checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_tca_nh4_1_0m_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: cu_tca_nh4_1_0m_a_sq

```
Bond precision:   C-C = 0.0098 A          Wavelength=1.54178

Cell:              a=20.9737(2)      b=20.9737(2)      c=20.9737(2)
                   alpha=90          beta=90           gamma=90
Temperature:       170 K

                 Calculated                  Reported
Volume           9226.3(3)                   9226.2(3)
Space group      I 2 3                       I 2 3
Hall group       I 2 2 3                     I 2 2 3
                 2(C21 H12 N O6), 2(C21 H15  2(C21 H12 N O6), 2(C21 H15
Moiety formula   N O6), 3(H O), 6(H4 N) [+   N O6), 6(H4 N), 1.5(H2 O2),
                 solvent]                    0.875[C3
Sum formula      C84 H81 N10 O27 [+ solvent] C86.62 H87.12 N10.88 O27.88
Mr               1662.59                     1726.63
Dx,g cm-3        1.197                       1.243
Z                4                           4
Mu (mm-1)        0.761                       0.789
F000             3484.0                      3624.0
F000'            3496.08
h,k,lmax                                     23,24,24
Nref                                         2724
Tmin,Tmax        0.759,0.815                 0.602,0.753
Tmin'            0.759

Correction method= # Reported T Limits: Tmin=0.602 Tmax=0.753
AbsCorr = NONE

Data completeness=                  Theta(max)= 66.444
```

R(reflections)= 0.0745(2004)

wR2(reflections)= 0.2270(2724)

S = 1.019 Npar= 184

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 C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.153
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .....      0.153 Report
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C00J Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.6 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O00M      0.207 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00979 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
              C21 H12 N O6
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595          2 Report
                2  0  4,   2  2  4,
```

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:C86.62 H87.12 N10.88 O27.88
           Atom count from the _atom_site data:  C84 H81 N10 O27
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  C86.62 H87.12 N10.88 O27.88
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        346.48    336.00   10.48
          H        348.48    324.00   24.48
          N         43.52     40.00    3.52
          O        111.52    108.00    3.52
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          6 Report
             H002  H00M  H00A  H00C  H00F  H00H
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C84 H81 N10 O27
             Rep.: C86.62 H87.12 N10.88 O27.88
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C21 H12 N O6), 2(C21 H15 N O6), 3(H O), 6(H4 N)
             Rep.: 2(C21 H12 N O6), 2(C21 H15 N O6), 6(H4 N), 1.5(H2 O2), 0.875
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.16 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H00M       Constrained at        0.5 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        712 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         36 Note
             O001    O002    H002    O003    O004    N005    N006    H00A
             H00C    H00F    H00H    C007    C008    C009    C00A    C00B
```

```
              H00B    C00C    C00D    H00D    C00E    H00E    N00F    C00G
              H00G    C00H    C00I    H00I    C00J    H00J    C00K    H00K
              C00L    H00L    O00M    H00M
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed         ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        44% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                0  1  1,   0  0  2,
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.20 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          3 Note
               -2  2  4,   2  0  4,   2  2  4,
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
   0 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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_RINTA01_cu_tca_nh4_1_0m_a_sq
;
PROBLEM: The value of Rint is greater than 0.12
RESPONSE: ...
;
_vrf_PLAT020_cu_tca_nh4_1_0m_a_sq
;
PROBLEM: The Value of Rint is Greater Than 0.12 .........      0.153 Report
RESPONSE: ...
;
_vrf_PLAT241_cu_tca_nh4_1_0m_a_sq
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of       C00J Check
RESPONSE: ...
;
_vrf_PLAT250_cu_tca_nh4_1_0m_a_sq
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.2 Note
RESPONSE: ...
;
_vrf_PLAT260_cu_tca_nh4_1_0m_a_sq
;
PROBLEM: Large Average Ueq of Residue Including      O00M      0.207 Check
RESPONSE: ...
;
_vrf_PLAT340_cu_tca_nh4_1_0m_a_sq
;
```

```
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.00979 Ang.
RESPONSE: ...
;
_vrf_PLAT790_cu_tca_nh4_1_0m_a_sq
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
RESPONSE: ...
;
_vrf_PLAT911_cu_tca_nh4_1_0m_a_sq
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.595          2 Report
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_nh4_1_0m_a_sq - ellipsoid plot