checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Red_CH3CN_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_CH3CN_120

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Bond precision:  C-C = 0.0240 A          Wavelength=0.71073

Cell:              a=45.272(7)      b=13.335(2)      c=24.665(4)
                   alpha=90         beta=90          gamma=90
Temperature:       120 K
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	Calculated	Reported
Volume	14890(4)	14890(4)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C62 H58 Cl8 Fe N10, 2(B F4), 2(C2 H3 N)	2(C62 H58 Cl8 Fe N10), 4(B F4), 4(C2 H3 N)
Sum formula	C66 H64 B2 Cl8 F8 Fe N12	C133 H128 B4 Cl16 F16 Fe2 N24
Mr	1538.37	3088.73
Dx,g cm-3	1.372	1.378
Z	8	4
Mu (mm-1)	0.557	0.558
F000	6304.0	6328.0
F000’	6318.66	
h,k,lmax	55,16,30	55,16,30
Nref	14647	14645
Tmin,Tmax	0.935,0.946	0.642,0.746
Tmin’	0.870	

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Correction method= # Reported T Limits: Tmin=0.642 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 25.999

R(reflections)= 0.1504( 6631)     wR2(reflections)= 0.4839( 14645)

S = 1.067                 Npar= 938
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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 A

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..... 0.48 Report

Author Response: The crystals suffered from a severe disorder of the lattice solvent molecules and a low reflective power.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.198

Author Response: The crystals suffered from a severe disorder of the lattice solvent molecules and a low reflective power.

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.198 Report

Author Response: The crystals suffered from a severe disorder of the lattice solvent molecules and a low reflective power.

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02402 Ang.

Author Response: The crystals suffered from a severe disorder of the lattice solvent molecules and a low reflective power.

Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 45% Check
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 6.00 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT082_ALERT_2_C High R1 Value ..... 0.15 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.11 Report
PLAT213_ALERT_2_C Atom C28 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C30 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C31 has ADP max/min Ratio ..... 3.1 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.7 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C1A --C2A . 5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Fe1 --N4 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cl1 --C13 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cl3 --C19 . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 --C4 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1A --C8A . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5 --C18 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5A --C6A . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C6A --C7A . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C10 --C11 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C16 --C17 . 0.17 Ang.

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PLAT234_ALERT_4_C Large Hirshfeld Difference C19A     --C20A     .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C24A     --C26A     .       0.22 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C6A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C11 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C22 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C18 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C24A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C28 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C28A Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        F1      0.179 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        F5      0.171 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       N1S      0.125 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       N2S      0.145 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       N3S      0.119 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       N4S      0.125 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C18A     -C23A           1.37 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C28      - C30      .       1.43 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -2.059 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         3 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         1 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      27.20 Check
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C133 H128 B4 Cl16 F16 Fe2 N24
           Atom count from _chemical_formula_moiety:C132 H128 B4 Cl16 F16 Fe2 N24
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:C133 H128 B4 Cl16 F16 Fe2 N24
           Atom count from the _atom_site data:  C132 H128 B4 Cl16 F16 Fe2 N24
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    4
          From the CIF: _chemical_formula_sum  C133 H128 B4 Cl16 F16 Fe2 N24
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        532.00    528.00    4.00
          H        512.00    512.00    0.00
          B         16.00     16.00    0.00
          Cl        64.00     64.00    0.00
          F         64.00     64.00    0.00
          Fe         8.00      8.00    0.00
          N         96.00     96.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        12 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        16 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      2.00 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.19 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    203.22 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         6 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        16 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        10 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
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PLAT300_ALERT_4_G Atom Site Occupancy of C29'       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C29A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C30'       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C30A       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 C31A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29E       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29F       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29H       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29I       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30E       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30F       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30H       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30I       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31E       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31F       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31H       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31I       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SC       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SC       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6SC       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N4S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8SC       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         4% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )       100% Note
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H6SA     ..H22      .       2.09 Ang.
                                                    x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H6SC     ..H22      .       2.06 Ang.
                                                    x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C6S      ..C22              3.10 Ang.
                                                    x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........         12 Note
PLAT721_ALERT_1_G Bond    Calc     0.98000, Rep     0.99760 Dev...       0.02 Ang.
              C2S      -H2SA            1.555   1.555 ........     #  175 Check
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PLAT721_ALERT_1_G Bond    Calc     0.98000, Rep     0.99850 Dev...       0.02 Ang.
              C2S      -H2SB           1.555   1.555 ........     #  176 Check
PLAT721_ALERT_1_G Bond    Calc     0.98000, Rep     0.99820 Dev...       0.02 Ang.
              C2S      -H2SC           1.555   1.555 ........     #  177 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      111.50 Dev...       1.50 Degree
              C1S     -C2S     -H2SB       1.555  1.555  1.555     #  318 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      111.40 Dev...       2.40 Degree
              C1S     -C2S     -H2SC       1.555  1.555  1.555     #  319 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      107.70 Dev...       2.30 Degree
              H2SA    -C2S     -H2SB       1.555  1.555  1.555     #  320 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      107.50 Dev...       1.50 Degree
              H2SA    -C2S     -H2SC       1.555  1.555  1.555     #  321 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      107.50 Dev...       1.50 Degree
              H2SB    -C2S     -H2SC       1.555  1.555  1.555     #  322 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          6 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (III)     .       3.75 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        112 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...         43 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
45 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
86 **ALERT level G** = General information/check it is not something unexpected

16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
33 ALERT type 2 Indicator that the structure model may be wrong or deficient
14 ALERT type 3 Indicator that the structure quality may be low
71 ALERT type 4 Improvement, methodology, query or suggestion
1 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 16/07/2020; check.def file version of 12/07/2020

Datablock Red_CH3CN_120 - ellipsoid plot