

1441
MW

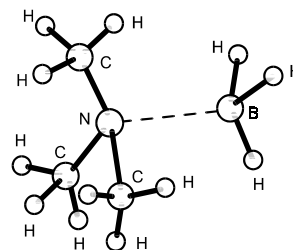
C₃H₁₂BN

Trimethylamine – borane (1/1)

C_{3v} (staggered
H₃B · NC₃ fragment)
(CH₃)₃N · BH₃

r_s	Å	θ_s	deg
B...N	1.638(10)	C–N...B	107.9(10)
C–N	1.483(10)	N...B–H	105.32(16)
B–H	1.211(3)		

Atom	z [Å] ^{a)}
N	–0.0042
B	1.6335



^{a)} Coordinates in principal axis system of (CH₃)₃¹⁴N · BH₃.

Cassoux, P., Kuczkowski, R.L., Bryan, P.S., Taylor, R.C.: Inorg. Chem. **14** (1975) 126.

ED, MW

r_g	Å ^{a)}	θ_α	deg ^{a)}
B...N	1.656(2)	N–C–H	109.0(2)
C–N	1.485(1)	H–B–H ^{b)}	113.4(4)
B–H	1.261(6)	C–N–C ^{b)}	109.4(2)
C–H	1.108(2)		

The potential barrier around the N...B bond was estimated to be higher than 5 kcal mol^{–1}.
The nozzle temperature was 346 K.

^{a)} Estimated limits of error.

^{b)} Dependent parameter.

Iijima, K., Adachi, N., Shibata, S.: Bull. Chem. Soc. Jpn. **57** (1984) 3269.