checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_tca_i6_0m

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: cu_tca_i6_0m

```
Bond precision:   C-C = 0.0079 A          Wavelength=1.54178

Cell:               a=20.959(1)      b=20.959(1)      c=20.959(1)
                    alpha=90         beta=90          gamma=90
Temperature:        170 K
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	Calculated	Reported
Volume	9206.9(13)	9206.9(13)
Space group	I 2 3	I 2 3
Hall group	I 2 2 3	I 2 2 3
Moiety formula	4(C21 H12 N O6), 4(C21 H15 N O6), C4 H4 I12, 6(H O), 12(H4 N)	2(C21 H12 N O6), 2(C21 H15 N O6), 6(H4 N), 1.5(H2 O2), 0.5(C4 H
Sum formula	C172 H166 I12 N20 O54	C86 H83 I6 N10 O27
Mr	4900.05	2450.02
Dx,g cm-3	1.768	1.768
Z	2	4
Mu (mm-1)	16.593	16.593
F000	4812.0	4812.0
F000'	4819.46	
h,k,lmax		24,25,21
Nref		2827
Tmin,Tmax	0.117,0.137	0.540,0.753
Tmin'	0.012	

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Correction method= # Reported T Limits: Tmin=0.540 Tmax=0.753
AbsCorr = NONE

Data completeness=                  Theta(max)= 68.285
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R(reflections)= 0.0696(2550) wR2(reflections)= 0.2132(2827)

S = 1.130 Npar= 189

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

PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor .... 4.6 Note

Author Response: Because photoactive CHI3 that encapsulated within the unit cell became disordered. Disordered singal of I atoms resluted in above alert.

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.500
From the CIF: _refine_ls_abs_structure_Flack_su 25.000
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: 4(C21 H12 N O6), 4(C21 H15 N O6), C4 H4 I12, 6(H O), 12(H4 N
Rep.: 2(C21 H12 N O6), 2(C21 H15 N O6), 6(H4 N), 1.5(H2 O2), 0.5(C
PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.17 Do !
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 2 Check
I1 C15
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C00K Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.7 Note

Author Response: Because photoactive CHI3 that encapsulated within the unit cell became disordered. Disordered singal of I atoms resluted in above alert.

PLAT260_ALERT_2_C Large Average Ueq of Residue Including O00M 0.149 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C21 H12 N O6
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by ..... 0.0022 Check
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.65Ang From O00M . -0.68 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H00M . -0.32 eA-3
PLAT987_ALERT_1_C The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 6 Report
H003 H00M H00C H00E H00F H00G
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.500 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.16 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report

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PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H15        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H00M       Constrained at        0.5 Check
PLAT417_ALERT_2_G Short Inter D-H..H-D       H00G     ..H00M     .        1.87 Ang.
                                  -1/2+z,3/2-x,3/2-y  =     18_466 Check
PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder           ! Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          36 Note
              O001    O002    O003    H003    O004    N005    H00C    H00E
              H00F    H00G    C006    N007    C008    C009    C00A    H00A
              C00B    H00B    C00C    C00D    H00D    N00E    C00F    C00G
              C00H    H00H    C00I    H00I    C00J    H00J    C00K    H00K
              C00L    H00L    O00M    H00M
PLAT721_ALERT_1_G Bond    Calc     0.93000, Rep     0.91970 Dev...        0.01 Ang.
              C15      -H15             1_555  12_676 ........     #   43 Check
PLAT721_ALERT_1_G Bond    Calc     0.93000, Rep     0.91970 Dev...        0.01 Ang.
              C15      -H15             1_555   6_467 ........     #   44 Check
PLAT721_ALERT_1_G Bond    Calc     0.93000, Rep     0.91970 Dev...        0.01 Ang.
              C15      -H15             1_555   1_555 ........     #   45 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       25.90 Deg.
              C15  -I1   -H15     1_555   1_555   6_467 ......     #   59 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       16.50 Deg.
              H15  -C15  -H15     6_467   1_555  12_676 ......     #   72 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       16.50 Deg.
              H15  -C15  -H15     1_555   1_555   6_467 ......     #   73 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       16.50 Deg.
              H15  -C15  -H15     1_555   1_555  12_676 ......     #   74 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                0  1  1,   0  0  2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
                0  3  3,
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.          4 Units
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          4 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  26 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  12 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  13 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_STRVA01_cu_tca_i6_0m
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
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;
_vrf_PLAT042_cu_tca_i6_0m
;
PROBLEM: Calc. and Reported MoietyFormula Strings Differ   Please Check
RESPONSE: ...
;
_vrf_PLAT057_cu_tca_i6_0m
;
PROBLEM: Correction for Absorption Required   RT(exp) ...   1.17 Do !
RESPONSE: ...
;
_vrf_PLAT202_cu_tca_i6_0m
;
PROBLEM: Isotropic non-H Atoms in Anion/Solvent ....   2 Check
RESPONSE: ...
;
_vrf_PLAT241_cu_tca_i6_0m
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of   C00K Check
RESPONSE: ...
;
_vrf_PLAT260_cu_tca_i6_0m
;
PROBLEM: Large Average Ueq of Residue Including   O00M   0.149 Check
RESPONSE: ...
;
_vrf_PLAT790_cu_tca_i6_0m
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd. #   1 Note
RESPONSE: ...
;
_vrf_PLAT927_cu_tca_i6_0m
;
PROBLEM: Reported and Calculated wR2 Differ by ....   0.0022 Check
RESPONSE: ...
;
_vrf_PLAT976_cu_tca_i6_0m
;
PROBLEM: Check Calcd Resid. Dens. 0.65Ang From O00M   .   -0.68 eA-3
RESPONSE: ...
;
_vrf_PLAT977_cu_tca_i6_0m
;
PROBLEM: Check Negative Difference Density on H00M   .   -0.32 eA-3
RESPONSE: ...
;
_vrf_PLAT987_cu_tca_i6_0m
;
PROBLEM: The Flack x is >> 0 - Do a BASF/TWIN Refinement   Please Check
RESPONSE: ...
;
end Validation Reply Form

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 14/11/2023; check.def file version of 14/09/2023

Datablock cu_tca_i6_0m - ellipsoid plot