

Datablock: VESTA_phase_1

Bond precision:		= 0.0000 Å	Wavelength=0.71073
Cell:	a=11.18878	b=11.18878	c=29.48594
	alpha=90	beta=90	gamma=90
Temperature	5 K		
:			
	Calculated	Reported	
Volume	3691.310	3691	
Space group	P 1	P 1	
Hall group	P 1	P 1	
Moiety formula	B16 Mn15 Ni	?	
Sum formula	B16 Mn15 Ni	Mn15B16Ni	
Mr	1055.75	1055.70	
Dx,g cm-3	0.475	0.000	
Z	1	1	
Mu (mm-1)	1.354	0.000	
F000	483.0	0.0	
F000'	488.41		
h,k,lmax			
Nref			
Tmin,Tmax			
Tmin'			
Correction method=	Not given		
Data completeness=	Theta (max)=		
R(reflections)=	wR2 (reflections)=		
S =	Npar=		

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 A

[PLAT602_ALERT_2_A](#) Solvent Accessible VOID(S) in Structure ! Check



Alert level B

[SYMMS02_ALERT_1_B](#) The unit-cell lengths a and c should be equal for a cubic cell

Cell	11.1888	11.1888	29.4859
Angles	90.0000	90.0000	90.0000

[PLAT049_ALERT_1_B](#) Calculated Density Less Than 1.0 gcm-3 0.4749 Check

[PLAT111_ALERT_2_B](#) ADDSYM Detects New (Pseudo) Centre of Symmetry . 100 %Fit

[PLAT112_ALERT_2_B](#) ADDSYM Detects New (Pseudo) Symm. Elem 4 100 %Fit

And 4 other PLAT112 Alerts

[PLAT112_ALERT_2_B](#) ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

[PLAT112_ALERT_2_B](#) ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

[PLAT112_ALERT_2_B](#) ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

[PLAT112_ALERT_2_B](#) ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

[PLAT113_ALERT_2_B](#) ADDSYM Suggests Possible Pseudo/New Space Group P4/mmm Check
Check Model Parameter Symmetry for Reflection Data Support



Alert level C

[CELLK01_ALERT_1_C](#) Check that the cell measurement temperature is in Kelvin.
Value of measurement temperature given = 5.000

[PLAT029_ALERT_3_C](#) _diffn_measured_fraction_theta_full value Low . 0.970 Why?

[PLAT034_ALERT_1_C](#) No Flack Parameter Given. Z > Si, NonCentro Please Do !

[PLAT041_ALERT_1_C](#) Calc. and Reported SumFormula Strings Differ Please Check

PLAT141_ALERT_4_C	s.u. on a - Axis Small or Missing	0.00000 Ang.
PLAT142_ALERT_4_C	s.u. on b - Axis Small or Missing	0.00000 Ang.
PLAT143_ALERT_4_C	s.u. on c - Axis Small or Missing	0.00000 Ang.
PLAT144_ALERT_4_C	s.u. on alpha Small or Missing	0.0000 Degree
PLAT145_ALERT_4_C	s.u. on beta Small or Missing	0.0000 Degree
PLAT146_ALERT_4_C	s.u. on gamma Small or Missing	0.0000 Degree
PLAT151_ALERT_1_C	No s.u. (esd) Given on Volume	Please Do !
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	4.0 Note



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT104_ALERT_1_G	The Reported Crystal System is Inconsistent with	P1 Check
PLAT110_ALERT_2_G	ADDSYM Detects Potential Lattice Translation ...	? Check
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem C	100 %Fit

And 14 other PLAT112 Alerts

PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	sub	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	b/2	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	361	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	a/2	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	311	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	631	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	131	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	331	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	121	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	221	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	521	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	151	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	251	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	551	100 %Fit

PLAT721_ALERT_1_G	Bond Calc	9.88409, Rep	2.00000 Dev...	7.88 Ang.
	MN1 -B1	1_555 1_555	#	2 Check

And 3 other PLAT721 Alerts

PLAT721_ALERT_1_G	Bond Calc	10.64960, Rep	2.00000 Dev...	8.65 Ang.
	MN1 -B2	1_555 1_555	#	3 Check
PLAT721_ALERT_1_G	Bond Calc	1.96152, Rep	2.00000 Dev...	0.04 Ang.
	B6 -NI1	1_555 1_555	#	5 Check
PLAT721_ALERT_1_G	Bond Calc	2.77582, Rep	2.80000 Dev...	0.02 Ang.
	MN7 -NI1	1_555 1_555	#	6 Check

PLAT722_ALERT_1_G	Angle Calc	15.07, Rep	26.50 Dev...	11.43 Degree
	B1 -MN1 -B2	1_555 1_555 1_555	#	1 Check
PLAT722_ALERT_1_G	Angle Calc	16.30, Rep	89.80 Dev...	73.50 Degree
	MN1 -B1 -MN2	1_555 1_555 1_555	#	2 Check
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found			Please Check
PLAT881_ALERT_1_G	No Datum for _diffrn_reflms_av_R_equivalents ...			Please Do !
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI			Please Do !
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT980_ALERT_1_G	No Anomalous Scattering Factors Found in CIF ...			Please Check

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

- 17 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
25 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
3 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

