checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Fe_tetrazol_RT_0ma_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_tetrazol_RT_0ma_a

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Bond precision:   C-C = 0.0140 A          Wavelength=1.54178

Cell:              a=22.5930(7)      b=22.5930(7)      c=7.4636(2)
                   alpha=90          beta=90           gamma=120
Temperature:       299 K

                 Calculated                Reported
Volume           3299.3(2)                 3299.3(2)
Space group      R -3                      R -3 :H
Hall group       -R 3                      -R 3
Moiety formula   C12 H6 Fe N12, 3(O)       C12 H6 Fe N12, 3(H2 O)
Sum formula      C12 H6 Fe N12 O3          C12 H12 Fe N12 O3
Mr               422.14                    428.14
Dx,g cm-3        1.275                     1.275
Z                6                         6
Mu (mm-1)        5.832                     5.821
F000             1272.0                    1272.0
F000'            1269.30
h,k,lmax         27,27,9                   27,27,9
Nref             1464                      862
Tmin,Tmax                                  0.500,0.900
Tmin'

Correction method= # Reported T Limits: Tmin=0.500 Tmax=0.900
AbsCorr = NUMERICAL

Data completeness= 0.589           Theta(max)= 72.347

R(reflections)= 0.0972( 841)                    wR2(reflections)=
                                                0.2661( 862)
S = 1.075                  Npar= 132
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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

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 6.00 Check
PLAT088_ALERT_3_B Poor Data / Parameter Ratio ..... 6.53 Note
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 567 Report

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Alert level C

DENSD01_ALERT_1_C The ratio of the submitted crystal density and that
calculated from the formula is outside the range 0.99 <> 1.01
Crystal density given = 1.275
Calculated crystal density = 1.293
PLAT031_ALERT_4_C Refined Extinction Parameter Within Range ..... 2.500 Sigma
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT046_ALERT_1_C Reported Z, MW and D(calc) are Inconsistent .... 1.293 Check
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
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.27 Report
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1W 0.111 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.014 Ang.
PLAT430_ALERT_2_C Short Inter D...A Contact N4 ..O2W . 2.89 Ang.
1/3+x-y,-1/3+x,5/3-z = 18_546 Check
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 83 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.548 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 9 Note
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 13.38 Check

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Alert level G

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:C12 H12 Fe1 N12 O3
Atom count from the _atom_site data: C12 H6 Fe1 N12 O3
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 6
From the CIF: _chemical_formula_sum C12 H12 Fe N12 O3
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	72.00	72.00	0.00
H	72.00	36.00	36.00
Fe	6.00	6.00	0.00
N	72.00	72.00	0.00
O	18.00	18.00	0.00

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 12 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0 0.963 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 28.85 Why ?

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PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          4 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C3         Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3A        Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3B        Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4         Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4A        Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4B        Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3         Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3A        Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3B        Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4         Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A        Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4B        Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1W        Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2W        Constrained at        0.4 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         22% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O1W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O2W Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.11 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (III)     .       3.92 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (II)      .       1.97 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         72 Note
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         26 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
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.          1 Info
PLAT982_ALERT_1_G The  C-f'=    0.0192 Deviates from  IT-value =       0.0181 Check
PLAT982_ALERT_1_G The Fe-f'=   -1.0935 Deviates from  IT-value =      -1.1336 Check
PLAT982_ALERT_1_G The  N-f'=    0.0330 Deviates from  IT-value =       0.0311 Check
PLAT982_ALERT_1_G The  O-f'=    0.0517 Deviates from  IT-value =       0.0492 Check
PLAT983_ALERT_1_G The Fe-f"=    3.1934 Deviates from  IT-Value =       3.1974 Check
PLAT983_ALERT_1_G The  O-f"=    0.0336 Deviates from  IT-Value =       0.0322 Check
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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
 15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 45 **ALERT level G** = General information/check it is not something unexpected

 18 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
 20 ALERT type 4 Improvement, methodology, query or suggestion
  4 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_tetrazol_RT_0ma_a - ellipsoid plot