checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: mm7

Bond precision: C-C = 0.0064 A Wavelength=0.71073

Cell: **a=9.6150(3) b=11.7549(4) c=17.2226(5)**
alpha=90 beta=105.283(3) gamma=90
Temperature: **123 K**

	Calculated	Reported
Volume	1877.72(11)	1877.72(10)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	C42 H45.90 Fe2 I2.10 O2	C21 H23 Fe I O
Sum formula	C42 H45.90 Fe2 I2.10 O2	C21 H23 Fe I O
Mr	960.88	474.14
Dx,g cm-3	1.699	1.677
Z	2	4
Mu (mm-1)	2.534	2.452
F000	954.4	944.0
F000'	954.07	
h,k,lmax	13,16,24	13,16,24
Nref	5564	5212
Tmin,Tmax	0.783,0.783	0.844,1.000
Tmin'	0.783	

Correction method= MULTI-SCAN

Data completeness= 0.937 Theta(max)= 30.150

R(reflections)= 0.0505(4244) wR2(reflections)= 0.1161(5212)

S = 1.128 Npar= 206

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) 5
PLAT420_ALERT_2_B D-H Without Acceptor O1 - H1 ... ?

Alert level C

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as

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           calculated from the _atom_site* data lies outside
           the range 0.99 <> 1.01
          From the CIF: _cell_formula_units_Z                  4
          From the CIF: _chemical_formula_weight          474.14
          TEST: Calculate formula weight from _atom_site_*
          atom     mass    num     sum
          I       126.90    1.05  133.29
          Fe       55.85    1.00   55.85
          O        16.00    1.00   16.00
          C        12.01   21.00  252.23
          H         1.01   22.95   23.13
          Calculated formula weight             480.50
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.15
PLAT410_ALERT_2_C Short Intra H...H Contact  H1A    ..  H16     ..       1.97 Ang.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT043_ALERT_1_C Check Reported Molecular Weight ................     474.14
PLAT045_ALERT_1_C Calculated and Reported Z Differ by ............       0.50 Ratio
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       3.34 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms ..          ?
PLAT721_ALERT_1_C Bond    Calc     1.43218, Rep     1.42000 Dev...       0.01 Ang.
             C9A  -C10A    1.555   1.555                   #         67
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Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C21 H23 Fe1 I1 O1
           Atom count from the _atom_site data:  C21 H22.94970 Fe1 I1.0503 O1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C21 H23 Fe I O
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         84.00     84.00    0.00
          H         92.00     91.80    0.20
          Fe         4.00      4.00    0.00
          I          4.00      4.20   -0.20
          O          4.00      4.00    0.00
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       6.50
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................      17.00 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          3
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          !
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   0 ALERT level A = In general: serious problem
   2 ALERT level B = Potentially serious problem
  11 ALERT level C = Check and explain
   7 ALERT level G = General alerts; check

   9 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
   2 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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*, 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 22/10/2010; check.def file version of 11/10/2010

Datablock mm7 - ellipsoid plot