



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2024byeb075b

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: 2024byeb075b

Bond precision:	Nb- O = 0.0027 Å		Wavelength=0.71073
Cell:	a=12.5355 (4)	b=12.5355 (4)	c=3.9213 (2)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	616.19 (5)	616.19 (5)	
Space group	P 4/m b m	P 4/m b m	
Hall group	-P 4 2ab	-P 4 2ab	
Moiety formula	Ce1.62 Fe0.11 Nb9.89 O30, 1.432 (Ba), 2.568 (K), 0.376 (Ca)	Ba0.715 Ca0.188 Ce0.812 Fe0.053 K1.285 Nb4.947 O15	
Sum formula	Ba1.43 Ca0.38 Ce1.62 Fe0.11 K2.57 Nb9.89 O30	Ba0.71 Ca0.19 Ce0.81 Fe0.05 K1.28 Nb4.95 O15	
Mr	1944.86	972.07	
Dx, g cm ⁻³	5.241	5.239	
Z	1	2	
Mu (mm ⁻¹)	10.286	10.278	
F000	879.1	879.0	
F000'	858.35		
h, k, lmax	17, 17, 5	17, 16, 5	
Nref	511	480	
Tmin, Tmax	0.814, 0.902	0.809, 1.000	
Tmin'	0.814		

Correction method= # Reported T Limits: Tmin=0.809 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.939 Theta(max)= 29.244

R(reflections)= 0.0188(427) wR2(reflections)=
0.0418(480)

S = 1.110 Npar= 44

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 C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
	Calc: Ba1.43 Ca0.38 Ce1.62 Fe0.11 K2.57 Nb9.89 O30		
	Rep.: Ba0.71 Ca0.19 Ce0.81 Fe0.05 K1.28 Nb4.95 O15		
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings Differ	Please Check
	Calc: Ce1.62 Fe0.11 Nb9.89 O30, 1.432(Ba), 2.568(K), 0.376(Ca)		
	Rep.: Ba0.715 Ca0.188 Ce0.812 Fe0.053 K1.285 Nb4.947 O15		
PLAT077_ALERT_4_C	Unit-Cell Contains Non-integer Number of Atoms	.	Please Check
PLAT213_ALERT_2_C	Atom O2	has ADP max/min Ratio	3.5 prolat
PLAT213_ALERT_2_C	Atom O4	has ADP max/min Ratio	3.4 prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 O	Ueq(max)/Ueq(min) Range	3.1 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		01 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		04 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		05 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Nb2 Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)		2.1 Note
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.016 Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.80Ang From O1	.	0.67 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.57Ang From O4	.	0.63 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.53Ang From O4	.	0.59 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.53Ang From O1	.	0.54 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.52Ang From O5	.	0.52 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.77Ang From O4	.	0.51 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.76Ang From O5	.	0.50 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.80Ang From O3	.	0.43 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.02Ang From O4	.	-0.65 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.98Ang From O4	.	-0.50 eA-3



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check	
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	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
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check

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PLAT200_ALERT_1_G Reported   _diffn_ambient_temperature ..... (K)          293 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd   1)          35% 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
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..      Please Do !
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]=      3.25 Note
                    1  1  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          29 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....          2.089 Note
                    Predicted wR2: Based on SigI**2  2.00 or SHELX Weight  3.76

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
18 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
7 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

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# start Validation Reply Form
_vrf_PLAT041_2024byeb075b
;
PROBLEM: Calc. and Reported SumFormula      Strings Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT042_2024byeb075b
;
PROBLEM: Calc. and Reported MoietyFormula Strings Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT077_2024byeb075b
;
PROBLEM: Unit-Cell Contains Non-integer Number of Atoms .      Please Check
RESPONSE: ...
;
_vrf_PLAT213_2024byeb075b
;
PROBLEM: Atom O2                      has ADP max/min Ratio .....      3.5 prolat
RESPONSE: ...
;
_vrf_PLAT220_2024byeb075b
;
PROBLEM: NonSolvent   Resd 1  0   Ueq(max)/Ueq(min) Range      3.1 Ratio
RESPONSE: ...
;
_vrf_PLAT241_2024byeb075b

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;
PROBLEM: High      'MainMol' Ueq as Compared to Neighbors of          01 Check
RESPONSE: ...
;
_vrf_PLAT242_2024byeb075b
;
PROBLEM: Low      'MainMol' Ueq as Compared to Neighbors of          Nb2 Check
RESPONSE: ...
;
_vrf_PLAT250_2024byeb075b
;
PROBLEM: Large U3/U1 Ratio for <U(i,j)> Tensor(Resd      1)          2.1 Note
RESPONSE: ...
;
_vrf_PLAT906_2024byeb075b
;
PROBLEM: Large K Value in the Analysis of Variance .....          2.016 Check
RESPONSE: ...
;
_vrf_PLAT975_2024byeb075b
;
PROBLEM: Check Calcd Resid. Dens.  0.80Ang From O1          .          0.67 eA-3
RESPONSE: ...
;
_vrf_PLAT976_2024byeb075b
;
PROBLEM: Check Calcd Resid. Dens.  1.02Ang From O4          .          -0.65 eA-3
RESPONSE: ...
;
# end Validation Reply Form

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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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found
