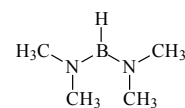


612 **C₄H₁₃BN₂**
ED, *ab initio* and DFT
calculations

***N,N,N',N'*-Tetramethylboranediamine**
Bis(dimethylamino)borane

C₂



| r_a | \AA^a | θ_a | deg a |
|-------------------|---------------------|---------------------|--------------------|
| B-H | 1.217 ^{b)} | N-B-N | 127.8(5) |
| B-N | 1.425(4) | B-N-C(1) | 119.9(3) |
| N-C(1) | 1.456(2) | B-N-C(2) | 127.3(2) |
| N-C(2) | 1.454 ^{c)} | N-C-H(1) | 110.3(2) |
| C-H ^{d)} | 1.106(1) | N-B-H | 116.1(2) |
| | | C-N-C | 112.7(3) |
| | | N-C-H ^{d)} | 111.4(2) |
| | | C(1)-N-B-N | -167.6(12) |
| | | C(2)-N-B-N | 14.7(15) |
| | | H(1)-C(1)-N-B | -3.1 ^{b)} |
| | | H(4)-C(2)-N-B | 13.9 ^{b)} |

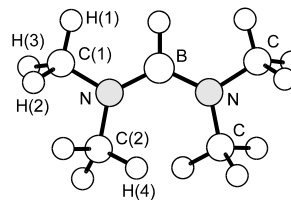
The nozzle temperature was 298 K.

^{a)} Estimated standard errors including a systematic error.

^{b)} Assumed at the value from 3PW91/6-311++G** calculations.

^{c)} Difference between the N-C(1) and N-C(2) bond lengths was assumed at the value from B3PW91/6-311++G** calculations.

^{d)} Average value.



Østby, K.-A., Fjeldberg, T., Gundersen, G.: J. Mol. Struct. **567-568** (2001) 247.