

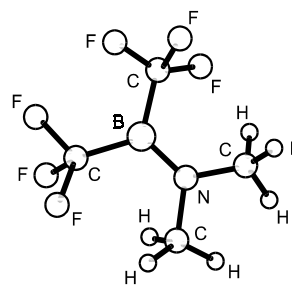
1620  
ED

**C<sub>4</sub>H<sub>6</sub>BF<sub>6</sub>N**

**(Dimethylamino)bis(trifluoromethyl)borane**

**C<sub>2</sub> assumed**  
(CF<sub>3</sub>)<sub>2</sub>B–N(CH<sub>3</sub>)<sub>2</sub>

| $r_a$ | Å <sup>a)</sup> | $\theta_a$            | deg <sup>a)</sup> |
|-------|-----------------|-----------------------|-------------------|
| B–C   | 1.623(4)        | C–B–C                 | 122.2(15)         |
| B–N   | 1.425(18)       | C–N–C                 | 110.7(37)         |
| C–N   | 1.453(7)        | F–C–F                 | 106.5(2)          |
| C–F   | 1.343(2)        | H–C–H                 | 108.9(14)         |
| C–H   | 1.079(9)        | $\tau(\text{N–C})^b)$ | 10 <sup>c)</sup>  |
|       |                 | $\tau(\text{B–N})^d)$ | 0 <sup>c)</sup>   |
|       |                 | $\tau(\text{B–C})^e)$ | 15.1(11)          |



C<sub>3v</sub> symmetry for the CF<sub>3</sub> and CH<sub>3</sub> groups and a planar configuration of the dimethylamino group were assumed. The CF<sub>3</sub> groups were assumed to be rotated around the B–C bonds in opposite directions, resulting in C<sub>2</sub> overall symmetry. These torsional angles should be considered effective values. The nozzle temperature was 30 °C.

<sup>a)</sup> Three times the estimated standard errors including a systematic error.

<sup>b)</sup> Torsional angle around the N–C bonds; for  $\tau(\text{N–C}) = 0^\circ$  two C–H bonds are staggered with respect to the B–N bond. The two N(CH<sub>3</sub>)<sub>2</sub> groups are rotated in opposite directions resulting in C<sub>2</sub> symmetry for the BN(CH<sub>3</sub>)<sub>2</sub> moiety.

<sup>c)</sup> Assumed.

<sup>d)</sup> Torsional angle around the B–N bond;  $\tau(\text{B–N}) = 0^\circ$  corresponds to the planar heavy-atom skeleton.

<sup>e)</sup> Torsional angle around the B–C bonds; for  $\tau(\text{B–C}) = 0^\circ$  two C–F bonds are staggered with respect to the B–N bond.

Hausser-Wallis, R., Oberhammer, H., Bürger, H., Pawelke, G.: J. Chem. Soc., Dalton Trans. (1987) 1839.