

**checkCIF/PLATON report**

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: ECKERMANNITE\_108401**

Bond precision:	= 0.0000 A	Wavelength=0.71070
Cell:	a=9.8087(7)      b=17.8448(13)      c=5.2905(4)	
	alpha=90      beta=103.660(1)      gamma=90	
Temperature:	293 K	
	Calculated	Reported
Volume	899.83(11)	899.83(11)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
	2(00.38 Si0.76),	
Moiety formula	0.034(Na4), 0.055(Na4), ?	
	2.48(Si), 11(O), 0.24(	
	Al0.33 Ca0.10 F0.24 Fe0.28 Al0.66 Ca0.20 F0.48 Fe0.55	
Sum formula	H0.87 Mg1.90 Na1.42 O11.76 H1.74 Mg3.79 Na2.84 O23.52	
	Si4	Si8
Mr	412.89	825.78
Dx,g cm-3	3.048	3.048
Z	4	2
Mu (mm-1)	1.456	1.456
F000	819.5	819.5
F000'	822.27	
h,k,lmax	13,25,7	13,25,7
Nref	1377	1377
Tmin,Tmax	0.900,0.943	0.830,0.962
Tmin'	0.840	

Correction method= MULTI-SCAN

Data completeness= 1.000      Theta(max)= 30.150

R(reflections)= 0.0290( 1085)      wR2(reflections)= wR= 0.0342( 1085)

S = \*\*\*\*\*      Npar= 128

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

CHEMW03\_ALERT\_2\_A ALERT: The ratio of given/expected molecular weight as calculated from the `_atom_site*` data lies outside the range 0.90 <> 1.10

From the CIF: `_cell_formula_units_Z` 2

From the CIF: `_chemical_formula_weight` 825.78

TEST: Calculate formula weight from `_atom_site_*`

atom	mass	num	sum
O	16.00	6.58	105.27
O2-	0.00	15.42	0.00
O-	0.00	1.52	0.00
F-	0.00	0.48	0.00
Si	28.09	6.20	174.13
Al3+	26.98	0.66	17.70
Si4+	28.09	1.80	50.55
Mg2+	24.31	3.79	92.21
Fe2+	55.85	0.19	10.61
Fe3+	55.85	0.36	20.10
Ca2+	40.08	0.20	8.02
Na+	22.99	2.84	65.20
H	1.01	1.74	1.75

Calculated formula weight 545.56

WEIGH01\_ALERT\_1\_A Unit weights are not acceptable for submissions to Acta

Crystallographica Section C.

n.b. unit is however a legal CIF keyword.

### Alert level B

PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	07B	..	2.67 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	06B	..	2.68 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	05B	..	2.69 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	01B	..	2.74 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	02B	..	2.75 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	03A	..	2.77 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	03A	..	03A	..	2.69 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	02B	..	06B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	02B	..	05B	..	2.67 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	02B	..	04B	..	2.75 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	02B	..	04B	..	2.82 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	04B	..	06B	..	2.61 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	04B	..	05B	..	2.67 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	05B	..	07B	..	2.56 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	05B	..	06B	..	2.63 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	05B	..	06B	..	2.68 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	06B	..	07B	..	2.62 Ang.

### Alert level C

REFNR01\_ALERT\_3\_C Ratio of reflections to parameters is < 10 for a centrosymmetric structure

sine(theta)/lambda 0.7067

Proportion of unique data used 0.7879

Ratio reflections to parameters 8.4766

PLAT077\_ALERT\_4\_C Unitcell contains non-integer number of atoms .. Please Check

PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 2.96 Report

PLAT213\_ALERT\_2\_C Atom A has ADP max/min Ratio ..... 4.0 oblate  
 PLAT430\_ALERT\_2\_C Short Inter D...A Contact O1B .. O4B .. 2.89 Ang.

### Alert level G

PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF Please Do !  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type O2- for O1B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type O- for O3A  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type F- for O3B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type O2- for O4B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type O2- for O5B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type O2- for O6B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type O2- for O7B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type SI for T1A  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type SI4+ for T1B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type SI for T2A  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type SI4+ for T2B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type MG2+ for M1A  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type FE2+ for M1B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type MG2+ for M2A  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type AL3+ for M2B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type FE3+ for M2C  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type MG2+ for M3A  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type FE2+ for M3B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type CA2+ for M4A  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type NA+ for M4B  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type NA+ for A  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type NA+ for AM  
 PLAT017\_ALERT\_1\_G Check Consistency of Scattering Type NA+ for A2  
 PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by ..... 2.00 Ratio  
 PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check  
 PLAT200\_ALERT\_1\_G Reported \_diffn\_ambient\_temperature ..... (K) 293 Check  
 PLAT301\_ALERT\_3\_G Main Residue Disorder ..... Percentage = 100 Note  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O1B Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O3A Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O2B Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O4B Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O5B Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O6B Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O7B Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O1A Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O2A Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O4A Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O6A Check  
 PLAT311\_ALERT\_2\_G Isolated Disordered Oxygen Atom (No H's ?) ..... O7A Check  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1A .. O1B .. 1.60 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1A .. O5B .. 1.62 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1A .. O6B .. 1.63 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1A .. O7B .. 1.64 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1A .. T2A .. 3.04 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1A .. T1A .. 3.08 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1A .. T2A .. 3.08 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1A .. O4B .. 3.21 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1A .. O2B .. 3.35 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T2A .. O4B .. 1.58 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T2A .. O2B .. 1.61 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T2A .. O5B .. 1.67 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T2A .. O6B .. 1.68 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T2A .. O4B .. 3.17 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1B .. O1B .. 1.60 Ang.  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact T1B .. O5B .. 1.62 Ang.

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PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 06B .. 1.63 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 07B .. 1.64 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 04B .. 3.21 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 02B .. 3.35 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 04B .. 1.58 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 02B .. 1.61 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 05B .. 1.67 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 06B .. 1.68 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 04B .. 3.17 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 23 Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found Please Check

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

27 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
58 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 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

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## Datablock: FLUORO-LEAKEITE\_BM\_1949\_151

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Bond precision:   = 0.0000 A                      Wavelength=0.71070

Cell:             a=9.7073(5)      b=17.7339(6)      c=5.2850(4)
                  alpha=90         beta=104.029(5)   gamma=90
Temperature:      293 K

                  Calculated                      Reported
Volume            882.67(9)                        882.67(9)
Space group       C 2/m                          C 2/m
Hall group        -C 2y                          -C 2y
Moiety formula    0.331(K4), 15.6(Si),
                  2.6(F), 45.4(O),                  ?
                  2.308(Fe), 0.012(Ca), 0.1
Sum formula       Al2.78 Ca0.01 F2.60 Fe2.31 Al1.39 Ca0.01 F1.30 Fe1.16
                  H K1.51 Li1.58 Mg3.73             H0.50 K0.76 Li0.79 Mg1.87
                  Na3.99 O45.40                     Na1.99 O22
Mr                1671.94                          836.07
Dx,g cm-3         3.145                            3.145
Z                 1                                2
Mu (mm-1)         2.019                            2.019
F000              824.5                            824.4
F000'             827.76
h,k,lmax          15,28,8                          15,28,8
Nref              2017                             2017
Tmin,Tmax         0.702,0.817                      0.773,0.900
Tmin'             0.540

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Correction method= PSI-SCAN

Data completeness= 1.000

Theta(max)= 35.010

R(reflections)= 0.0186( 1062)

wR2(reflections)= wR= 0.0306(1062)

S = \*\*\*\*\*

Npar= 118

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

CHEMW03\_ALERT\_2\_A ALERT: The ratio of given/expected molecular weight as calculated from the \_atom\_site\* data lies outside the range 0.90 <> 1.10

From the CIF: \_cell\_formula\_units\_Z 2

From the CIF: \_chemical\_formula\_weight 836.07

TEST: Calculate formula weight from \_atom\_site\*

atom	mass	num	sum
O	16.00	6.26	100.15
O2-	0.00	16.44	0.00
F-	0.00	1.30	0.00
Al3+	26.98	1.27	34.32
Si4+	28.09	2.64	74.15
Al	26.98	0.12	3.24
Si	28.09	5.16	144.92
Mg2+	24.31	1.87	45.33
Fe2+	55.85	0.35	19.32
Fe3+	55.85	0.81	45.12
Li+	6.94	0.79	5.48
Na+	22.99	1.99	45.84
Ca2+	40.08	0.01	0.24
K+	0.00	0.76	0.00
H	1.01	0.50	0.50

Calculated formula weight 518.62

WEIGH01\_ALERT\_1\_A Unit weights are not acceptable for submissions to Acta Crystallographica Section C.  
n.b. unit is however a legal CIF keyword.

### Alert level B

PLAT430_ALERT_2_B	Short Inter D...A Contact	O1B	..	O2B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O1B	..	O1B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O1B	..	O6B	..	2.67 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O1B	..	O7B	..	2.68 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O1B	..	O5B	..	2.68 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O1B	..	O4B	..	2.77 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O2B	..	O5B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O2B	..	O6B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O2B	..	O4B	..	2.73 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O2B	..	O4B	..	2.75 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O4B	..	O6B	..	2.59 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O4B	..	O5B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O5B	..	O7B	..	2.58 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O5B	..	O6B	..	2.64 Ang.

PLAT430_ALERT_2_B	Short Inter D...A Contact	O5B	..	O6B	..	2.66	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O6B	..	O7B	..	2.60	Ang.

### ● Alert level C

REFNR01\_ALERT\_3\_C Ratio of reflections to parameters is < 10 for a centrosymmetric structure

sine(theta)/lambda	0.8073
Proportion of unique data used	0.5265
Ratio reflections to parameters	9.0000

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT077_ALERT_4_C	Unitcell contains non-integer number of atoms ..		Please Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	O1B .. O2B ..	2.86 Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact	O2B .. O4B ..	2.89 Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact	O4B .. O4B ..	2.89 Ang.

### ● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF	Please Do !
PLAT017_ALERT_1_G	Check Consistency of Scattering Type O2-	for	O1B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type O2-	for	O3A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type F-	for	O3B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type O2-	for	O4B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type O2-	for	O5B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type O2-	for	O6B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type O2-	for	O7B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type AL3+	for	T1A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type SI4+	for	T1B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type AL	for	T1C
PLAT017_ALERT_1_G	Check Consistency of Scattering Type SI	for	T1D
PLAT017_ALERT_1_G	Check Consistency of Scattering Type SI	for	T2A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type SI4+	for	T2B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type MG2+	for	M1A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type FE2+	for	M1B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type AL3+	for	M2A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type FE3+	for	M2B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type MG2+	for	M3A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type LI+	for	M3B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type NA+	for	M4A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type CA2+	for	M4B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type K+	for	AM
PLAT017_ALERT_1_G	Check Consistency of Scattering Type K+	for	A
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by .....		0.50 Ratio
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	(K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	(K)	293 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	Percentage =	100 Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O1B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O2B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O4B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O5B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O6B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O7B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O1A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O3A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O2A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O4A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O5A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O6A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O7A Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	T1D .. O1B ..	1.60 Ang.

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PLAT432_ALERT_2_G Short Inter X...Y Contact T1D .. 06B .. 1.63 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1D .. 05B .. 1.63 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1D .. 07B .. 1.63 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1D .. T2A .. 3.02 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1D .. T2A .. 3.08 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1D .. T1D .. 3.09 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1D .. 04B .. 3.17 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1D .. 02B .. 3.31 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1D .. 03B .. 3.32 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2A .. 04B .. 1.59 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2A .. 02B .. 1.62 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2A .. 05B .. 1.66 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2A .. 06B .. 1.66 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2A .. 04B .. 3.13 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2A .. 01B .. 3.39 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 01B .. 1.60 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 06B .. 1.63 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 05B .. 1.63 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 07B .. 1.63 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 04B .. 3.17 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 02B .. 3.31 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T1B .. 03B .. 3.32 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 04B .. 1.59 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 02B .. 1.62 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 05B .. 1.66 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 06B .. 1.66 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 04B .. 3.13 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact T2B .. 01B .. 3.39 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 23 Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found Please Check

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29 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
62 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 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

```

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## Datablock: FLUORO-LEAKEITE\_570725

---

```

Bond precision:   = 0.0000 A                               Wavelength=0.71070

Cell:             a=9.7094(6)    b=17.7305(12)    c=5.2815(3)
                  alpha=90      beta=104.040(1)   gamma=90
Temperature:      293 K

```

	Calculated	Reported
Volume	882.06(10)	882.06(10)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
	00.64 Si0.64, 0.042(K4),	
Moiety formula	1.31(Si), 0.32(F),	?
	5.04(O), 0.281(Fe),	
	Al0.35 Ca F0.32 Fe0.28	Al1.38 Ca0.01 F1.28 Fe1.13
Sum formula	H0.11 K0.19 Li0.16 Mg0.51	H0.42 K0.76 Li0.65 Mg2.04
	Na0.50 O5.68 S	Na1.99 O22
Mr	209.36	837.39
Dx,g cm-3	3.153	3.153
Z	8	2
Mu (mm-1)	2.004	2.004
F000	826.1	826.1
F000'	829.37	
h,k,lmax	13,24,7	13,24,7
Nref	1325	1321
Tmin,Tmax	0.687,0.887	0.812,0.937
Tmin'	0.663	

Correction method= MULTI-SCAN

Data completeness= 0.997

Theta(max)= 29.960

R(reflections)= 0.0212( 1217)

wR2(reflections)= wR= 0.0203( 1217)

S = \*\*\*\*\*

Npar= 123

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

CHEMW03\_ALERT\_2\_A ALERT: The ratio of given/expected molecular weight as calculated from the \_atom\_site\* data lies outside the range 0.90 <> 1.10

From the CIF: \_cell\_formula\_units\_Z

2

From the CIF: \_chemical\_formula\_weight

837.39

TEST: Calculate formula weight from \_atom\_site\_\*

atom	mass	num	sum
O	16.00	5.96	95.35
O2-	0.00	16.76	0.00
F-	0.00	1.28	0.00
Al3+	26.98	1.26	34.05
Si4+	28.09	2.88	80.89
Al	26.98	0.12	3.24
Si	28.09	4.92	138.18
Mg2+	24.31	2.04	49.66
Fe2+	55.85	0.31	17.09
Fe3+	55.85	0.82	45.68



Li+	6.94	0.65	4.52
Na+	22.99	1.99	45.80
Ca <sup>2+</sup>	40.08	0.01	0.32
K+	0.00	0.76	0.00
H	1.01	0.42	0.42

Calculated formula weight	515.20
---------------------------	--------

WEIGH01\_ALERT\_1\_A Unit weights are not acceptable for submissions to Acta Crystallographica Section C.

n.b. unit is however a legal CIF keyword.

PLAT213\_ALERT\_2\_A Atom A has ADP max/min Ratio ..... 5.1 oblate

### Alert level B

PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	02B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	01B	..	2.67 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	06B	..	2.67 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	07B	..	2.67 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	05B	..	2.68 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	01B	..	04B	..	2.78 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	02B	..	05B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	02B	..	06B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	02B	..	04B	..	2.73 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	02B	..	04B	..	2.75 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	04B	..	06B	..	2.58 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	04B	..	05B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	05B	..	07B	..	2.57 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	05B	..	06B	..	2.64 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	05B	..	06B	..	2.66 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	06B	..	07B	..	2.60 Ang.

### Alert level C

REFNR01\_ALERT\_3\_C Ratio of reflections to parameters is < 10 for a centrosymmetric structure

sine(theta)/lambda 0.7027

Proportion of unique data used 0.9213

Ratio reflections to parameters 9.8943

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT077_ALERT_4_C	Unitcell contains non-integer number of atoms	..	Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	....	2.85 Report
PLAT430_ALERT_2_C	Short Inter D...A Contact	01B .. 02B ..	2.87 Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact	02B .. 04B ..	2.90 Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact	04B .. 04B ..	2.89 Ang.

### Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF	Please Do !
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	O2- for	01B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	O2- for	03A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	F- for	03B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	O2- for	04B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	O2- for	05B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	O2- for	06B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	O2- for	07B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	AL3+ for	T1A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	SI4+ for	T1B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	AL for	T1C
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	SI for	T1D
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	SI for	T2A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	SI4+ for	T2B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type	MG2+ for	M1A

PLAT017_ALERT_1_G	Check Consistency of Scattering Type FE2+	for	M1B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type AL3+	for	M2A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type FE3+	for	M2B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type MG2+	for	M3A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type LI+	for	M3B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type NA+	for	M4A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type CA2+	for	M4B
PLAT017_ALERT_1_G	Check Consistency of Scattering Type K+	for	A
PLAT017_ALERT_1_G	Check Consistency of Scattering Type K+	for	AM
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by .....	4.00	Ratio
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	100	Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	01B	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	02B	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	04B	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	05B	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	06B	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	07B	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	01A	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	03A	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	02A	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	04A	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....	07A	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	01B ..	1.60 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	06B ..	1.62 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	05B ..	1.63 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	07B ..	1.63 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	T2A ..	3.02 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	T2A ..	3.08 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	T1D ..	3.09 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	04B ..	3.17 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	02B ..	3.32 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1D ..	03B ..	3.32 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2A ..	04B ..	1.59 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2A ..	02B ..	1.62 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2A ..	05B ..	1.66 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2A ..	06B ..	1.66 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2A ..	04B ..	3.13 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2A ..	01B ..	3.39 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1B ..	01B ..	1.60 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1B ..	06B ..	1.62 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1B ..	05B ..	1.63 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1B ..	07B ..	1.63 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1B ..	04B ..	3.17 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1B ..	02B ..	3.32 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T1B ..	03B ..	3.32 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2B ..	04B ..	1.59 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2B ..	02B ..	1.62 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2B ..	05B ..	1.66 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2B ..	06B ..	1.66 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2B ..	04B ..	3.13 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact T2B ..	01B ..	3.39 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	23	Note
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check

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

28 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 62 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 2 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

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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**

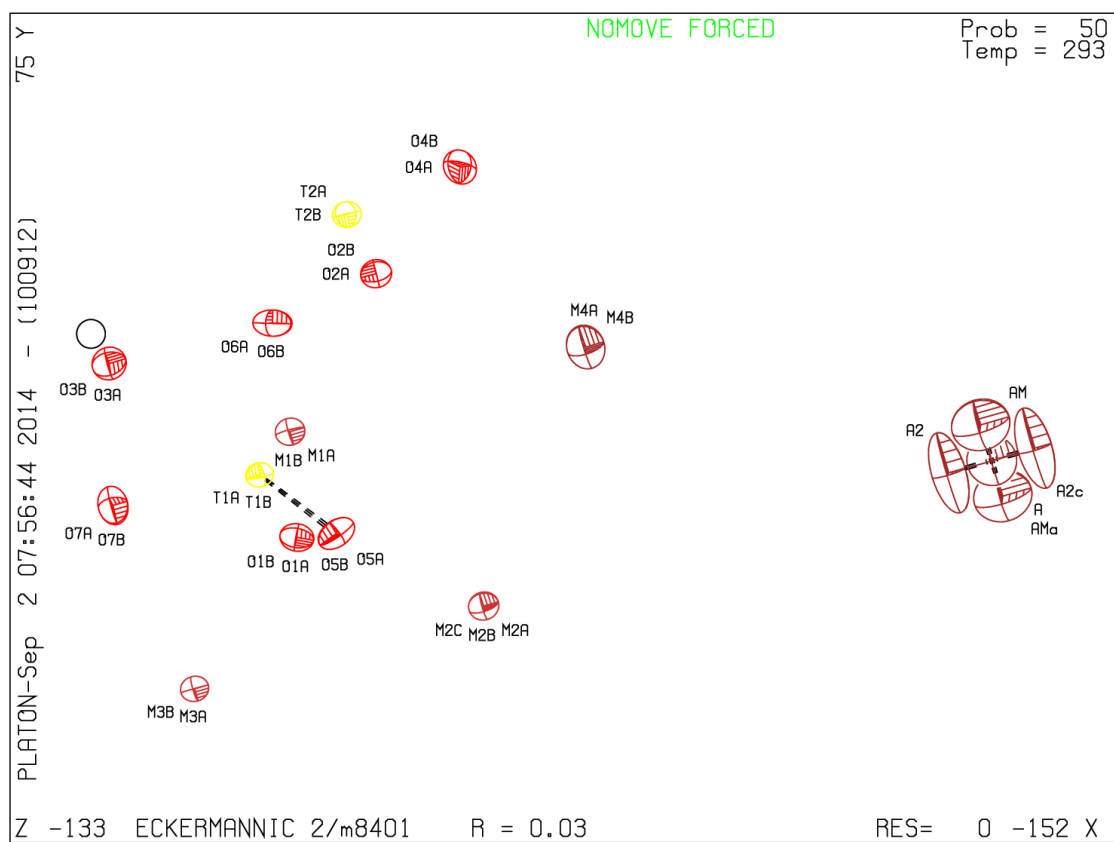
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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**

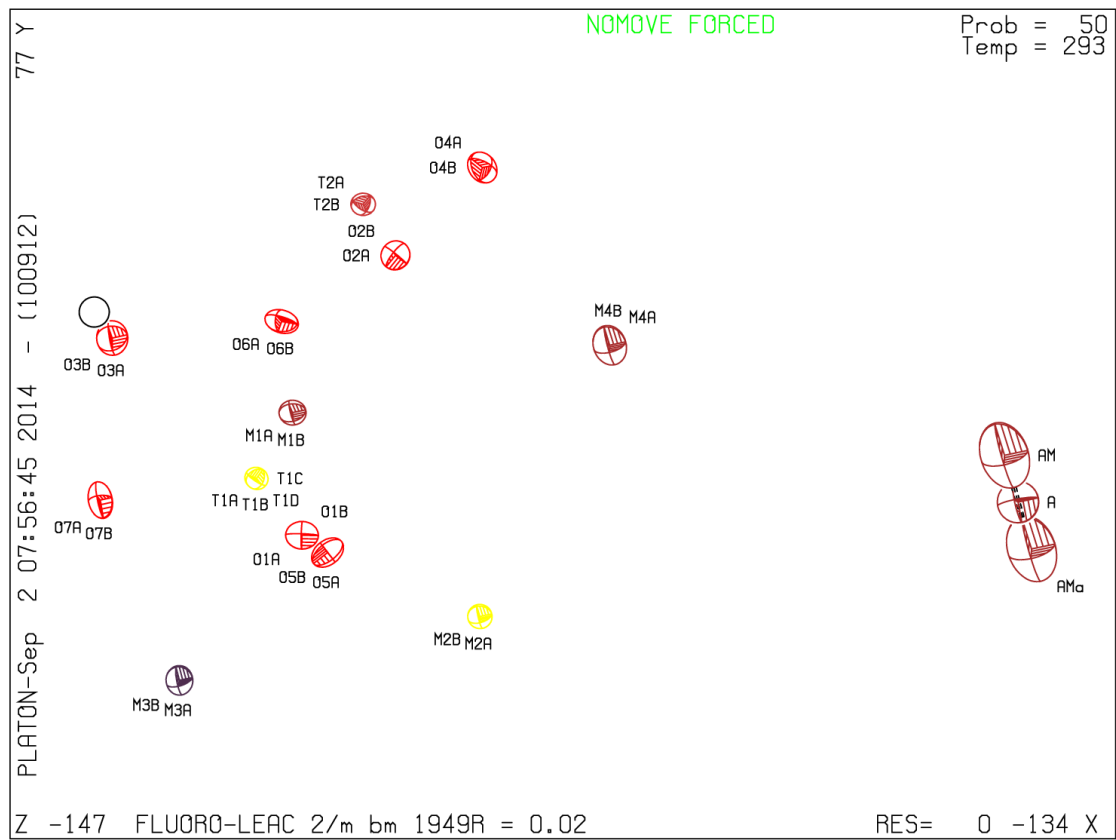
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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**PLATON version of 20/08/2014; check.def file version of 18/08/2014**



Datablock FLUORO-LEAKEITE\_BM\_1949\_151 - ellipsoid plot



Datablock FLUORO-LEAKEITE\_570725 - ellipsoid plot

