checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Fe_trz_hexa_420K_a

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: Fe_trz_hexa_420K_a

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Bond precision:   C-C = 0.0030 A          Wavelength=1.54178

Cell:             a=22.1736(14)      b=22.1736(14)      c=7.0796(5)
                  alpha=90           beta=90            gamma=120
Temperature:      273 K

                 Calculated                Reported
Volume           3014.5(4)                 3014.5(4)
Space group      R -3 m                    R -3 m :H
Hall group       -R 3 2"                   -R 3 2"
Moiety formula   C12 H9 Fe N12             ?
Sum formula      C12 H9 Fe N12             C108 H72 Fe6 N36
Mr               377.16                    2209.11
Dx,g cm-3        1.247                     1.217
Z                6                         1
Mu (mm-1)        6.202                     6.103
F000             1146.0                    1128.0
F000'            1142.43
h,k,lmax         27,27,8                   26,27,8
Nref             725                       725
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 1.000           Theta(max)= 72.333

R(reflections)= 0.0266( 698)                    wR2(reflections)=
                                                0.0986( 725)
S = 0.945                  Npar= 60
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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

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PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by ..       8.98 Check
PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor ....        5.1 Note
PLAT601_ALERT_2_B Unit Cell Contains Solvent Accessible VOIDS of .        155 Ang**3
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Alert level C

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       1.62 %
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT085_ALERT_2_C SHELXL Default Weighting Scheme is not Optimized     Please Check
PLAT215_ALERT_3_C Disordered C2        has ADP max/min Ratio .....        3.6 Note
PLAT215_ALERT_3_C Disordered C3        has ADP max/min Ratio .....        3.5 Note
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT245_ALERT_2_C U(iso) H2        Smaller than U(eq) C2        by      0.016 Ang**2
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N3       --H3N      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N4       --H4N      .     Please Check
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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:C108 H72 Fe6 N36
           Atom count from the _atom_site data:  C72 H54 Fe6 N72
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    1
           From the CIF: _chemical_formula_sum  C108 H72 Fe6 N36
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        108.00     72.00   36.00
           H         72.00     54.00   18.00
           Fe         6.00      6.00    0.00
           N         36.00     72.00  -36.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     6.0000 Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        273 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --N1       .        6.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe2      --N2       .        5.9 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of C2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3         Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3N        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4N        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        24% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C2              2.38 Ang.
                                  2/3-x,1/3-x+y,4/3-z  =     12_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C2              2.38 Ang.
                                    2/3-x,1/3-y,4/3-z  =     25_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C3              2.40 Ang.
                                    2/3-x,1/3-y,4/3-z  =     25_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C3              2.40 Ang.
                                  2/3-x,1/3-x+y,4/3-z  =     12_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C1              2.79 Ang.
                                  2/3-x,1/3-x+y,4/3-z  =     12_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C2       ..C3              1.38 Ang.
                                  2/3-x,1/3-x+y,4/3-z  =     12_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C2       ..C3              1.48 Ang.
                                    2/3-x,1/3-y,4/3-z  =     25_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C2       ..C2              2.63 Ang.
                                  2/3-x,1/3-x+y,4/3-z  =     12_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C2       ..C2              2.69 Ang.
                                    2/3-x,1/3-y,4/3-z  =     25_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C3       ..C3              2.70 Ang.
                                  2/3-x,1/3-x+y,4/3-z  =     12_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C3       ..C3              2.74 Ang.
                                    2/3-x,1/3-y,4/3-z  =     25_556 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      24.20 Deg.
              C2   -C1   -C2     24_555   1_555   1_555 ......     #   37 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      20.60 Deg.
              C3   -C1   -C3     24_555   1_555   1_555 ......     #   42 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
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.          5 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
34 **ALERT level G** = General information/check it is not something unexpected

15 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
23 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 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

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 18/12/2021; check.def file version of 18/12/2021

Datablock Fe_trz_hexa_420K_a - ellipsoid plot