

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deynekoite_na

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: deynekoite_na

Bond precision:	P- O = 0.0057 A	Wavelength=0.56087	
Cell:	a=10.3516(3)	b=10.3516(3)	c=37.1599(17)
	alpha=90	beta=90	gamma=120
Temperature:	296 K		
	Calculated	Reported	
Volume	3448.4(3)	3448.4(3)	
Space group	R 3 c	R 3 c	
Hall group	R 3 -2"c	R 3 -2"c	
Moiety formula	Fe0.58 Mg0.42 O24 P6, H0.27 Ca9 Fe0.576 H0.266 Mg0.424 O4 P, 9(Ca), 0.1(Na)	Na0.095 O28 P7	
Sum formula	Ca9 Fe0.58 H0.27 Mg0.42 Na0.10 O28 P7	Ca9 H0.27 Fe0.57 Mg0.42 Na0.09 O28 P7	
Mr	1070.56	1070.41	
Dx, g cm-3	3.093	3.093	
Z	6	6	
Mu (mm-1)	1.548	1.530	
F000	3182.6	3182.0	
F000'	3195.95		
h, k, lmax	14, 14, 52	14, 14, 49	
Nref	2255[1131]	1915	
Tmin, Tmax	0.955, 0.970	0.989, 1.000	
Tmin'	0.955		

Correction method= # Reported T Limits: Tmin=0.989 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.69/0.85

Theta(max)= 23.265

R(reflections)= 0.0407(1682)

wR2(reflections)=
0.0675(1915)

S = 1.044

Npar= 149

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

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree
PLAT430_ALERT_2_B Short Inter D...A Contact 01 ..010A . 2.59 Ang.
x,-1+y,z = 1_545 Check
PLAT430_ALERT_2_B Short Inter D...A Contact 02 ..07 . 2.76 Ang.
2/3-x+y,-2/3+y,-1/6+z = 11_544 Check

● 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 = 1.546
Value of mu given = 1.530
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.560
From the CIF: _refine_ls_abs_structure_Flack_su 0.090
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
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 6.79 Note
PLAT213_ALERT_2_C Atom O4 has ADP max/min Ratio 3.5 oblate
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) 09 Check
PLAT430_ALERT_2_C Short Inter D...A Contact 02 ..03 . 2.86 Ang.
1-x+y,-x,z = 3_655 Check
PLAT430_ALERT_2_C Short Inter D...A Contact 06 ..07 . 2.86 Ang.
2-y,1+x-y,z = 2_765 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.672 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 0.56 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.01Ang From O2 . 0.49 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From O3 . 0.48 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.69Ang From O6 . 0.46 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.70Ang From O6 . 0.46 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.84Ang From O9 . 0.43 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.05Ang From O4 . 0.42 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.63Ang From O5 . 0.41 eA-3

● Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:H0.27 Ca9 Fe0.57 Mg0.42 Na.09 O2
Atom count from the _atom_site data: H0.267 Ca9 Fe0.576 Mg0.424 Na.1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 6

From the CIF: _chemical_formula_sum Ca9 H0.27 Fe0.57 Mg0.42 Na0.09 O28
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Ca	54.00	54.00	0.00
H	1.62	1.60	0.02
Fe	3.42	3.46	-0.04
Mg	2.52	2.54	-0.02
Na	0.54	0.60	-0.06
O	168.00	168.00	-0.00
P	42.00	42.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
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
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	2	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	9%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	67%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	5.27	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 6)	0.03	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # Ca	3	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # Ca	4	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4	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	109	Note
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	3	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	3	Units
PLAT982_ALERT_1_G	The Ca-f' = 0.1624 Deviates from IT-value =	0.1611	Check
PLAT982_ALERT_1_G	The Fe-f' = 0.2928 Deviates from IT-value =	0.2886	Check
PLAT982_ALERT_1_G	The Mg-f' = 0.0310 Deviates from IT-value =	0.0298	Check
PLAT983_ALERT_1_G	The Ca-f" = 0.1939 Deviates from IT-Value =	0.1926	Check
PLAT983_ALERT_1_G	The Fe-f" = 0.5488 Deviates from IT-Value =	0.5448	Check

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

14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 16 ALERT type 2 Indicator that the structure model may be wrong or deficient
 5 ALERT type 3 Indicator that the structure quality may be low
 13 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.

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