checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_230103_zhj_nh2_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: mo_230103_zhj_nh2_0m

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Bond precision:   C-C = 0.0087 A          Wavelength=0.71073

Cell:               a=28.216(9)      b=13.252(2)      c=14.528(3)
                    alpha=90         beta=90          gamma=90
Temperature:        170 K

                 Calculated                Reported
Volume           5432(2)                   5432(2)
Space group      P 21 21 2                 P 21 21 2
Hall group       P 2 2ab                   P 2 2ab
Moiety formula   C56 H60 I N4 O8 Si2       C56 H60 I N4 O8 Si2
Sum formula      C56 H60 I N4 O8 Si2       C56 H61 I N4 O8 Si2
Mr               1100.16                   1101.16
Dx,g cm-3        1.345                     1.346
Z                4                         4
Mu (mm-1)        0.690                     0.690
F000             2276.0                    2280.0
F000'            2275.63
h,k,lmax         39,18,20                  38,18,20
Nref             16096[ 8799]              15884
Tmin,Tmax        0.767,0.813               0.663,0.746
Tmin'            0.718

Correction method= # Reported T Limits: Tmin=0.663 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.81/0.99        Theta(max)= 30.159

R(reflections)= 0.0439( 11790)                wR2(reflections)=
                                              0.1185( 15884)
S = 1.035                 Npar= 811
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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 C

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C17      --C18      .      0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C18 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C24 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C47 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C10 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C14 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C35 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00868 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X       H1B      ..H36C     .      2.05 Ang.
                                                 x,y,1+z  =     1_556 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N1       --H1A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N1       --H1B      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N3       --H3A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N3       --H3B      .     Please Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..         1 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.08Ang From C7      .      0.52 eA-3
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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:   C56 H61 I1 N4 O8 Si2
           Atom count from _chemical_formula_moiety:C56 H60 I1 N4 O8 Si2
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:C56 H61 I1 N4 O8 Si2
           Atom count from the _atom_site data:  C56 H60 I1 N4 O8 Si2
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    4
          From the CIF: _chemical_formula_sum  C56 H61 I N4 O8 Si2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        224.00    224.00    0.00
          H        244.00    240.00    4.00
          I          4.00      4.00    0.00
          N         16.00     16.00    0.00
          O         32.00     32.00    0.00
          Si         8.00      8.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         40 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         39 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         44 Report
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PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        25% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C7       - C8       .       1.55 Ang.
PLAT410_ALERT_2_G Short Intra H...H Contact  H28      ..H48      .       2.08 Ang.
                                                      x,y,z  =     1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H34B     ..H40A     .       2.03 Ang.
                                                      x,y,z  =     1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H44A     ..H46      .       1.93 Ang.
                                                      x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H37C     ..H44      .       2.12 Ang.
                                                      x,y,z  =     1_555 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         26 Check
PLAT791_ALERT_4_G Model has Chirality at C8          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C32         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C33         (Sohnke SpGr)          S Verify
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        585 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         20 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
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
0 **ALERT level B** = A potentially serious problem, consider carefully
19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
53 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 24 ALERT type 2 Indicator that the structure model may be wrong or deficient
 32 ALERT type 3 Indicator that the structure quality may be low
  9 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
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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 28/11/2022; check.def file version of 28/11/2022

Datablock mo_230103_zhj_nh2_0m - ellipsoid plot