checkCIF/PLATON report

Structure factors have been supplied for datablock(s) p4mmm_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: p4mmm_a_sq

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Bond precision:   C-C = 0.0105 A          Wavelength=0.70000

Cell:               a=25.252(4)      b=25.252(4)      c=25.552(5)
                    alpha=90         beta=90          gamma=90
Temperature:        298 K
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	Calculated	Reported
Volume	16294(6)	16294(6)
Space group	P 4/m m m	P 4/m m m
Hall group	-P 4 2	-P 4 2
Moiety formula	C72 H40 Fe N4 O16 Zr3 [+ solvent]	?
Sum formula	C72 H40 Fe N4 O16 Zr3 [+ solvent]	C144 H96 Fe2 N8 O32 Zr6
Mr	1546.59	3109.30
Dx,g cm-3	0.315	0.317
Z	2	1
Mu (mm-1)	0.144	0.144
F000	1548.0	1564.0
F000'	1528.07	
h,k,lmax	29,29,29	29,20,29
Nref	7480	7438
Tmin,Tmax	0.983,0.999	0.979,0.999
Tmin'	0.979	

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Correction method= # Reported T Limits: Tmin=0.979 Tmax=0.999
AbsCorr = NONE

Data completeness= 0.994           Theta(max)= 24.013
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R(reflections)= 0.0683(5330)

wR2(reflections)= 0.2391(7438)

S = 1.052 Npar= 163

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

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PLAT213_ALERT_2_B Atom Fe1             has ADP max/min Ratio .....        4.3 prolat
PLAT213_ALERT_2_B Atom N2              has ADP max/min Ratio .....        4.5 prolat
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  Zr1      --O3       .       10.5 s.u.
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        Zr2 Check
PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor ....        7.9 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..         10 Check
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Alert level C

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CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           Greenish
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5813
PLAT213_ALERT_2_C Atom N1              has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C11             has ADP max/min Ratio .....        3.6 prolat
PLAT213_ALERT_2_C Atom C13             has ADP max/min Ratio .....        3.5 prolat
PLAT213_ALERT_2_C Atom C14             has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C15             has ADP max/min Ratio .....        3.8 prolat
PLAT213_ALERT_2_C Atom C16             has ADP max/min Ratio .....        3.6 prolat
PLAT215_ALERT_3_C Disordered C9        has ADP max/min Ratio .....        3.3 Note
PLAT215_ALERT_3_C Disordered C10       has ADP max/min Ratio .....        3.1 Note
PLAT215_ALERT_3_C Disordered C17       has ADP max/min Ratio .....        3.5 Note
PLAT215_ALERT_3_C Disordered C18       has ADP max/min Ratio .....        3.7 Note
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Zr2      --O3       .        6.9 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Zr2      --O4       .        7.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C2       --C7       .       0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         N2 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
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Zr1 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        C12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Zr1      0.178 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C2       -C7       .       1.35 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01047 Ang.
PLAT752_ALERT_4_C Angle   Calc       90.00, Rep       90.00 ......  Senseless s.u.
              N2      -FE1     -N1         1_555  1_555  1_555     #   58 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         10 Note
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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.581         34 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          3 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.78Ang From Fe1             1.89 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.71Ang From O3      .       0.44 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:C144 H96 Fe2 N8 O32 Zr6
           Atom count from the _atom_site data:  C144 H80 Fe2 N8 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    1
          From the CIF: _chemical_formula_sum  C144 H96 Fe2 N8 O32 Zr6
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        144.00    144.00    0.00
          H         96.00     80.00   16.00
          Fe         2.00      2.00    0.00
          N          8.00      8.00    0.00
          O         32.00     32.00    0.00
          Zr         6.00      6.00    0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         14 Report
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       5.89 Why ?
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.70000 Ang.
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C9         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         14% Note
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........           ! Info
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          8 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Zr1       (IV)      .       3.98 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zr2       (IV)      .       4.02 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (II)      .       2.17 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         73 Note
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 !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        39% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.6 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           9 Units
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
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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
   6 ALERT level B = A potentially serious problem, consider carefully
  36 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  36 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  34 ALERT type 2 Indicator that the structure model may be wrong or deficient
  15 ALERT type 3 Indicator that the structure quality may be low
  16 ALERT type 4 Improvement, methodology, query or suggestion
   5 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 p4mmm_a_sq - ellipsoid plot