checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo221124a

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: mo221124a

```
Bond precision:   C-C = 0.0061 A          Wavelength=0.71073

Cell:           a=11.359(3)        b=13.185(3)       c=16.123(4)
                alpha=76.717(5)    beta=75.085(5)    gamma=69.919(5)
Temperature:    296 K
```

	Calculated	Reported
Volume	2164.8(9)	2164.8(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H42 Cl2 Ni O2 P2 Si, C H2 Cl2	C42 H42 Cl2 Ni O2 P2 Si, C H2 Cl2
Sum formula	C43 H44 Cl4 Ni O2 P2 Si	C43 H44 Cl4 Ni O2 P2 Si
Mr	883.30	883.32
Dx,g cm-3	1.355	1.355
Z	2	2
Mu (mm-1)	0.831	0.831
F000	916.0	916.0
F000'	918.67	
h,k,lmax	16,18,23	16,18,22
Nref	13194	11764
Tmin,Tmax	0.905,0.936	0.906,1.000
Tmin'	0.905	

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Correction method= # Reported T Limits: Tmin=0.906 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.892            Theta(max)= 30.478

R(reflections)= 0.0527( 4896)                    wR2(reflections)=
                                                 0.1216( 11764)
S = 0.838                  Npar= 478
```

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

```
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..        42% Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C19 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C25 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C39 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Si1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C17 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C29 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl3      0.173 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00611 Ang.
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          5 Note
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.005 Degree
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         2% Note
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O1       .      145.6 Degree
PLAT410_ALERT_2_G Short Intra H...H Contact  H38      ..H35      .       1.73 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H42      ..H43      .       1.93 Ang.
                                                    x,y,z  =      1_555 Check
PLAT793_ALERT_4_G Model has Chirality at C1          (Centro SPGR)          S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       1429 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 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
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  12 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 28/11/2022; check.def file version of 28/11/2022

Datablock mo221124a - ellipsoid plot