checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: A-BA4NB2O9_1273K_phase_1

Bond precision: Nb- O = 0.0180 A Wavelength=0.71073

Cell: **a=10.3829(3)** **b=10.3829(3)** **c=8.5722(8)**
alpha=90 **beta=90** **gamma=120**
Temperature: **?**

	Calculated	Reported
Volume	800.31(8)	800.32(13)
Space group	P -6 2 c	P -6 2 c
Hall group	P -6c -2c	?
Moiety formula	2(Nb2 O9), Nb2, 9(O), 12(Ba)	?
Sum formula	Ba12 Nb6 O27	Ba6 NB3.00 O13.50
Mr	2637.42	1318.68
Dx,g cm-3	5.472	0.000
Z	1	2
Mu (mm-1)	16.626	0.000
F000	1134.0	0.0
F000’	1118.02	
h,k,lmax		
Nref		
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= **Theta(max)=**

R(reflections)= **wR2(reflections)=**

S = **Npar=**

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

ATOM007_ALERT_1_A _atom_site_aniso_label is missing
Unique label identifying the atom site.
PLAT430_ALERT_2_A Short Inter D...A Contact O3 .. O4 .. 2.52 Ang.
PLAT091_ALERT_1_A No Wavelength found in CIF - 0.71079 Ang Assumed ?
PLAT197_ALERT_1_A Missing _cell_measurement_temperature ..... ?

Alert level B

```
CELLV02_ALERT_1_B  The supplied cell volume s.u. differs from that
            calculated from the cell parameter s.u.'s by > 4
            Calculated cell volume su =       8.78
            Cell volume su given      =      13.00
PLAT430_ALERT_2_B Short Inter D...A Contact  O4     ..  O4      ..       2.66 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact  O4     ..  O4      ..       2.66 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA1    --  BA1     ..       4.29 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA1    --  BA1     ..       4.29 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA1    --  BA2     ..       4.09 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA1    --  BA2     ..       4.12 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA1    --  BA2     ..       4.09 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA1    --  BA2     ..       4.12 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA2    --  BA1     ..       4.09 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA2    --  BA1     ..       4.12 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA2    --  BA1     ..       4.09 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA2    --  BA1     ..       4.12 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA2    --  BA2     ..       4.29 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:   BA2    --  BA2     ..       4.29 Ang.
```

Alert level C

```
PLAT034_ALERT_1_C No Flack Parameter Given. Z .GT. Si, NonCentro .          ?
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT045_ALERT_1_C Calculated and Reported Z Differ by ............       0.50 Ratio
PLAT076_ALERT_1_C Occupancy       0.50 less than 1.0 for Sp.pos  .         O4
PLAT152_ALERT_1_C Supplied and Calc Volume s.u. Inconsistent .....          ?
PLAT194_ALERT_1_C Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_C Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_C Missing _cell_measurement_theta_min   datum ....          ?
PLAT731_ALERT_1_C Bond    Calc     3.76(4), Rep   3.763(19) ......       2.11 su-Ra
             NB2  -BA2     1.555   2.665
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA1    --  BA2     ..       4.00 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA1    --  BA2     ..       4.00 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA1    --  NB1     ..       3.69 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA1    --  NB1     ..       3.69 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA1    --  NB2     ..       3.51 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA1    --  NB2     ..       3.51 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA2    --  BA1     ..       4.00 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA2    --  BA1     ..       4.00 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA2    --  NB1     ..       3.54 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA2    --  NB1     ..       3.54 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA2    --  NB2     ..       3.76 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA2    --  NB2     ..       3.76 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB1    --  BA1     ..       3.69 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB1    --  BA1     ..       3.69 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB1    --  BA1     ..       3.69 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB1    --  BA2     ..       3.54 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB1    --  BA2     ..       3.54 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB1    --  BA2     ..       3.54 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB2    --  BA1     ..       3.51 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB2    --  BA1     ..       3.51 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB2    --  BA1     ..       3.51 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB2    --  BA2     ..       3.76 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB2    --  BA2     ..       3.76 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NB2    --  BA2     ..       3.76 Ang.
```

Alert level G

```
PLAT301_ALERT_3_G Note Main Residue  Disorder ....................      14.00 Perc.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      37.10 Deg.
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             BA1  -O3   -O3      6.655   1.555   4.556
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         !
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   4 ALERT level A = In general: serious problem
  15 ALERT level B = Potentially serious problem
  33 ALERT level C = Check and explain
   3 ALERT level G = General alerts; check

  49 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: A-BA4NB2O9_1273K_phase_2

Bond precision: Nb-Nb = 0.0001 A Wavelength=0.71073

Cell: a=3.33572(8) b=3.33572(8) c=3.33572(8)
alpha=90 beta=90 gamma=90
Temperature: ?

	Calculated	Reported
Volume	37.12(1)	37.12(1)
Space group	I m -3 m	I m 3 m
Hall group	-I 4 2 3	?
Moiety formula	Nb	?
Sum formula	Nb	Nb
Mr	92.91	92.91
Dx,g cm-3	8.313	0.000
Z	2	2
Mu (mm-1)	14.709	0.000
F000	82.0	0.0
F000’	77.78	
h,k,lmax		
Nref		
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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

ATOM007_ALERT_1_A _atom_site_aniso_label is missing
Unique label identifying the atom site.
SYMMG01_ALERT_1_A Unrecognised _symmetry_space_group_name_H-M
International Tables space group number is not in the CIF
From the CIF: _symmetry_space_group_name_H-M I m 3 m
Int. Tables space group number for I m 3 m is 0
SYMMG02_ALERT_1_A Supplied _symmetry_space_group_name_H-M not recognised
From the CIF: _symmetry_equiv_pos_as_xyz
+x,+y,+z
+z,+x,+y
+y,+z,+x
+x,+y,-z
-z,+x,+y
+y,-z,+x
-z,+x,-y
-y,-z,+x
+y,-z,-x
-x,+y,-z
-z,-x,+y
+x,-y,-z
+y,+x,+z
+z,+y,+x
+x,+z,+y
+y,+x,-z
-z,+y,+x
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+z,+x,-y
-x,+y,+z
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-x,-z,-y
-y,-x,+z
+z,-y,-x
-x,+z,-y
+z,-y,+x
+x,+z,-y
-x,+z,+y
+y,-x,+z
+z,+y,-x

-y,+x,+z
+x+1/2,+y+1/2,+z+1/2
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-y+1/2,+x+1/2,-z+1/2
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-y+1/2,+z+1/2,+x+1/2
+x+1/2,-y+1/2,+z+1/2
+z+1/2,+x+1/2,-y+1/2
-x+1/2,+y+1/2,+z+1/2
-y+1/2,-x+1/2,-z+1/2
-z+1/2,-y+1/2,-x+1/2
-x+1/2,-z+1/2,-y+1/2
-y+1/2,-x+1/2,+z+1/2
+z+1/2,-y+1/2,-x+1/2
-x+1/2,+z+1/2,-y+1/2
+z+1/2,-y+1/2,+x+1/2
+x+1/2,+z+1/2,-y+1/2
-x+1/2,+z+1/2,+y+1/2
+y+1/2,-x+1/2,+z+1/2
+z+1/2,+y+1/2,-x+1/2
-y+1/2,+x+1/2,+z+1/2

These symops generate the Hall space group symbol -i_4_2_3
which is equivalent to the H-M space group symbol i_m_-3_m

PLAT091_ALERT_1_A No Wavelength found in CIF - 0.71079 Ang Assumed ?
PLAT197_ALERT_1_A Missing _cell_measurement_temperature ..... ?

Alert level C

PLAT194_ALERT_1_C Missing _cell_measurement_reflns_used datum .... ?
PLAT195_ALERT_1_C Missing _cell_measurement_theta_max datum .... ?
PLAT196_ALERT_1_C Missing _cell_measurement_theta_min datum .... ?
PLAT731_ALERT_1_C Bond Calc 3.33570(10), Rep 3.3357(2) ..... 2.30 su-Ra
NB -NB 1.555 1.455

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PLAT731_ALERT_1_C Bond    Calc 3.33570(10), Rep   3.3357(2) ......       2.30 su-Ra
              NB   -NB      1.555   1.545
PLAT731_ALERT_1_C Bond    Calc 3.33570(10), Rep   3.3357(2) ......       2.30 su-Ra
              NB   -NB      1.555   1.554
PLAT731_ALERT_1_C Bond    Calc 3.33570(10), Rep   3.3357(2) ......       2.30 su-Ra
              NB   -NB      1.555   1.556
PLAT731_ALERT_1_C Bond    Calc 3.33570(10), Rep   3.3357(2) ......       2.30 su-Ra
              NB   -NB      1.555   1.565
PLAT731_ALERT_1_C Bond    Calc 3.33570(10), Rep   3.3357(2) ......       2.30 su-Ra
              NB   -NB      1.555   1.655
```

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5 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
9 **ALERT level C** = Check and explain
0 **ALERT level G** = General alerts; check

14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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.

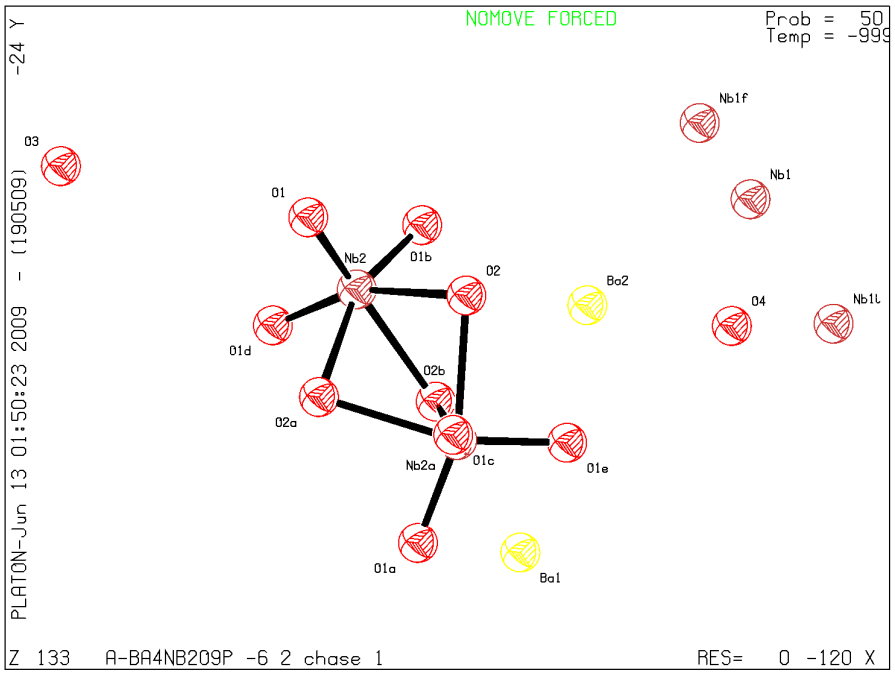
Publication of your CIF in other journals

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

PLATON version of 19/05/2009; check.def file version of 13/05/2009

Datablock A-BA4NB2O9_1273K_phase_1 - No thermal parameters given. Plot performed with default spheres.

Datablock A-BA4NB2O9_1273K_phase_1 - ellipsoid plot



Datablock A-BA4NB2O9_1273K_phase_2 - No thermal parameters given. Plot performed with default spheres.

Datablock A-BA4NB2O9_1273K_phase_2 - ellipsoid plot

