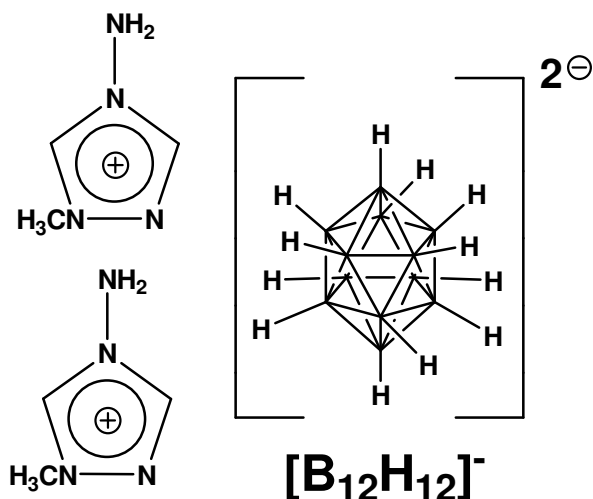




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Datablock: 1

Bond precision: N- C = 0.0040 Å Wavelength=0.71073
Cell: a=7.036(6) b=12.707(10) c=10.176(8)
alpha=90 beta=93.001(10) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	908.6(13)	908.6(12)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	B12 H12, 2(C3 H7 N4)	?
Sum formula	C6 H26 B12 N8	C6 H26 B12 N8
Mr	340.07	340.07
Dx, g cm ⁻³	1.243	1.243
Z	2	2
Mu (mm ⁻¹)	0.071	0.071
F000	356.0	356.0
F000'	356.04	
h, k, lmax	8, 15, 12	8, 15, 12
Nref	1696	1697
Tmin, Tmax	0.981, 0.987	0.981, 0.987
Tmin'	0.981	

Correction method= MULTII-SCAN

Data completeness= 1.001 Theta(max)= 25.460
R(reflections)= 0.0657(1277) wR2(reflections)= 0.1921(1697)
S = 1.030 Npar= 170

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 B

PLAT390_ALERT_3_B	Deviating Methyl C3	X-C-H Bond Angle	123.00
Deg.			
PLAT391_ALERT_3_B	Deviating Methyl C3	H-C-H Bond Angle	99.00
Deg.			
PLAT415_ALERT_2_B	Short Inter D-H..H-X	H4 .. H10 ..	2.08
Ang.			

● Alert level C

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.98
PLAT420_ALERT_2_C	D-H Without Acceptor N4 - H9 ...	?
PLAT194_ALERT_1_C	Missing _cell_measurement_reflms_used datum	?
PLAT195_ALERT_1_C	Missing _cell_measurement_theta_max datum	?
PLAT196_ALERT_1_C	Missing _cell_measurement_theta_min datum	?

● Alert level G

PLAT066_ALERT_1_G	Predicted and Reported Transmissions Identical .	?
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.23

Ratio

0 **ALERT level A** = In general: serious problem

3 **ALERT level B** = Potentially serious problem

5 **ALERT level C** = Check and explain

2 **ALERT level G** = General alerts; check

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

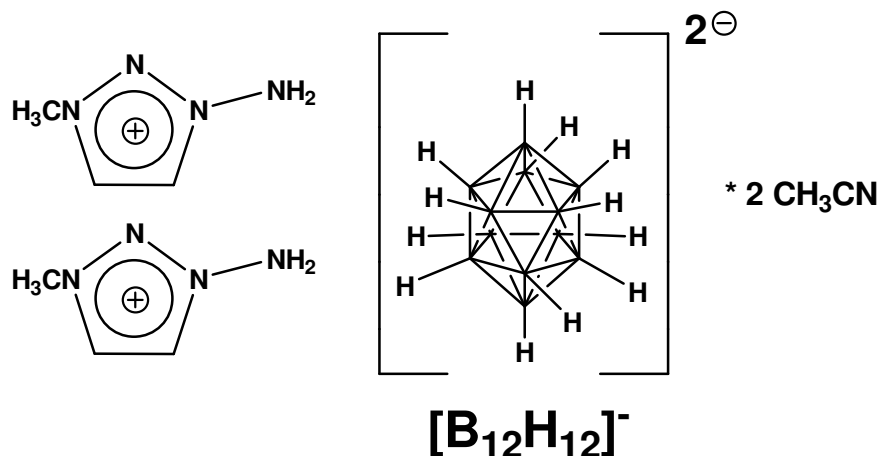
2 ALERT type 2 Indicator that the structure model may be wrong or deficient

3 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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Datablock: 2

Bond precision:	C-C = 0.0045 Å	Wavelength=0.71073
Cell:	a=11.590(5) b=8.959(4) c=12.229(5)	
	alpha=90 beta=102.668(9) gamma=90	
Temperature:	296 K	

	Calculated	Reported
Volume	1238.9(9)	1238.9(9)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	B ₁₂ H ₁₂ , 2(C ₃ H ₇ N ₄), 2(C ₂ H ₃ N)	?
Sum formula	C ₁₀ H ₃₂ B ₁₂ N ₁₀	C ₁₀ H ₃₂ B ₁₂ N ₁₀
Mr	422.18	422.18
Dx, g cm ⁻³	1.132	1.132
Z	2	2
Mu (mm ⁻¹)	0.066	0.066
F ₀₀₀	444.0	444.0
F ₀₀₀ '	444.06	
h, k, l _{max}	15, 11, 16	15, 11, 16
N _{ref}	3044	2895
T _{min} , T _{max}	0.980, 0.989	0.973, 0.989
T _{min} '	0.973	

Correction method= MULTI-SCAN

Data completeness= 0.951 Theta(max)= 28.190

R(reflections)= 0.0628(1676) wR₂(reflections)= 0.1993(2895)

S = 1.036 N_{par}= 168

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 B

PLAT029_ALERT_3_B	_diffn_measured_fraction_theta_full	Low	0.95
PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)		2

Author Response: The molecule consists only of light weight H, C, B and N atoms and there was just no significant intensity at angles >28.19 deg.

● Alert level C

PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	N1
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	N3
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C5
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds (x 1000)	Ang ...	5
PLAT194_ALERT_1_C	Missing _cell_measurement_reflms_used	datum	?
PLAT195_ALERT_1_C	Missing _cell_measurement_theta_max	datum	?
PLAT196_ALERT_1_C	Missing _cell_measurement_theta_min	datum	?

● Alert level G

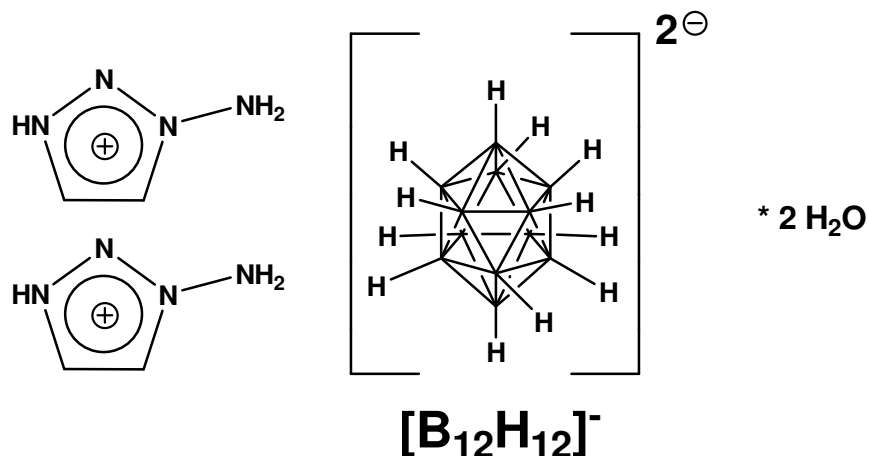
PLAT066_ALERT_1_G	Predicted and Reported Transmissions Identical	.	?
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.21

Ratio

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

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

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Datablock: 3

Bond precision:	C-C = 0.0030 Å	Wavelength=1.54178
Cell:	a=7.3950(5) b=16.8827(12) c=7.3580(7)	
	alpha=90 beta=97.048(5) gamma=90	
Temperature:	296 K	
	Calculated	Reported
Volume	911.69(12)	911.69(12)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	B ₁₂ H ₁₂ , 2(C ₂ H ₅ N ₄), 2(H ₂ O)	?
Sum formula	C ₄ H ₂₆ B ₁₂ N ₈ O ₂	C ₄ H ₂₆ B ₁₂ N ₈ O ₂
Mr	348.05	348.05
Dx, g cm ⁻³	1.268	1.268
Z	2	2
Mu (mm ⁻¹)	0.629	0.629
F000	364.0	364.0
F000'	364.92	
h, k, lmax	8, 19, 8	8, 19, 5
Nref	1555	958
Tmin, Tmax	0.791, 0.860	0.787, 0.860
Tmin'	0.787	
Correction method=	MULTI-SCAN	
Data completeness=	0.616	Theta(max)= 64.730
R(reflections)=	0.0508(936)	wR2(reflections)= 0.1230(958)
S =	1.087	Npar= 171

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

REFLT03_ALERT_3_A	Reflection count < 85% complete (theta max?)	
	From the CIF: <code>_diffn_refl_theta_max</code>	64.73
	From the CIF: <code>_diffn_refl_theta_full</code>	64.73
	From the CIF: <code>_reflns_number_total</code>	958
	TEST2: Reflns within <code>_diffn_refl_theta_max</code>	
	Count of symmetry unique reflns	1555
	Completeness (<code>_total/calc</code>)	61.61%
REFNR01_ALERT_3_A	Ratio of reflections to parameters is < 6 for a centrosymmetric structure	
	<code>sine(theta)/lambda</code>	0.5865
	Proportion of unique data used	1.0000
	Ratio reflections to parameters	5.6023
PLAT022_ALERT_3_A	Ratio Unique / Expected Reflections too Low	0.62
PLAT029_ALERT_3_A	<code>_diffn_meas_fraction_theta_full</code> Low	0.62
PLAT088_ALERT_3_A	Poor Data / Parameter Ratio	5.60

Author Response: The crystal was of very poor quality and the molecule consists only of light weight H, C, B and N atoms which contribute to no significant intensity at high angles.

●Alert level C

THETM01_ALERT_3_C	The value of <code>sine(theta_max)/wavelength</code> is less than 0.590	
	Calculated <code>sin(theta_max)/wavelength</code> =	0.5865
PLAT415_ALERT_2_C	Short Inter D-H...H-X	H4 .. H12 .. 2.12 Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor	N4 - H10 ... ?
PLAT194_ALERT_1_C	Missing <code>_cell_measurement_reflns_used</code> datum	?
PLAT195_ALERT_1_C	Missing <code>_cell_measurement_theta_max</code> datum	?
PLAT196_ALERT_1_C	Missing <code>_cell_measurement_theta_min</code> datum	?
PLAT952_ALERT_1_C	Reported and Calculated Lmax Values Differ by ..	3

●Alert level G

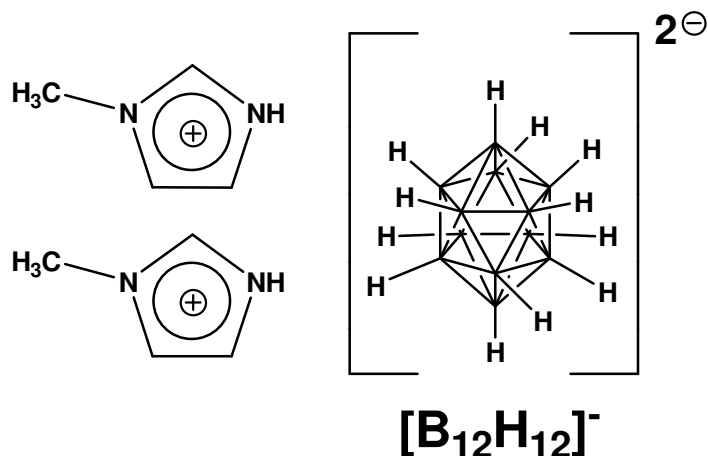
REFLT03_ALERT_1_G	ALERT: Expected hkl max differ from CIF values	
	From the CIF: <code>_diffn_refl_theta_max</code>	64.73
	From the CIF: <code>_reflns_number_total</code>	958
	From the CIF: <code>_diffn_refl_limit_max hkl</code>	8. 19. 5.
	From the CIF: <code>_diffn_refl_limit_min hkl</code>	-8. -13. -5.
	TEST1: Expected hkl limits for theta max	
	Calculated maximum hkl	8. 19. 8.
	Calculated minimum hkl	-8. -19. -8.
PLAT066_ALERT_1_G	Predicted and Reported Transmissions Identical .	?
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.24
	Ratio	

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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

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Datablock: 4

Bond precision:	C-C = 0.0070 Å	Wavelength=0.71073
Cell:	a=7.535(4) b=15.011(7) c=8.168(4)	
	alpha=90 beta=90.329(7) gamma=90	
Temperature:	296 K	

	Calculated	Reported
Volume	923.9(8)	923.8(7)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	B ₁₂ H ₁₂ , 2(C ₄ H ₇ N ₂)	?
Sum formula	C ₈ H ₂₆ B ₁₂ N ₄	C ₈ H ₂₆ B ₁₂ N ₄
Mr	308.05	308.05
Dx, g cm ⁻³	1.107	1.107
Z	2	2
Mu (mm ⁻¹)	0.058	0.058
F ₀₀₀	324.0	324.0
F ₀₀₀ '	324.04	
h, k, l _{max}	10, 19, 10	9, 19, 10
N _{ref}	2255	2050
T _{min} , T _{max}	0.993, 0.995	0.970, 0.995
T _{min} '	0.970	

Correction method= MULTI-SCAN

Data completeness= 0.909 Theta(max)= 28.160

R(reflections)= 0.0785(1397) wR2(reflections)= 0.1725(2050)

S = 1.195 Npar= 139

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

[PLAT029_ALERT_3_A](#) _diffn_measured_fraction_theta_full Low 0.91

Author Response: The crystal was rather small and the molecule consists only of light weight H, C, B and N atoms and there was just no significant intensity at angles >28.16 deg.

●Alert level B

[PLAT031_ALERT_4_B](#) Refined Extinction Parameter within Range 1.00
Sigma

●Alert level C

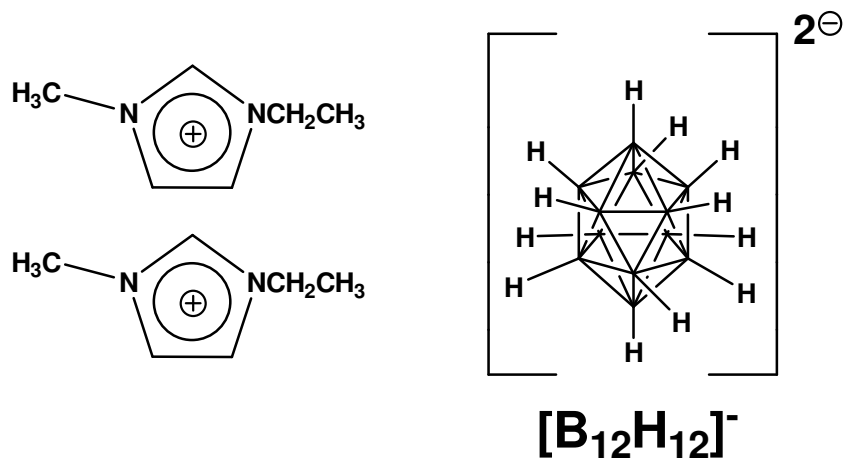
[REFLT03_ALERT_3_C](#) Reflection count < 95% complete
From the CIF: _diffn_reflms_theta_max 28.16
From the CIF: _diffn_reflms_theta_full 28.16
From the CIF: _reflns_number_total 2050
TEST2: Reflms within _diffn_reflms_theta_max
Count of symmetry unique reflms 2255
Completeness (_total/calc) 90.91%
[PLAT242_ALERT_2_C](#) Check Low Ueq as Compared to Neighbors for N1
[PLAT245_ALERT_2_C](#) U(iso) H5 Smaller than U(eq) B5 by ... 0.01
AngSq
[PLAT340_ALERT_3_C](#) Low Bond Precision on C-C Bonds (x 1000) Ang ... 7
[PLAT415_ALERT_2_C](#) Short Inter D-H..H-X H2 .. H7 .. 2.11
Ang.
[PLAT152_ALERT_1_C](#) Supplied and Calc Volume s.u. Inconsistent ?
[PLAT194_ALERT_1_C](#) Missing _cell_measurement_reflms_used datum ?
[PLAT195_ALERT_1_C](#) Missing _cell_measurement_theta_max datum ?
[PLAT196_ALERT_1_C](#) Missing _cell_measurement_theta_min datum ?

●Alert level G

[PLAT066_ALERT_1_G](#) Predicted and Reported Transmissions Identical . ?
[PLAT720_ALERT_4_G](#) Number of Unusual/Non-Standard Labels 3
[PLAT764_ALERT_4_G](#) Overcomplete CIF Bond List Detected (Rep/Expd) . 1.24
Ratio

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

5 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
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check



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Datablock: 5

Bond precision: C-C = 0.0030 A Wavelength=0.71073
Cell: a=8.2681(17) b=8.6731(16) c=8.8457(16)
alpha=69.757(2) beta=84.526(2) gamma=67.521(1)
Temperature: 296 K

	Calculated	Reported
Volume	549.43(18)	549.43(18)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	B ₁₂ H ₁₂ , 2(C ₆ H ₁₁ N ₂)	?
Sum formula	C ₁₂ H ₃₄ B ₁₂ N ₄	C ₁₂ H ₃₄ B ₁₂ N ₄
Mr	364.15	364.15
Dx, g cm ⁻³	1.101	1.101
Z	1	1
Mu (mm ⁻¹)	0.058	0.058
F000	194.0	194.0
F000'	194.03	
h, k, lmax	11, 11, 11	10, 11, 11
Nref	2766	2514
Tmin, Tmax	0.981, 0.991	0.978, 0.991
Tmin'	0.978	

Correction method= MULTI-SCAN

Data completeness= 0.909 Theta(max)= 28.440

R(reflections)= 0.0495(2207) wR2(reflections)= 0.1501(2514)

S = 1.078 Npar= 196

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

[PLAT029_ALERT_3_A](#) _diffn_measured_fraction_theta_full Low 0.91

Author Response: The molecule consists only of light weight H, C, B and N atoms and there was just no significant intensity at angles >28.44 deg.

Alert level C

[REFLT03_ALERT_3_C](#) Reflection count < 95% complete

From the CIF: _diffn_reflms_theta_max 28.44

From the CIF: _diffn_reflms_theta_full 28.44

From the CIF: _reflns_number_total 2514

TEST2: Reflms within _diffn_reflms_theta_max

Count of symmetry unique reflms 2766

Completeness (_total/calc) 90.89%

[PLAT194_ALERT_1_C](#) Missing _cell_measurement_reflms_used datum ?

[PLAT195_ALERT_1_C](#) Missing _cell_measurement_theta_max datum ?

[PLAT196_ALERT_1_C](#) Missing _cell_measurement_theta_min datum ?

Alert level G

[PLAT066_ALERT_1_G](#) Predicted and Reported Transmissions Identical . ?

[PLAT764_ALERT_4_G](#) Overcomplete CIF Bond List Detected (Rep/Expd) . 1.22

Ratio

1 **ALERT level A** = In general: serious problem

0 **ALERT level B** = Potentially serious problem

4 **ALERT level C** = Check and explain

2 **ALERT level G** = General alerts; check

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

2 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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