

No syntax errors found.
Please wait while processing

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

Datablock: BaBH42-NH3

Bond precision:	= 0.0000 A	Wavelength=0.71073
Cell:	a=5.08626(8) b=9.37609(16) c=12.9631(2)	
	alpha=90 beta=90 gamma=90	
Temperature:	368 K	
	Calculated	Reported
Volume	618.200(17)	618.203(18)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	H3 N, 2(B H4), Ba	Ba(Bh4)2(Nh3)
Sum formula	B2 Ba H11 N	BaNb2H11
Mr	184.05	184.05
Dx,g cm-3	1.977	0.000
Z	4	2
Mu (mm-1)	6.270	0.000
F000	336.0	0.0
F000'	334.79	
h,k,lmax	3,6,9	
Nref	238[161]	
Tmin,Tmax		
Tmin'		
Correction method=	Not given	
Data completeness=	0.00/0.00	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

[GEOM001_ALERT_1_A](#) _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.

[GEOM002_ALERT_1_A](#) _geom_bond_atom_site_label_2 is missing
Label identifying the atom site 2.

[GEOM003_ALERT_1_A](#) _geom_bond_distance is missing
Distance between atom sites 1 and 2.

[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.

[PLAT043_ALERT_1_A](#) Calculated and Reported Mol. Weight Differ by .. 92.02 Check

[PLAT699_ALERT_1_A](#) Missing _exptl_crystal_description Value Please Do !

Alert level C

[REFI015_ALERT_1_C](#) _refine_ls_shift/su_max is missing
Maximum shift/s.u. ratio after final refinement cycle.
The following tests will not be performed
SHFSU_01

[CRYSC01_ALERT_1_C](#) No recognised colour has been given for crystal colour.

[PLAT041_ALERT_1_C](#) Calc. and Reported SumFormula Strings Differ Please Check

[PLAT415_ALERT_2_C](#) Short Inter D-H..H-X H5 ..H9 . 2.09 Ang.

[PLAT420_ALERT_2_C](#) D-H Without Acceptor N1 --H11 . Please Check

Alert level G

[FORMU01_ALERT_1_G](#) There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is

usually due to the moiety formula being in the wrong format.

Atom count from `_chemical_formula_sum`: H11 B2 Ba1 N1

Atom count from `_chemical_formula_moiety`:

[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`: H11 B2 Ba1 N1

Atom count from the `_atom_site` data: H22 B4 Ba2 N2

[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` BaNB2H11

TEST: Compare cell contents of formula and `atom_site` data

WARNING: Unexpected atom type is in site list: Ba

WARNING: Unexpected atom type is in site list: B

WARNING: Unexpected atom type is in site list: N

WARNING: Formula and `atom_type_symbol` element names mismatch.

atom	Z*formula	cif sites	diff
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BaNB	4.00	0.00	4.00
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H	22.00	44.00	-22.00
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WARNING: Site labels do not match formula elements

[PLAT007 ALERT 5 G](#) Number of Unrefined Donor-H Atoms 3 Report

[PLAT042 ALERT 1 G](#) Calc. and Reported MoietyFormula Strings Differ Please Check

[PLAT045 ALERT 1 G](#) Calculated and Reported Z Differ by a Factor ... 2.00 Check

[PLAT769 ALERT 4 G](#) CIF Embedded explicitly supplied scattering data Please Note

[PLAT982 ALERT 1 G](#) The B-f' = 0.0000 Deviates from IT-value = 0.0013 Check

And 2 other PLAT982 Alerts

More ...

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

- 18 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
- 0 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

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 10/08/2020; check.def file version of 06/08/2020

Datablock BaBH42-NH3 - ellipsoid plot



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