

checkCIF/PLATON report (publication check)

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: _Mo134La

Bond precision: La- O = 0.0169 Å Wavelength=0.71075
 Cell: a=35.530(16) b=37.05(2) c=36.11(2)
 alpha=90 beta=119.85(2) gamma=90
 Temperature: 173 K

	Calculated	Reported
Volume	41228(38)	4123
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Cl4 La10 Mo134 O520, 10(Na)	H516 CL4 LA10 MO134 NA10 O664
Sum formula	Cl4 La10 Mo134 Na10 O520	H516 CL4 LA10 MO134 NA10 O664
Mr	22936.76	25760.40
Dx, g cm-3	1.848	2.075
Z	2	2
Mu (mm-1)	2.555	2.574
F000	21072.0	24408.0
F000'	20616.65	
h, k, lmax	46, 48, 46	46, 48, 46
Nref	94596	94422
Tmin, Tmax	0.635, 0.773	0.510, 0.773
Tmin'	0.592	

Correction method= NUMERICAL
 Data completeness= 0.998 Theta(max)= 27.490
 R(reflections)= 0.0923(52411) wR2(reflections)= 0.2841(94422)
 S = 1.012 Npar= 1940

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

[REFI014_ALERT_1_G](#) _refine_ls_hydrogen_treatment is missing
 Code for H-atom treatment.
 The following tests will not be performed
 HYDTR_01

[GEOM006_ALERT_1_A](#) _geom_angle_atom_site_label_2 is missing
 Label identifying the atom site 2.

[GEOM007_ALERT_1_A](#) _geom_angle_atom_site_label_3 is missing
 Label identifying the atom site 3.

[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 *****
 TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
Mo	95.94	134.00	12855.96
O	16.00	520.00	8319.48
La	138.91	10.00	1389.06
Cl	35.45	4.00	141.81
Na	22.99	10.00	229.90
H	1.01	0.00	0.00

Calculated formula weight 22936.21

PLAT220_ALERT_2_A	Large Non-Solvent	Mo	Ueq(max)/Ueq(min) ...	7.22	Ratio
PLAT220_ALERT_2_A	Large Non-Solvent	O	Ueq(max)/Ueq(min) ...	10.00	Ratio
PLAT242_ALERT_2_A	Check Low	Ueq as Compared to Neighbors for		La1	
PLAT242_ALERT_2_A	Check Low	Ueq as Compared to Neighbors for		0195	
PLAT242_ALERT_2_A	Check Low	Ueq as Compared to Neighbors for		0206	
PLAT242_ALERT_2_A	Check Low	Ueq as Compared to Neighbors for		0225	
PLAT602_ALERT_2_A	VERY LARGE Solvent Accessible VOID(S) in Structure			!	
PLAT043_ALERT_1_A	Check Reported Molecular Weight			25760.40	
PLAT044_ALERT_1_A	Calculated and Reported Dx Differ			?	
PLAT150_ALERT_1_A	Volume as Calculated Differs from that Given			4123.00	Ang-3

Alert level B

[CHEMS01_ALERT_1_B](#) The sum formula contains elements in the wrong order.
 H precedes Cl
 Sequence must be alphabetical for inorganic structures.

[DIFMN02_ALERT_2_B](#) The minimum difference density is < -0.1*ZMAX*1.00
 _refine_diff_density_min given = -6.130
 Test value = -5.700

[DIFMX01_ALERT_2_B](#) The maximum difference density is > 0.1*ZMAX*1.00
 _refine_diff_density_max given = 8.970
 Test value = 5.700

[PLAT097_ALERT_2_B](#) Large Reported Max. (Positive) Residual Density 8.97 eA-3
[PLAT098_ALERT_2_B](#) Large Reported Min. (Negative) Residual Density -6.13 eA-3
[PLAT241_ALERT_2_B](#) Check High Ueq as Compared to Neighbors for Mo67
[PLAT242_ALERT_2_B](#) Check Low Ueq as Compared to Neighbors for La3
[PLAT242_ALERT_2_B](#) Check Low Ueq as Compared to Neighbors for Mo60
[PLAT242_ALERT_2_B](#) Check Low Ueq as Compared to Neighbors for Mo63
[PLAT242_ALERT_2_B](#) Check Low Ueq as Compared to Neighbors for O220

Alert level C

[DIFMN03_ALERT_1_C](#) The minimum difference density is < -0.1*ZMAX*0.75
 The relevant atom site should be identified.

[DIFMX02_ALERT_1_C](#) The maximum difference density is > 0.1*ZMAX*0.75
 The relevant atom site should be identified.

[RFACR01_ALERT_3_C](#) The value of the weighted R factor is > 0.25
 Weighted R factor given 0.284

[PLAT084_ALERT_2_C](#) High R2 Value 0.28
[PLAT165_ALERT_3_C](#) Nr. of Status R Flagged Non-Hydrogen Atoms 18
[PLAT241_ALERT_2_C](#) Check High Ueq as Compared to Neighbors for Mo45
[PLAT241_ALERT_2_C](#) Check High Ueq as Compared to Neighbors for Mo57
[PLAT241_ALERT_2_C](#) Check High Ueq as Compared to Neighbors for Mo61
[PLAT241_ALERT_2_C](#) Check High Ueq as Compared to Neighbors for Mo62
[PLAT242_ALERT_2_C](#) Check Low Ueq as Compared to Neighbors for La2
[PLAT242_ALERT_2_C](#) Check Low Ueq as Compared to Neighbors for La4
[PLAT242_ALERT_2_C](#) Check Low Ueq as Compared to Neighbors for La5
[PLAT242_ALERT_2_C](#) Check Low Ueq as Compared to Neighbors for O174
[PLAT242_ALERT_2_C](#) Check Low Ueq as Compared to Neighbors for O202
[PLAT242_ALERT_2_C](#) Check Low Ueq as Compared to Neighbors for O208
[PLAT242_ALERT_2_C](#) Check Low Ueq as Compared to Neighbors for O231
[PLAT041_ALERT_1_C](#) Calc. and Reported SumFormula Strings Differ ?
[PLAT042_ALERT_1_C](#) Calc. and Reported MoietyFormula Strings Differ ?
[PLAT068_ALERT_1_C](#) Reported F000 Differs from Calcd (or Missing)... ?
[PLAT151_ALERT_1_C](#) No su (esd) Given on Volume ?
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... M057
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... M061
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... M062
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... M067
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 072
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 073
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 074
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 075
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 084
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 085
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 086
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 087
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 088
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 089
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... 090
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... O102
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... O103
[PLAT161_ALERT_4_C](#) Missing or Zero su (esd) on x-coordinate for ... O104
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... M057
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... M061
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... M062
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... M067
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... 072
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[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... 088
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... 089
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... 090
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... O102
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... O103
[PLAT162_ALERT_4_C](#) Missing or Zero su (esd) on y-coordinate for ... O104
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... M057
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... M061

[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... M062
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... M067
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 072
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 073
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 074
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 075
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 084
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 085
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 086
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 087
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 088
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 089
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 090
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 0102
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 0103
[PLAT163_ALERT_4_C](#) Missing or Zero su (esd) on z-coordinate for ... 0104
[PLAT711_ALERT_1_C](#) BOND Unknown or Inconsistent Label 0328
 NA(5) 0(328)
[PLAT751_ALERT_4_C](#) Bond Calc 2.18487, Rep 2.184(14) Senseless su
 MO(57-0(195 1.555 1.555
[PLAT751_ALERT_4_C](#) Bond Calc 2.18730, Rep 2.19(2) Senseless su
 MO(57-0(221 1.555 1.555
[PLAT751_ALERT_4_C](#) Bond Calc 2.17832, Rep 2.178(15) Senseless su
 MO(61-0(206 1.555 1.555
[PLAT751_ALERT_4_C](#) Bond Calc 2.03553, Rep 2.035(19) Senseless su
 MO(61-0(224 1.555 1.555
[PLAT751_ALERT_4_C](#) Bond Calc 2.16309, Rep 2.163(16) Senseless su
 MO(62-0(225 1.555 1.555
[PLAT751_ALERT_4_C](#) Bond Calc 2.00670, Rep 2.01(2) Senseless su
 MO(62-0(226 1.555 1.555
[PLAT751_ALERT_4_C](#) Bond Calc 2.28485, Rep 2.28(2) Senseless su
 MO(67-0(231 1.555 1.555

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: H516 Cl4 La10 Mo134 Na10 O664
 Atom count from the _atom_site data: Cl4 La10 Mo134 Na10 O520
[CELLZ01_ALERT_1_G](#) Difference between formula and atom_site contents detected.
[CELLZ01_ALERT_1_G](#) ALERT: Large difference may be due to a
 symmetry error - see SYMMG tests
 From the CIF: _cell_formula_units_Z 2
 From the CIF: _chemical_formula_sum H516 Cl4 La10 Mo134 Na10 O664
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
H	1032.00	0.00	1032.00
Cl	8.00	8.00	0.00
La	20.00	20.00	0.00
Mo	268.00	268.00	0.00
Na	20.00	20.00	0.00
O	1328.00	1040.00	288.00

[PLAT072_ALERT_2_G](#) SHELXL First Parameter in WGHT Unusually Large.. 0.16

13 **ALERT level A** = In general: serious problem

10 **ALERT level B** = Potentially serious problem

82 **ALERT level C** = Check and explain

5 **ALERT level G** = General alerts; check

16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

31 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

61 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

[PUBL002_ALERT_1_A](#) The contact author's address is missing,
 _publ_contact_author_address.

[PUBL012_ALERT_1_A](#) _publ_section_abstract is missing.
 Abstract of paper in English.

Alert level G

[PUBL013_ALERT_1_G](#) The _publ_section_comment (discussion of study) is

missing. This is required for a full paper submission (but is optional for an electronic paper).

[PUBL017_ALERT_1_G](#) The _publ_section_references section is missing or empty.

2 **ALERT level A** = Data missing that is essential or data in wrong format
 2 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should always 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 nature of your study may justify the reported deviations from the submission requirements of the journal and these should be commented upon in the discussion or experimental section of a paper - after all, they might represent an interesting feature.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a [basic structural check](#) is run on the final version of your CIF prior to submission.

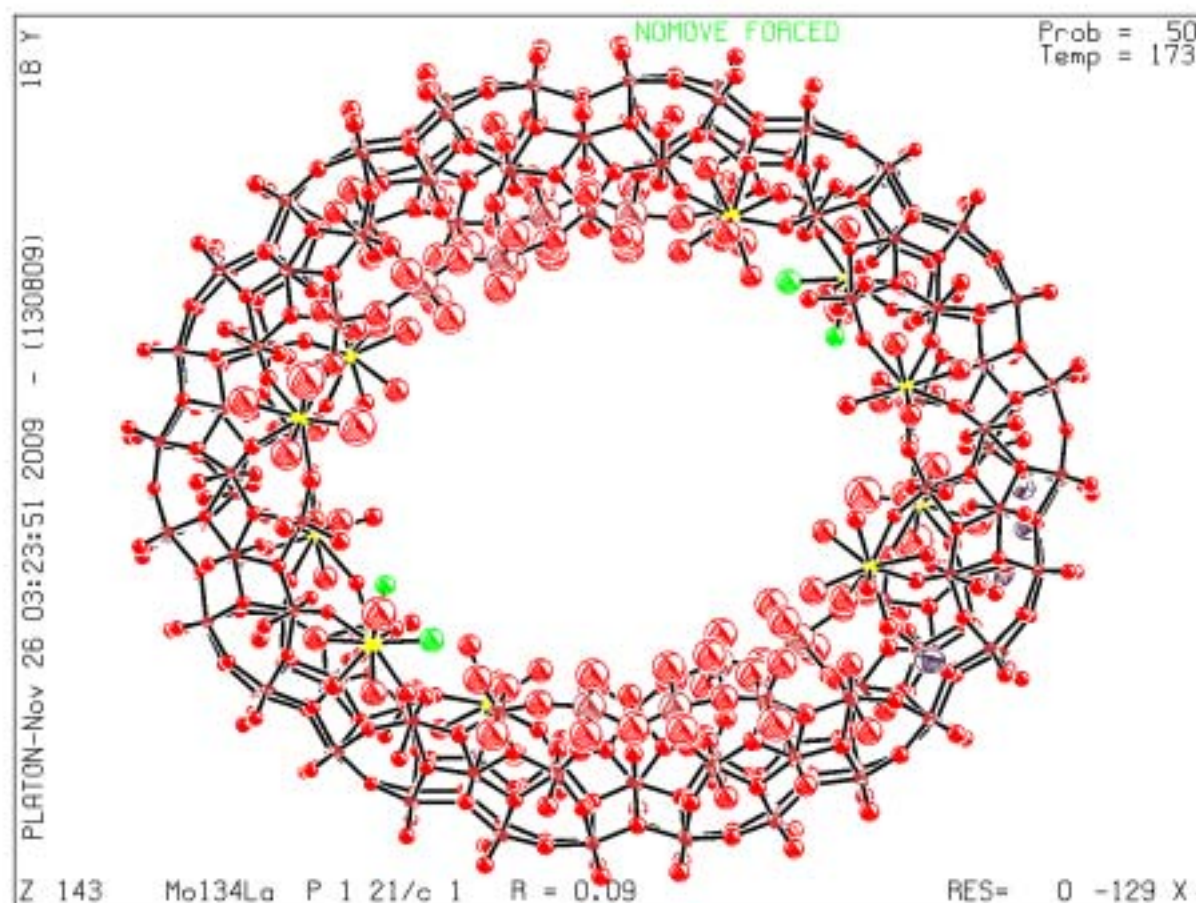
```
# start Validation Reply Form
_vrf_PUBL002_GLOBAL
;
PROBLEM: The contact author's address is missing,
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_GEOM006_Mo134La
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_Mo134La
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_CHEMW03_Mo134La
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT220_Mo134La
;
PROBLEM: Large Non-Solvent    Mo      Ueq(max)/Ueq(min) ...      7.22 Ratio
RESPONSE: ...
;
_vrf_PLAT242_Mo134La
;
PROBLEM: Check Low          Ueq as Compared to Neighbors for      La1
RESPONSE: ...
;
_vrf_PLAT602_Mo134La
;
PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure      !
RESPONSE: ...
;
_vrf_PLAT043_Mo134La
;
PROBLEM: Check Reported Molecular Weight .....      25760.40
RESPONSE: ...
;
_vrf_PLAT044_Mo134La
```

```
;
PROBLEM: Calculated and Reported Dx Differ ..... ?
RESPONSE: ...
;
_vrf_PLAT150__Mo134La
;
PROBLEM: Volume as Calculated Differs from that Given ... 4123.00 Ang-3
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via [the web](#). If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic [submission](#) or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 13/08/2009; check.def file version of 12/08/2009

Datablock _Mo134La - ellipsoid plot



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