

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB1

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: MAB1

Bond precision:	O- B = 0.0017 A	Wavelength=0.71075	
Cell:	a=8.2773(1)	b=20.5277(3)	c=8.0133(1)
	alpha=90	beta=91.283(1)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	1361.23(3)	1361.23(3)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	B4 H4 O9, H16 N4 Ni O2, H2 O	B4 H4 O9, H16 N4 Ni O2, H2 O	
Sum formula	B4 H22 N4 Ni O12	B4 H22 N4 Ni O12	
Mr	372.15	372.16	
Dx,g cm-3	1.816	1.816	
Z	4	4	
Mu (mm-1)	1.492	1.492	
F000	776.0	776.0	
F000'	777.81		
h,k,lmax	10,26,10	10,26,10	
Nref	3132	3128	
Tmin,Tmax	0.807,0.914	0.873,1.000	
Tmin'	0.788		

Correction method= # Reported T Limits: Tmin=0.873 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.481

R(reflections)= 0.0216(3021) wR2(reflections)= 0.0528(3128)

S = 1.027 Npar= 278

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

PLAT420_ALERT_2_C	D-H Bond Without Acceptor N12	--H12E	.	Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		2 Report



Alert level G

PLAT794_ALERT_5_G	Tentative Bond Valency for Nil	(II)	.	1.92	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.9	Low

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

0 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
1 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 13/07/2021; check.def file version of 13/07/2021

Datablock MAB1 - ellipsoid plot

