checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Red_H2O_120

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: Red_H2O_120

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Bond precision:  C-C = 0.0053 A          Wavelength=0.71073

Cell:           a=16.9032(12)    b=21.2547(15)     c=17.4043(12)
                alpha=90         beta=91.033(2)    gamma=90
Temperature:    120 K
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	Calculated	Reported
Volume	6251.9(8)	6251.9(8)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C62 H58 Cl8 Fe N10), 4(BF4), H2 O	2(C62 H58 Cl8 Fe N10), 4(BF4), H2 O
Sum formula	C124 H118 B4 Cl16 F16 Fe2 N20 O	C124 H118 B4 Cl16 F16 Fe2 N20 O
Mr	2930.53	2930.52
Dx,g cm-3	1.557	1.557
Z	2	2
Mu (mm-1)	0.659	0.659
F000	2996.0	2996.0
F000’	3003.31	
h,k,lmax	21,27,22	21,27,22
Nref	13645	13643
Tmin,Tmax	0.888,0.936	0.654,0.746
Tmin’	0.794	

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Correction method= # Reported T Limits: Tmin=0.654 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 27.000

R(reflections)= 0.0521( 7932)     wR2(reflections)= 0.1237( 13643)

S = 0.993                 Npar= 841
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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 C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
          Rint given   0.142
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.2 Ratio
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        C28 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -3.013 Report
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.142 Report
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         B1 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         B2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1W       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1WA      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1WB      Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )       1.50 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl2A     ..Cl2A            3.25 Ang.
                                              1-x,-y,1-z  =      3_656 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (III)     .       3.78 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...         13 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 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
   2 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 16/07/2020; check.def file version of 12/07/2020

Datablock Red_H2O_120 - ellipsoid plot