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:   Si- O = 0.0058 A         Wavelength=0.71073

Cell:              a=5.2271(5)     b=5.4198(4)          c=7.0466(6)
                   alpha=90        beta=90.011(7)       gamma=90
Temperature:       170 K

                 Calculated                 Reported
Volume           199.63(3)                  199.63(3)
Space group      P n                        P n
Hall group       P -2yac                    P -2yac
Moiety formula   Co O4 Si, 2(Na)            Co O4 Si, 2(Na)
Sum formula      Co Na2 O4 Si               Co Na2 O4 Si
Mr               197.00                     197.00
Dx,g cm-3        3.277                      3.277
Z                2                          2
Mu (mm-1)        4.691                      4.691
F000             190.0                      190.0
F000'            191.04
h,k,lmax                                    7,7,9
Nref                                        909
Tmin,Tmax        0.721,0.910                0.838,1.181
Tmin'            0.490

Correction method= # Reported T Limits: Tmin=0.838 Tmax=1.181
AbsCorr = MULTI-SCAN

Data completeness=                  Theta(max)= 29.956

R(reflections)= 0.0247( 894)                    wR2(reflections)=
                                                0.0636( 909)
S = 1.028                  Npar= 74
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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

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.77 Note
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report
-6 0 2, -4 0 2, -5 0 3, -3 0 3, -5 1 3, -4 0 4,

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (II) . 1.99 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! 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 7 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.25 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law (0 0 1) Est.d BASF 0.32 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.0 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 60.0 Degree

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
4 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 14/11/2023; check.def file version of 14/09/2023

Datablock shelx - ellipsoid plot