

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dravite, mg-lucc

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: mg-lucc

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Bond precision:      O- B = 0.0070 Å      Wavelength=1.54184

Cell:                      a=15.9863(3)              b=15.9863(3)              c=7.22426(15)  
                                alpha=90              beta=90              gamma=120

Temperature:              293 K

	Calculated	Reported
Volume	1598.90(7)	1598.89(6)
Space group	R 3 m	R 3 m
Hall group	R 3 -2"	R 3 -2"
Moiety formula	Al18 B9 Fe4.46 H9 Mg4.55 O90 Si18, 2.37(O), 0.63(F), 1.68(Ca),	Al6 B3 Ca0.561 F0.212 Fe1.484 H3 Mg1.516 Na0.439 O30.788 Si6
Sum formula	Al18 B9 Ca1.68 F0.63 Fe4.46 H9 Mg4.55 Na1.32 O92.37 Si18	Al6 H3 B3 Ca0.56 F0.21 Fe1.48 Mg1.52 Na0.44 O30.79 Si6
Mr	3044.49	1014.79
Dx, g cm <sup>-3</sup>	3.162	3.162
Z	1	3
Mu (mm <sup>-1</sup> )	17.183	17.175
F000	1503.1	1503.0
F000'	1512.69	
h, k, lmax	20, 20, 9	20, 20, 9
Nref	846[ 428]	786
Tmin, Tmax	0.445, 0.685	0.391, 1.000
Tmin'	0.404	

Correction method= # Reported T Limits: Tmin=0.391 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.84/0.93

Theta(max)= 77.616

R(reflections)= 0.0187( 779)

wR2(reflections)=  
0.0502( 786)

S = 1.069

Npar= 94

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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 B

PLAT090\_ALERT\_3\_B Poor Data / Parameter Ratio (Zmax > 18) ..... 4.53 Note

**Author Response: The crystal is very small of 0.05 mm thickness. The experiment already took 64 h on an in-house diffractometer.**

PLAT430\_ALERT\_2\_B Short Inter D...A Contact O1W ..O2 . 2.76 Ang.  
1-y,1+x-y,z = 2\_665 Check

**Author Response: There is no visible H position from the residual density map to form O1w\_H...O2 hydrogen bond.**

PLAT430\_ALERT\_2\_B Short Inter D...A Contact O1W ..O2 . 2.76 Ang.  
-x+y,1-x,z = 3\_565 Check

**Author Response: There is no visible H position from the residual density map to form O1w\_H...O2 hydrogen bond.**

PLAT430\_ALERT\_2\_B Short Inter D...A Contact O1W ..O2 . 2.76 Ang.  
x,y,z = 1\_555 Check

**Author Response: There is no visible H position from the residual density map to form O1w\_H...O2 hydrogen bond.**



#### Alert level C

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT077\_ALERT\_4\_C Unitcell Contains Non-integer Number of Atoms .. Please Check  
PLAT752\_ALERT\_4\_C Angle Calc 120.04, Rep 120.1(2) ..... Senseless s.u.  
O8 -B -O2 1\_555 1\_555 1\_555 # 121 Check



#### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 2 Note  
PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 1 Info  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.333 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	3	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffraction_ambient_temperature ..... (K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	10%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5 )	100%	Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	01W	Check
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O5 .	132.1	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	6	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	2	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please Check

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 6 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  
 11 ALERT type 4 Improvement, methodology, query or suggestion  
 2 ALERT type 5 Informative message, check

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## Datablock: dravite

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Bond precision:    O- B = 0.0050 A                      Wavelength=1.54184

Cell:                      a=15.97377(14)              b=15.97377(14)              c=7.22644(7)  
                               alpha=90                      beta=90                      gamma=120

Temperature:            292 K

	Calculated	Reported
Volume	1596.87(3)	1596.87(3)
Space group	R 3 m	R 3 m
Hall group	R 3 -2"	R 3 -2"
Moiety formula	Al18 B9 Fe3.87 H9 Mg5.13 O93 Si18, 3(Ca0.05), 2.85(Na)	Al6 B3 Ca0.046 Fe1.289 H3 Mg1.711 Na0.954 O31 Si6
Sum formula	Al18 B9 Ca0.15 Fe3.87 H9 Mg5.13 Na2.85 O93 Si18	Al6 H3 B3 Ca0.05 Fe1.29 Mg1.71 Na0.95 O31 Si6
Mr	2998.01	999.28
Dx, g cm <sup>-3</sup>	3.118	3.117
Z	1	3
Mu (mm <sup>-1</sup> )	15.257	15.251
F000	1480.5	1480.0
F000'	1490.43	
h,k,lmax	20,20,9	20,20,9
Nref	846[ 428]	845
Tmin,Tmax	0.652,0.846	0.443,1.000
Tmin'	0.412	

Correction method= # Reported T Limits: Tmin=0.443 Tmax=1.000  
AbsCorr = MULTISCAN

Data completeness= 1.97/1.00      Theta(max)= 77.763

R(reflections)= 0.0154( 842)      wR2(reflections)=  
0.0397( 845)  
S = 1.125      Npar= 93

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 B

PLAT090\_ALERT\_3\_B Poor Data / Parameter Ratio (Zmax > 18) ..... 4.60 Note

**Author Response: The data collection strategy was set to correspond to the  
magnesio\_lucchesiite experiment.**



#### Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula	Strings Differ	Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..		Please Check

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.333	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing .....	0.00007	Ang.
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	2	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	10%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100%	Note
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PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O5 .	132.5	Degree
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PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	2	Note

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1 ALERT type 5 Informative message, check
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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.



