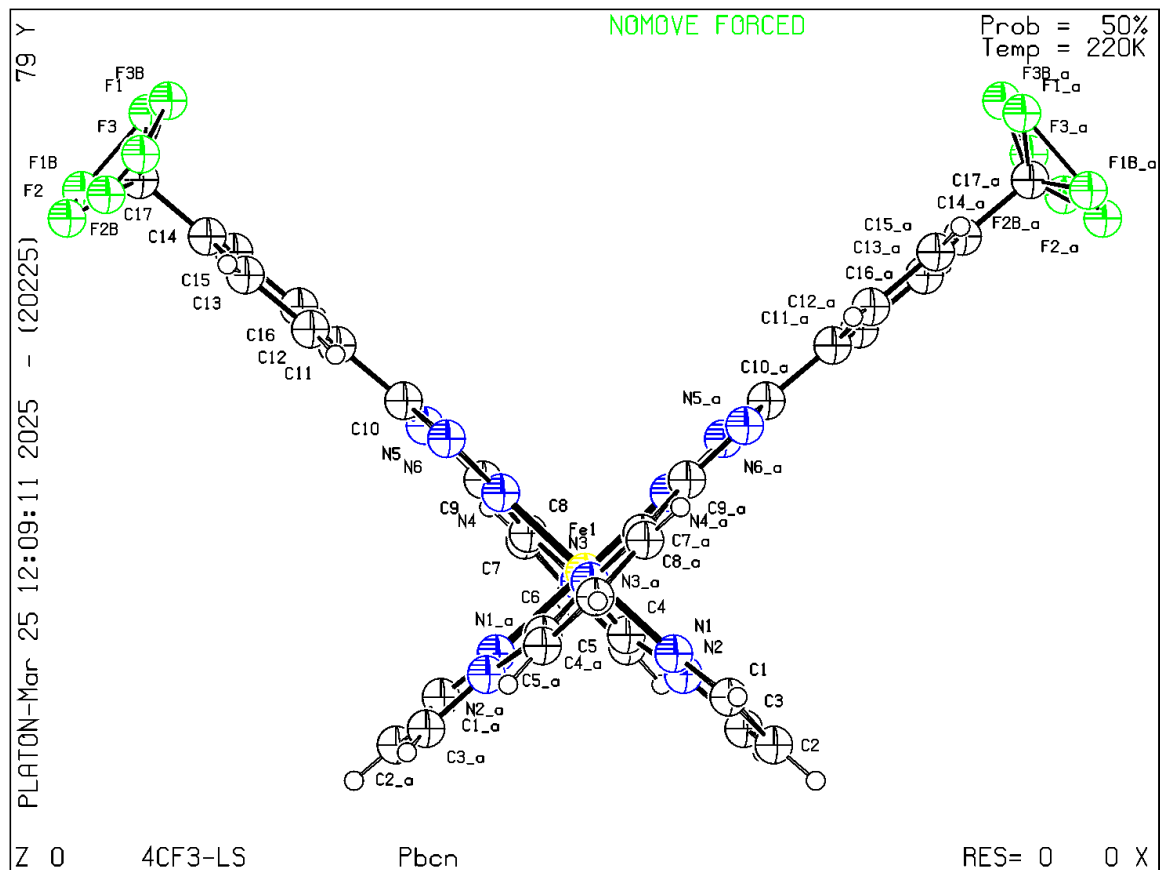
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CCDC_2468401

1 (HS)

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Datablock: 4CF3-HS

Bond precision: C-C = 0.0953 Å Wavelength=0.72979

Cell: a=12.85389 (16) b=9.5164 (2) c=27.1630 (5)
 alpha=90 beta=90 gamma=90

Temperature: 317 K

	Calculated	Reported
Volume	3322.65 (10)	3322.65 (11)
Space group	P b c n	Pbcn
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C34 H20 F6 Fe N12	C34 H20 F6 Fe N12
Sum formula	C34 H20 F6 Fe N12	C34 H20 F6 Fe N12
Mr	766.47	766.47
Dx, g cm ⁻³	1.532	1.532
Z	4	4
Mu (mm ⁻¹)	0.570	0.000
F000	1552.0	0.0
F000'	1554.20	
h, k, lmax		
Nref		
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= Theta (max)=

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

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PLAT341_ALERT_3_A Low Bond Precision on C-C Bonds 0.09533 Ang.

Author Response: The structure was solved and refined from powder X-ray diffraction data by the Rietveld method. The lower precision of bond lengths is typical for powder data and is considered acceptable for the present discussion.

 Alert level G

PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.72979 Ang.
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 10 Note
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at 0.5 Check
F1 F1B F2 F2B F3 F3B
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 11% Note
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C14 - C17 . 1.51 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (II) . 2.29 Info

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