checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cmmm_a_sq

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: cmmm_a_sq

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Bond precision:   C-C = 0.0044 A          Wavelength=0.70000

Cell:               a=26.924(5)      b=41.374(8)      c=26.072(5)
                    alpha=90         beta=90          gamma=90
Temperature:        298 K
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	Calculated	Reported
Volume	29043(10)	29043(10)
Space group	C m m m	C m m m
Hall group	-C 2 2	-C 2 2
Moiety formula	C94 H55 Fe N6 O16 Zr3 [+ solvent]	?
Sum formula	C94 H55 Fe N6 O16 Zr3 [+ solvent]	C188 H126 Fe2 N12 O32 Zr6
Mr	1853.95	3724.02
Dx,g cm-3	0.424	0.426
Z	4	2
Mu (mm-1)	0.166	0.166
F000	3740.0	3772.0
F000'	3700.33	
h,k,lmax	38,58,37	38,58,37
Nref	23064	22997
Tmin,Tmax	0.971,0.998	0.968,0.998
Tmin'	0.967	

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Correction method= # Reported T Limits: Tmin=0.968 Tmax=0.998
AbsCorr = NONE

Data completeness= 0.997           Theta(max)= 29.858
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R(reflections)= 0.0564(19264)

wR2(reflections)= 0.1738(22997)

S = 0.967 Npar= 318

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

PLAT213_ALERT_2_B Atom O2 has ADP max/min Ratio ..... 4.2 prolat
PLAT213_ALERT_2_B Atom C28 has ADP max/min Ratio ..... 4.2 prolat
PLAT213_ALERT_2_B Atom C29 has ADP max/min Ratio ..... 4.8 prolat
PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 7.9 Ratio
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C29 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Zr02 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT334_ALERT_2_B Small <C-C> Benzene Dist. C27 -C28_e . 1.32 Ang.
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 7 Check

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Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
Reddish
PLAT213_ALERT_2_C Atom Zr01 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom O1 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C3 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C4 has ADP max/min Ratio ..... 3.7 prolat
PLAT213_ALERT_2_C Atom C5 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C6 has ADP max/min Ratio ..... 3.6 prolat
PLAT213_ALERT_2_C Atom C7 has ADP max/min Ratio ..... 3.6 prolat
PLAT213_ALERT_2_C Atom C8 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C13 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom C16 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C30 has ADP max/min Ratio ..... 3.1 prolat
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.1 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C9 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C10 Check
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 C13 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Zr01 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C11 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.5 Note
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C2 -C7 . 1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C8 -C13 . 1.36 Ang.

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PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          9 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         40 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          4 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          7 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.58Ang From O4              1.63 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.52Ang From O2      .       0.93 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.53Ang From O2      .       0.79 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.66Ang From O1      .       0.52 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.45Ang From O1      .       0.50 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.02Ang From O2      .      -1.06 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From O1      .      -0.76 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.99Ang From O2      .      -0.70 eA-3
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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:C188 H126 Fe2 N12 O32 Zr6
           Atom count from the _atom_site data:  C188 H110 Fe2 N12 O32 Zr6
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C188 H126 Fe2 N12 O32 Zr6
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        376.00    376.00    0.00
          H        252.00    220.00   32.00
          Fe         4.00      4.00    0.00
          N         24.00     24.00    0.00
          O         64.00     64.00    0.00
          Zr        12.00     12.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...          2 Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      33.30 Why ?
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.70000 Ang.
PLAT300_ALERT_4_G Atom Site Occupancy of C19        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )          6% Note
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          2 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          8 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Zr01      (IV)      .       4.07 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zr02      (IV)      .       4.05 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         20 Note
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PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
  11 ALERT level B = A potentially serious problem, consider carefully
  41 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  29 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  49 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
  14 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 28/11/2022; check.def file version of 28/11/2022

Datablock cmmm_a_sq - ellipsoid plot