

1700  
MW

**C<sub>4</sub>H<sub>7</sub>N**

**3-Butynylamine**  
3-Butyn-1-amine

**C<sub>1</sub>** (conformer I)  
**C<sub>1</sub>** (conformer II)  
HC≡C-CH<sub>2</sub>-CH<sub>2</sub>-NH<sub>2</sub>

$r_0$	Å	$\theta_0$	deg
C(1)≡C(2)	1.207 <sup>a)</sup>	C(3)-C(2)≡C(1)	180.00 <sup>a)</sup>
C(1)-H	1.060 <sup>a)</sup>	H-C(1)≡C(2)	180.00 <sup>a)</sup>
C(2)-C(3)	1.459 <sup>a)</sup>	C(2)-C(3)-H	109.47 <sup>a)</sup>
C(3)-C(4)	1.548 <sup>a)</sup>	C(2)-C(3)-C(4)	111.70 <sup>a)</sup>
C(4)-N	1.475 <sup>a)</sup>	C(4)-N-H	111.00 <sup>a)</sup>
C-H	1.091 <sup>a)</sup>	C(3)-C(4)-N	108.3(15) (I)
N-H	1.017 <sup>a)</sup>		113.5(15) (II)
		C(3)-C(4)-N-H <sup>b)</sup>	60 or 180 <sup>a)</sup>
		C(2)-C(3)-C(4)-N <sup>b)</sup>	63(3) (I)
			60(3) (II)

Conformer I is more stable than II  
and any other by 1.5(20) and at least  
3 kJ mol<sup>-1</sup>, respectively.

<sup>a)</sup> Assumed.

<sup>b)</sup> From *syn*.

Braathen, O.-A., Marstokk, K.-H.,  
Møllendal, H.: Acta Chem. Scand.,  
Ser. A **39** (1985) 209.

