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

CIF dictionary
Interpreting this report

Datablock: 160312ET_1_work6

Bond precision: C-C = 0.0069 A Wavelength=0.71073
Cell: a=15.8696(4) b=19.5070(5) c=32.5981(8)
alpha=97.1881(12) beta=102.1501(12) gamma=104.3036(13)
Temperature: 140 K

	Calculated	Reported
Volume	9390.9(4)	9390.9(4)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C80 H136 Fe4 O20 S2, 0.375(C4 H10 O)	C80 H136 Fe4 O20 S2,(C4 H10 O)0.375
Sum formula	C81.50 H139.75 Fe4 O20.38 S2	C81.50 H139.75 Fe4 O20.38 S2
Mr	1733.21	1733.20
Dx,g cm-3	1.226	1.226
Z	4	4
Mu (mm-1)	0.712	0.712
F000	3711.0	3711.0
F000'	3719.02	
h,k,lmax	20,24,41	20,24,41
Nref	41033	39675
Tmin,Tmax	0.653,0.758	0.663,0.769
Tmin'	0.632	

Correction method= # Reported T Limits: Tmin=0.663
Tmax=0.769 AbsCorr = MULTI-SCAN
Data completeness= 0.967 Theta(max)= 27.010
R(reflections)= 0.0602(27095) wR2(reflections)= 0.1754(39675)
S = 1.040 Npar= 2008

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) ..... 8 Report
C175 C176 C177 C178 C47A etc.

Author Response: Isotropic refinement was used for disordered C atoms of tBu groups with SOF < 2/3 (C175,C176,C177,C178,C47A,C48A,C49A,C50A in the Main Residues) and for C and O atoms of minority thioacetyl components and of solvent molecules

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C19 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 C43 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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.967 Why?
PLAT213_ALERT_2_C Atom C112 has ADP max/min Ratio ..... 3.3 prolat
And 6 other PLAT213 Alerts

PLAT213_ALERT_2_C Atom C128 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C133 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C22 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C44 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom C54 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom C60A has ADP max/min Ratio ..... 3.2 prolat

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.8 Ratio
And 3 other PLAT220 Alerts

PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 5.3 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 5.3 Ratio

PLAT220_ALERT_2_C NonSolvent Resd 2 O Ueq(max)/Ueq(min) Range 4.0 Ratio

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 6.3 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O11 Check
And 2 other PLAT241 Alerts

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C12 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C14 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C103 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 C107 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 C111 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 C127 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 C131 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 C143 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 C23 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 C27 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 C35 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 C51 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 C55 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 C72 Check

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

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00689 Ang.

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         71 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         19 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..       0.63 mm
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      19.70 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of S7         Constrained at       0.25 Check
And 9 other PLAT300 Alerts

PLAT300_ALERT_4_G Atom Site Occupancy of O43        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C165       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C166       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C181       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16O       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16P       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16Q       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18C       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18D       Constrained at       0.25 Check

PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        17% Note
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  2  )        11% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )       6.55 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )       4.70 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C73 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C80 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H12J     ..H91      .       1.94 Ang.
                                               x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H88      ..H12D     .       1.93 Ang.
                                               x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H91      ..H16D     .       2.06 Ang.
                                               x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H17      ..H62A     .       2.03 Ang.
                                               x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H12U     ..H16N     .       2.13 Ang.
                                           1-x,-y,1-z  =      2_656 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H13J     ..H15F     .       1.86 Ang.
                                          1-x,1-y,1-z  =      2_666 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          34 Note
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Fe2      --Fe3       ..       5.36 Ang.
And 5 other PLAT774 Alerts

PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Fe2      --Fe4       ..       5.35 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Fe3      --Fe4       ..       5.35 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Fe6      --Fe7       ..       5.40 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Fe6      --Fe8       ..       5.44 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Fe7      --Fe8       ..       5.27 Ang.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         282 Check
             C47A -C12  -C47B    1.555   1.555   1.555            32.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         773 Check
             C119 -C89  -C175    1.555   1.555   1.555            18.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         851 Check
             C167 -C90  -C123    1.555   1.555   1.555            23.70 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #           3 Note
             C4 H10 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #           4 Note
             C4 H10 O
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (III)     .       3.25 Info
And 7 other PLAT794 Alerts

PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (III)     .       3.16 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe3       (III)     .       3.18 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe4       (III)     .       3.16 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe5       (III)     .       3.25 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe6       (III)     .       3.15 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe7       (III)     .       3.16 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe8       (III)     .       3.17 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        365 Note
PLAT899_ALERT_4_G SHELXL97  is Deprecated and Succeeded by SHELXL/       2018 Note
```

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

  7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 38 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
 24 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

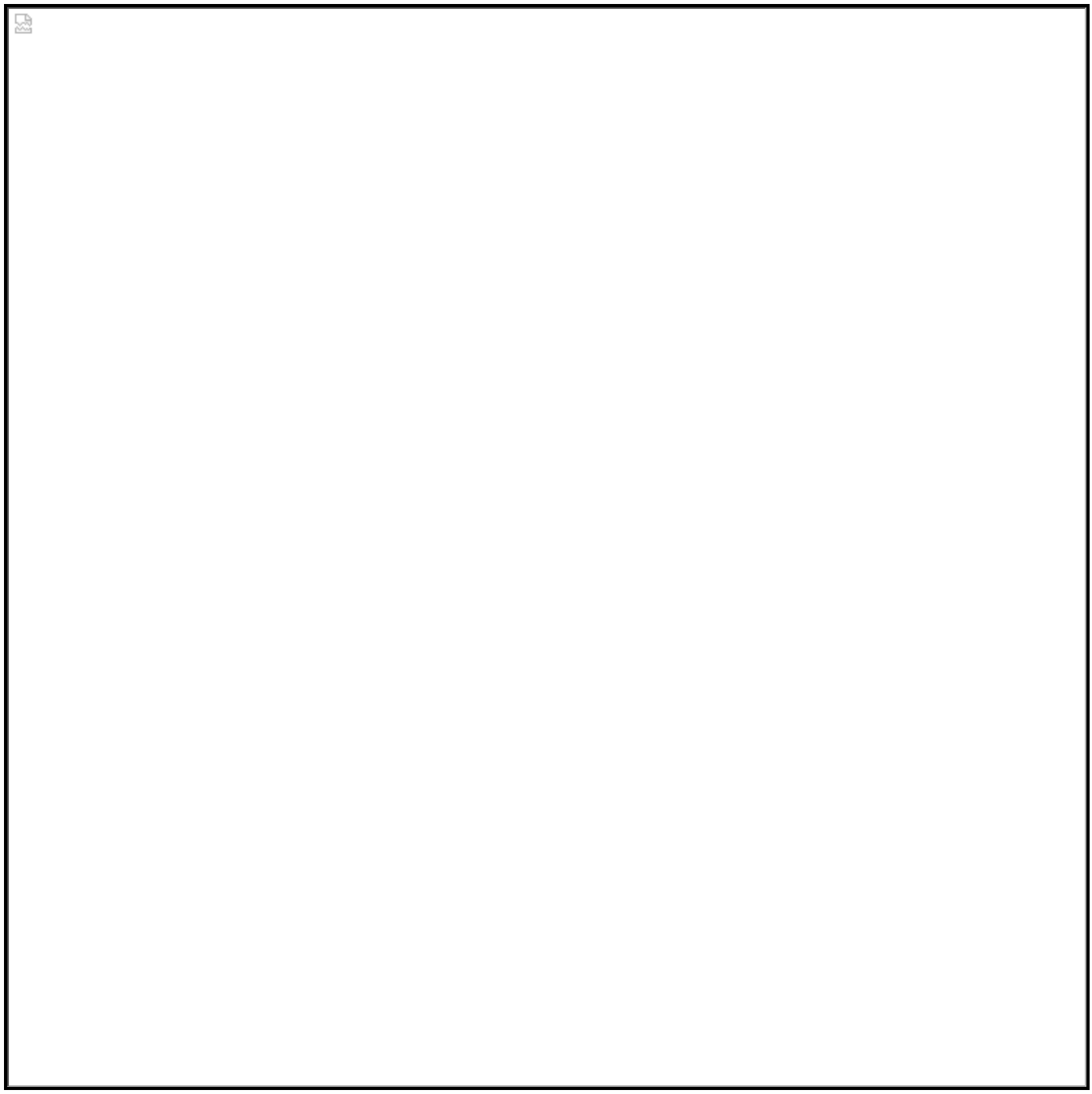
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 160312ET_1_work6 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry