checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:    P- O = 0.0014 A           Wavelength=0.71073

Cell:           a=6.3677(2)        b=9.3316(4)        c=10.8478(4)
                alpha=65.191(1)    beta=80.533(1)     gamma=73.042(1)
Temperature:    293 K

                Calculated                   Reported
Volume          559.00(4)                    559.00(4)
Space group     P -1                         P -1
Hall group      -P 1                         -P 1
Moiety formula  Fe Ni3 O28 P8, 7(Na)         Fe Na7 Ni3 O28 P8
Sum formula     Fe Na7 Ni3 O28 P8            Fe Na7 Ni3 O28 P8
Mr              1088.61                      1088.67
Dx,g cm-3       3.234                        3.234
Z               1                            1
Mu (mm-1)       3.972                        3.972
F000            531.0                        531.0
F000'           533.64
h,k,lmax        10,15,17                     10,15,17
Nref            5150                         5143
Tmin,Tmax       0.494,0.573                  0.626,0.748
Tmin'           0.301

Correction method= # Reported T Limits: Tmin=0.626 Tmax=0.748
AbsCorr = MULTI-SCAN

Data completeness= 0.999              Theta(max)= 35.630


R(reflections)= 0.0261( 4998)                      wR2(reflections)=
                                                   0.0663( 5143)
S = 1.089                   Npar= 215
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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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DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
              The relevant atom site should be identified.
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ      Please Check
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density      2.38 eA-3
PLAT214_ALERT_2_C Atom Na2        (Anion/Solvent) ADP max/min Ratio      4.1 prolat
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         5 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.71Ang From Na1           2.15 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.68Ang From Na1          -1.57 eA-3
PLAT974_ALERT_2_C Check Calcd Negative Resid. Density on        Ni2    -1.25 eA-3
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⚪ Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        3 Info
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.001 Degree
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records        1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records        1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)      293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ni1        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1        Constrained at      0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        5% Note
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O3        .    133.0 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Ni2       (II)       .     2.02 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL   2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        1 Note
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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
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   6 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 10/05/2023; check.def file version of 10/05/2023