

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) DiammineNickelNitrate

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: DiammineNickelNitrate

Bond precision: O- N = 0.0525 A Wavelength=1.54056

Cell: a=11.0628(5) b=6.0454(3) c=9.3526(4)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	625.49(5)	625.49(5)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	H6 N4 Ni O6	H6 N4 Ni O6
Sum formula	H6 N4 Ni O6	H6 N4 Ni1 O6
Mr	216.78	216.80
Dx,g cm-3	2.302	2.302
Z	4	4
Mu (mm-1)	4.504	4.578
F000	440.0	440.0
F000'	429.54	
h,k,lmax	11,6,9	
Nref	756[409]	
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.00/0.00 Theta(max)=

R(reflections)= 0.0333(0) wR2(reflections)= wR= 0.0443(0)

S = 2.510 Npar= 68

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

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies
outside the range 0.99 <> 1.01

Calculated value of mu = 4.656

Value of mu given = 4.578

Author Response: Mu as calculated by Jana2006. No absorption correction applied.



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6	Report
PLAT092_ALERT_4_G	Check: Wavelength given is not Cu,Ga,Mo,Ag,In Ka	1.54056	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6	Note
PLAT982_ALERT_1_G	The N-f' = 0.033 Deviates from the IT-value	0.031	Check
PLAT982_ALERT_1_G	The Ni-f' = -3.119 Deviates from the IT-value	-3.001	Check
PLAT982_ALERT_1_G	The O-f' = 0.052 Deviates from the IT-value	0.050	Check

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
7 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 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 24/11/2016; check.def file version of 23/11/2016

