No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: fe4ch2sac_8_work3

Bond precision: C-C = 0.0057 A Wavelength=0.71073
Cell: a=15.9287(6) b=24.8996(11) c=26.7398(12)
alpha=68.529(2) beta=77.634(2) gamma=81.590(2)
Temperature: 120 K

	Calculated	Reported
Volume	9613.6(7)	9613.6(7)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C80 H136 Fe4 O20 S2, C4 H10 O	C80 H136 Fe4 O20 S2, C4 H10 O
Sum formula	C84 H146 Fe4 O21 S2	C84 H146 Fe4 O21 S2
Mr	1779.53	1779.53
Dx,g cm-3	1.230	1.229
Z	4	4
Mu (mm-1)	0.697	0.697
F000	3816.0	3816.0
F000'	3824.06	
h,k,lmax	19,30,33	19,30,33
Nref	38523	38056
Tmin,Tmax	0.703,0.846	0.713,0.850
Tmin'	0.689	

Correction method= # Reported T Limits: Tmin=0.713
Tmax=0.850 AbsCorr = MULTI-SCAN
Data completeness= 0.988 Theta(max)= 26.180
R(reflections)= 0.0505(26267) wR2(reflections)= 0.1455(38056)
S = 1.012 Npar= 2054

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

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 3 Report
O41 C161 C162

Author Response: Isotropic refinement was found preferable for the extensively overlapping acetyl moieties of disordered thioacetyl group in MOL2 (O40,C159,C160,O41,C161,C162)

PLAT213_ALERT_2_B Atom C112 has ADP max/min Ratio ..... 4.3 prolat

Author Response: Methyl C atoms of tBu groups undergoing rotational disorder

PLAT213_ALERT_2_B Atom C44 has ADP max/min Ratio ..... 4.1 prolat

Author Response: Methyl C atoms of tBu groups undergoing rotational disorder

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 6.1 Ratio

Author Response: Larger than usual Ueq values are associated with some methyl C atoms of tBu groups, which undergo rotational disorder, and to C and O atoms of thioacetyl groups

PLAT220_ALERT_2_B NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 7.6 Ratio

Author Response: Larger than usual Ueq values are associated with some methyl C atoms of tBu groups, which undergo rotational disorder, and to C and O atoms of thioacetyl groups

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C109 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C41 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.05 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 2.23 eA-3
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 5 Check
Ox2A Cx6A Cx5A Cx7A Cx8A
PLAT213_ALERT_2_C Atom C110 has ADP max/min Ratio ..... 3.1 prolat

Author Response: Methyl C atoms of tBu groups undergoing rotational disorder

PLAT213_ALERT_2_C Atom C30A has ADP max/min Ratio ..... 3.1 prolat

Author Response: Methyl C atoms of tBu groups undergoing rotational disorder

PLAT213_ALERT_2_C Atom C43 has ADP max/min Ratio ..... 3.6 prolat

Author Response: Methyl C atoms of tBu groups undergoing rotational disorder

PLAT213_ALERT_2_C Atom C47 has ADP max/min Ratio ..... 3.2 prolat

Author Response: Methyl C atoms of tBu groups undergoing rotational disorder

PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.7 Ratio

Author Response: Larger than usual Ueq values are associated with some methyl C atoms of tBu groups, which undergo rotational disorder, and to C and O atoms of thioacetyl groups

PLAT220_ALERT_2_C NonSolvent Resd 2 O Ueq(max)/Ueq(min) Range 4.4 Ratio

Author Response: Larger than usual Ueq values are associated with some methyl C atoms of tBu groups, which undergo rotational disorder, and to C and O atoms of thioacetyl groups

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 7.1 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 8.3 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C125 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C133 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C141 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C29 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C45 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C53 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C61 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C65 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C75 Check

Author Response: Quaternary C atoms of tBu groups, whose methyl C atoms have much larger Ueq values due to rotational disorder

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of Ox1 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Cx1 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Cx3 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Ox1 0.137 Check
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C41 - C44 . 1.43 Ang.
And 2 other PLAT360 Alerts

PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond Cx2 - Cx1 . 1.40 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond Cx3 - Cx4 . 1.39 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 57 Note
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 14.27 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 12% Note
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 2) 8% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 4) 8.27 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 5) 6.73 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C156 Check
And 2 other PLAT380 Alerts

PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C76 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C80 Check

PLAT412_ALERT_2_G Short Intra XH3 .. XHn H91 ..Hy3G . 2.01 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H103 ..Hy9H . 2.12 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H11 ..H39A . 2.05 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H11 ..Hx2G . 2.02 Ang.
x,y,z = 1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn Hy8J ..Hx1B . 2.12 Ang.
1-x,1-y,1-z = 2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C126 ..Cx14 3.11 Ang.
-1+x,y,z = 1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C155 ..Cx22 3.13 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 214 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C69 --Cx18 1.74 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C133 --C163 1.71 Ang.
PLAT774_ALERT_1_G Check X-Y Bond in CIF: Fe2 --Fe3 .. 5.35 Ang.
And 5 other PLAT774 Alerts

PLAT774_ALERT_1_G Check X-Y Bond in CIF: Fe2 --Fe4 .. 5.36 Ang.
PLAT774_ALERT_1_G Check X-Y Bond in CIF: Fe3 --Fe4 .. 5.31 Ang.
PLAT774_ALERT_1_G Check X-Y Bond in CIF: Fe6 --Fe7 .. 5.37 Ang.
PLAT774_ALERT_1_G Check X-Y Bond in CIF: Fe6 --Fe8 .. 5.43 Ang.
PLAT774_ALERT_1_G Check X-Y Bond in CIF: Fe7 --Fe8 .. 5.29 Ang.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 162 Check
C31A -C29 -C31B 1.555 1.555 1.555 38.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 168 Check
C32A -C29 -C32B 1.555 1.555 1.555 42.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 172 Check
C30A -C29 -C30B 1.555 1.555 1.555 42.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 191 Check
C39 -C37 -CX24 1.555 1.555 1.555 38.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 248 Check
CX20 -C69 -C72 1.555 1.555 1.555 42.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 450 Check
C118 -C117 -CX16 1.555 1.555 1.555 39.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 486 Check
C165 -C133 -C134 1.555 1.555 1.555 43.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 527 Check
CX12 -C149 -C152 1.555 1.555 1.555 39.40 Deg.
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (III) . 3.27 Info
And 7 other PLAT794 Alerts

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PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (III)     .       3.18 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe3       (III)     .       3.18 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe4       (III)     .       3.19 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe5       (III)     .       3.27 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe6       (III)     .       3.18 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe7       (III)     .       3.17 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe8       (III)     .       3.19 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         50 Note
PLAT899_ALERT_4_G SHELXL97  is Deprecated and Succeeded by SHELXL/       2018 Note
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  7 ALERT level B = A potentially serious problem, consider carefully
 28 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 47 ALERT level G = General information/check it is not something unexpected

  8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 39 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
 20 ALERT type 4 Improvement, methodology, query or suggestion
  9 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

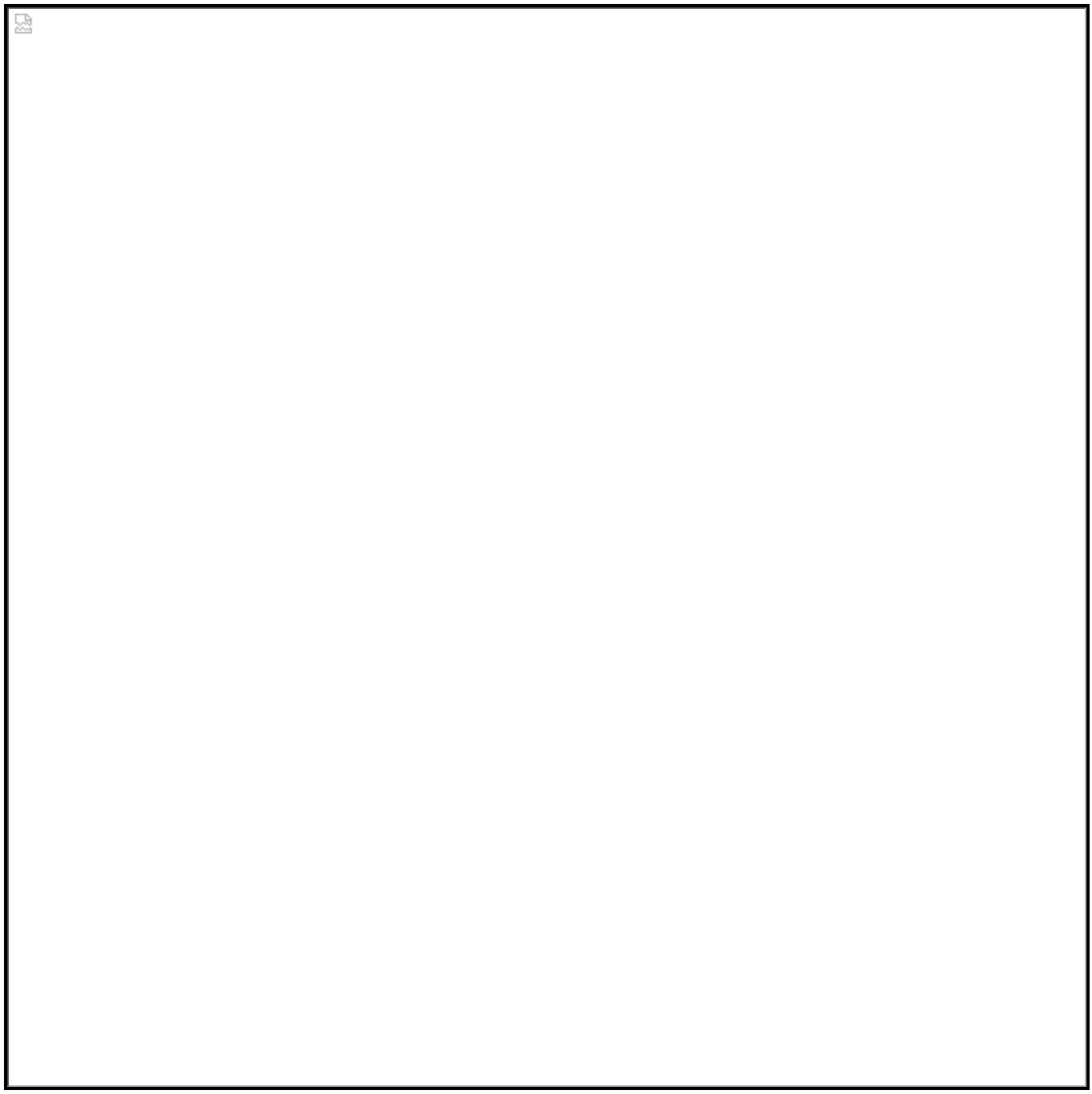
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 18/09/2020; check.def file version of 20/08/2020

Datablock fe4ch2sac_8_work3 - ellipsoid plot



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