No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: BaBH42-2NH3

Bond precision: = 0.0000 A   Wavelength=0.71073

Cell: a=6.7784(2)   b=6.7175(2)   c=8.6991(3)
             alpha=90   beta=90   gamma=90

Temperature: 248 K

	Calculated	Reported
Volume	396.10(2)	396.10(2)
Space group	P n c 2	P n c 2
Hall group	P 2 -2bc	P 2 -2bc
Moiety formula	H6 N2, 2(B H4), Ba	Ba(Bh4)2(Nh3)2
Sum formula	B2 Ba H14 N2	BaB2N2H14
Mr	201.08	201.08
Dx,g cm-3	1.686	0.000
Z	2	2
Mu (mm-1)	4.903	0.000
F000	188.0	0.0
F000'	187.39	
h,k,lmax	4,4,6	
Nref	153[86]	
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.
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value ....   Please Do !

🟠Alert level B

PLAT415_ALERT_2_B Short Inter D-H..H-X   H3   ..H5   .   1.91 Ang.
                                        1-x,1-y,z =   4_665 Check

🟡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
PLAT353_ALERT_3_C Long   N-H (N0.87,N1.01A) N1   - H5   .   1.05 Ang.
And 2 other PLAT353 Alerts
More ...

PLAT420_ALERT_2_C	D-H Without Acceptor	N1_b	--H6	.	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N1	--H7	.	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: H14 B2 Ba1 N2
         Atom count from _chemical_formula_moiety:
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 BaB2N2H14
         TEST: Compare cell contents of formula and atom_site data
         WARNING: Unexpected atom type is in site list: B
         WARNING: Unexpected atom type is in site list: Ba
         WARNING: Formula and atom_type_symbol element names mismatch.

         atom   Z*formula cif sites diff
         BaB   4.00   0.00   4.00
         N   4.00   4.00   0.00
         H   28.00   28.00   0.00
          WARNING: Site labels do not match formula elements
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   2 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please 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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   6 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
   8 **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

  16 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
   3 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 BaBH42-2NH3 - ellipsoid plot