checkCIF/PLATON report

Structure factors have been supplied for datablock(s) yellow_ch3cn_293

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: yellow_ch3cn_293

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Bond precision:  C-C = 0.0151 A          Wavelength=0.71073

Cell:             a=43.047(14)      b=14.742(6)     c=23.161(6)
                  alpha=90          beta=90         gamma=90
Temperature:      293 K
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	Calculated	Reported
Volume	14698(9)	14699(8)
Space group	F d d 2	F d d 2
Hall group	F 2 -2d	F 2 -2d
Moiety formula	C62 H58 Cl8 Fe N10, 2(B F4), 2(C2 H3 N)	C62 H58 Cl8 Fe N10, 2(B F4), 2(C2 H3 N)
Sum formula	C66 H64 B2 Cl8 F8 Fe N12	C66 H64 B2 Cl8 F8 Fe N12
Mr	1538.36	1538.36
Dx,g cm-3	1.390	1.390
Z	8	8
Mu (mm-1)	0.565	0.565
F000	6304.0	6304.0
F000’	6318.66	
h,k,lmax	54,18,29	54,18,29
Nref	8030[4117]	8029
Tmin,Tmax	0.873,0.893	0.453,0.746
Tmin’	0.868	

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Correction method= # Reported T Limits: Tmin=0.453 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.95/1.00      Theta(max)= 26.999

R(reflections)= 0.0656( 3666)     wR2(reflections)= 0.1776( 8029)

S = 0.939                 Npar= 474
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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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.216
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01512 Ang.

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.590
From the CIF: _refine_ls_abs_structure_Flack_su 0.050
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 46% Check
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C24 --C27' . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C24A --C27A . 0.19 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C15 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C24 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C24A Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C1S Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including F1 0.156 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N1S 0.181 Check
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 34 Ang**3
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 0.59 Check

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Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 9 Report
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.216 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 6 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 7 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of B1 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 15% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H2 ..H25A . 2.08 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H2A ..H25G . 2.14 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 3 Note
PLAT721_ALERT_1_G Bond Calc 0.97000, Rep 0.96000 Dev... 0.01 Ang.
C26A -H26F 1.555 1.555 ..... # 84 Check
PLAT721_ALERT_1_G Bond Calc 0.97000, Rep 0.96000 Dev... 0.01 Ang.
C27A -H27D 1.555 1.555 ..... # 88 Check
PLAT721_ALERT_1_G Bond Calc 0.97000, Rep 0.96000 Dev... 0.01 Ang.
C26" -H26I 1.555 1.555 ..... # 102 Check
PLAT722_ALERT_1_G Angle Calc 108.00, Rep 109.50 Dev... 1.50 Degree
H27D -C27A -H27E 1.555 1.555 1.555 # 163 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C24 --C25' 1.73 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (II) . 2.15 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 55 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 1 Check

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

  7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 13 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
  9 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 10/08/2020; check.def file version of 06/08/2020

Datablock yellow_ch3cn_293 - ellipsoid plot