checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Negevite

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: Negevite

```
Bond precision:  P- P = 0.0011 A         Wavelength=0.71073

Cell:              a=5.4816(5)      b=5.4816(5)      c=5.4816(5)
                   alpha=90         beta=90          gamma=90
Temperature:       293 K

                Calculated                Reported
Volume          164.71(5)                 164.71(5)
Space group     P a -3                    P a -3
Hall group      -P 2ac 2ab                ?
Moiety formula  Ni P2                     ?
Sum formula     Ni P2                     Ni P2
Mr              120.63                    120.65
Dx,g cm-3       4.865                     4.865
Z               4                         4
Mu (mm-1)       13.090                    13.090
F000            232.0                     232.0
F000'           234.18
h,k,lmax        7,7,7                     7,7,7
Nref            62                        62
Tmin,Tmax       0.877,0.877               0.629,0.746
Tmin'           0.877

Correction method= # Reported T Limits: Tmin=0.629 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 26.988

R(reflections)= 0.0173( 52)       wR2(reflections)= 0.0366( 62)

S = 1.115                  Npar= 6
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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 G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  P1       ..P1               3.36 Ang.
                                            1-x,1/2+y,1/2-z  =      3_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  P1       ..P1               3.36 Ang.
                                            1/2-x,1-y,1/2+z  =      2_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  P1       ..P1               3.36 Ang.
                                            1/2+x,1/2-y,1-z  =      4_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  P1       ..P1               3.36 Ang.
                                           1-x,-1/2+y,1/2-z  =      3_645 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  P1       ..P1               3.36 Ang.
                                           -1/2+x,1/2-y,1-z  =      4_456 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  P1       ..P1               3.36 Ang.
                                           1/2-x,1-y,-1/2+z  =      2_564 Check
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
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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
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   0 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 07/08/2019; check.def file version of 30/07/2019

Datablock Negevite - ellipsoid plot