checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Nickolayite_Holotype, Nickolayite_low_Mo

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: Nickolayite_Holotype

Bond precision: Fe- P = 0.0009 A Wavelength=0.71073

Cell: a=5.9519(5) b=3.7070(3) c=6.8465(6)
alpha=90 beta=90 gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	151.06(2)	151.06(2)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	Fe4 Mo3.52 Ni0.48 P4	?
Sum formula	Fe4 Mo3.52 Ni0.48 P4	Fe Mo0.88 Ni0.12 P
Mr	713.16	178.29
Dx,g cm-3	7.839	7.840
Z	1	4
Mu (mm-1)	18.770	18.770
F000	325.3	325.0
F000'	321.18	
h,k,lmax	8,5,9	8,5,9
Nref	251	251
Tmin,Tmax	0.337,0.472	0.574,1.000
Tmin'	0.312	

Correction method= # Reported T Limits: Tmin=0.574 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 29.875

R(reflections)= 0.0174(251) wR2(reflections)= 0.0435(251)

S = 1.136 Npar= 20

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

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.2500 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
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
PLAT300_ALERT_4_G Atom Site Occupancy of Mo1 Constrained at 0.88 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ni1 Constrained at 0.12 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 49% Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check
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
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

2 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
2 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

Datablock: Nickolayite_low_Mo

Bond precision: Fe- P = 0.0012 A Wavelength=0.71073

Cell:	a=5.8544(6)	b=3.6241(4)	c=6.7182(7)
	alpha=90	beta=90	gamma=90
Temperature:	296 K		

	Calculated	Reported
Volume	142.54(3)	142.54(3)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	Fe5.80 Mo1.80 Ni0.40 P4	?
Sum formula	Fe5.80 Mo1.80 Ni0.40 P4	Fe1.45 Mo0.45 Ni0.10 P
Mr	643.98	161.00
Dx,g cm-3	7.502	7.502
Z	1	4
Mu (mm-1)	20.422	20.422
F000	297.6	298.0
F000'	297.06	
h,k,lmax	8,5,9	8,4,9
Nref	238	235
Tmin,Tmax	0.375,0.542	0.049,1.000
Tmin'	0.346	

Correction method= # Reported T Limits: Tmin=0.049 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 29.917

R(reflections)= 0.0224(205) wR2(reflections)= 0.0415(235)

S = 1.144 Npar= 19

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

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.059 Check

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Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.2500 Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
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
PLAT300_ALERT_4_G	Atom Site Occupancy of Mo1 Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ni1 Constrained at	0.1 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fe1 Constrained at	0.45 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	49% Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note

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PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.1 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       60.0 Degree
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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

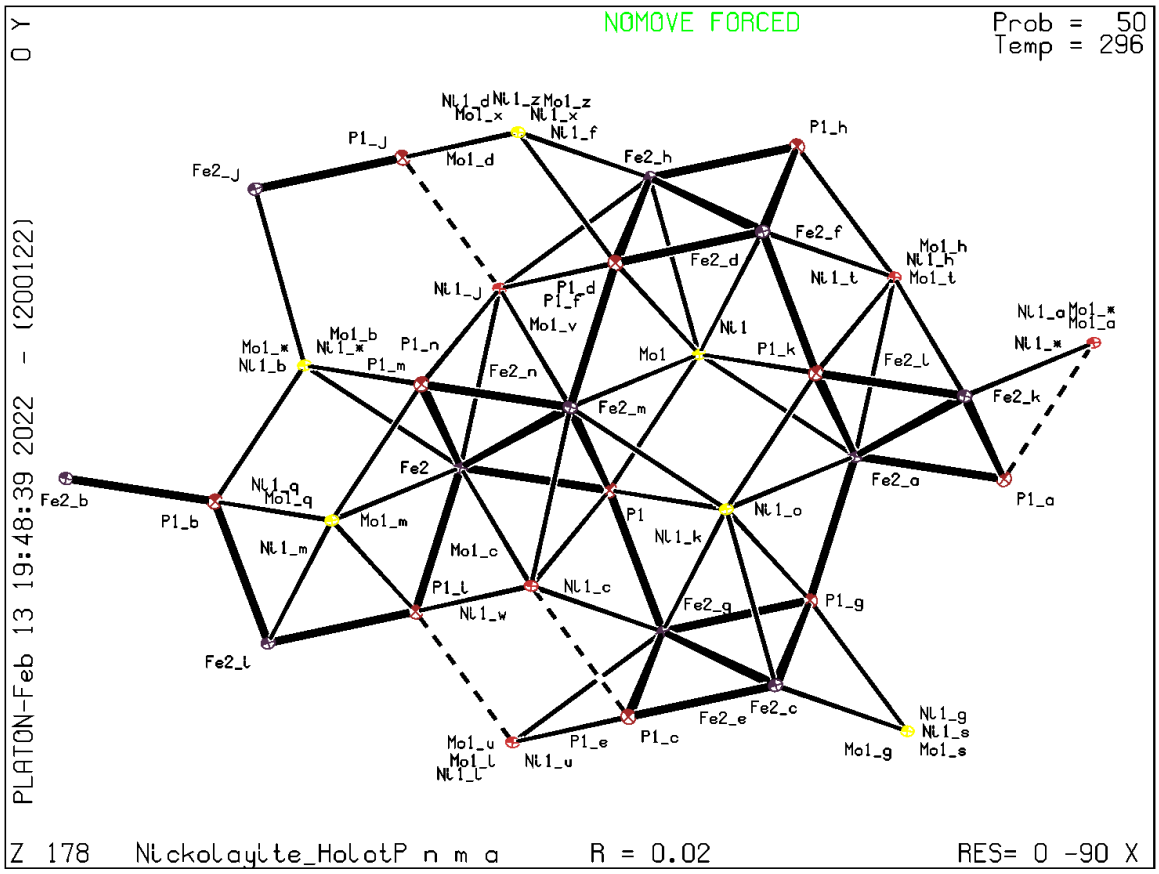
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 20/01/2022; check.def file version of 19/01/2022

Datablock Nickolayite_Holotype - ellipsoid plot



Datablock Nickolayite_low_Mo - ellipsoid plot