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: BaZnNCN2

Bond precision: N- C = 0.0077 A Wavelength=1.54180

Cell: a=11.93398(5) b=11.92746(6) c=6.84528(3)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	974.372(8)	974.371(7)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	?
Moiety formula	C8 N16 Zn4, 4(Ba)	?
Sum formula	C8 Ba4 N16 Zn4	C2 Ba N4 Zn
Mr	1131.12	282.76
Dx,g cm-3	3.855	0.000
Z	2	8
Mu (mm-1)	67.458	0.000
F000	1008.0	0.0
F000’	990.90	
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 G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.25 Check
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..............    0.00006 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00003 Ang.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT202_ALERT_3_G Isotropic non-H Atoms in Anion/Solvent .........          1 Check
PLAT981_ALERT_1_G No non-zero f" Anomalous Scattering Values Found     Please Check
PLAT986_ALERT_1_G No non-zero f’ Anomalous Scattering Values Found     Please Check
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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
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   6 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
   1 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: LiF

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Bond precision:  N- C = 0.0000 A         Wavelength=1.54180

Cell:            a=4.02645(1)     b=4.02645(1)     c=4.02645(1)
                 alpha=90         beta=90          gamma=90
Temperature:     293 K

                 Calculated                Reported
Volume           65.278(1)                 65.278(1)
Space group      F m -3 m                  F m -3 m
Hall group       -F 4 2 3                  ?
Moiety formula   F, Li                     ?
Sum formula      F Li                      F Li
Mr               25.94                     25.94
Dx,g cm-3        2.639                     0.000
Z                4                         4
Mu (mm-1)        3.087                     0.000
F000             48.0                      0.0
F000’            48.29
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 G

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 1	0.02 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 2	0.02 Check
PLAT981_ALERT_1_G	No non-zero f" Anomalous Scattering Values Found	Please Check
PLAT986_ALERT_1_G	No non-zero f’ Anomalous Scattering Values Found	Please Check

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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
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

4 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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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

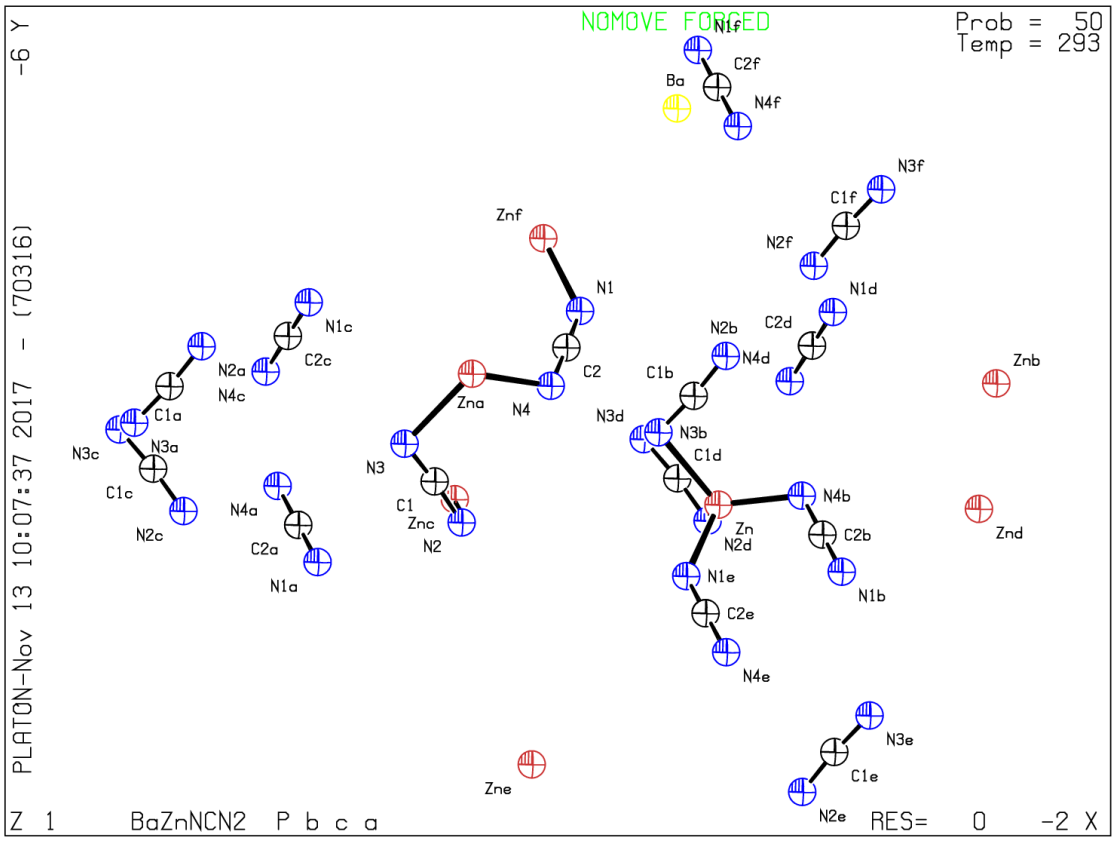
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

PLATON version of 09/11/2017; check.def file version of 08/11/2017

Datablock BaZnNCN2 - ellipsoid plot



Datablock LiF - ellipsoid plot