

1111  
MW

**C<sub>3</sub>H<sub>3</sub>N**

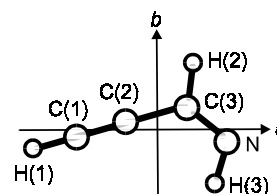
**(Z)-2-Propynimine**  
(Z)-2-Propynylideneamine

**C<sub>s</sub>**  
HC≡C–CH=NH

$r_s$	Å	$\theta_s$	deg
C(1)–H	1.057(3)	H–C(1)≡C(2)	179.3(8)
C(1)≡C(2)	1.207(6)	C(1)≡C(2)–C(3)	180.8(11)
C(2)–C(3)	1.431(6)	C(2)–C(3)–H	123.3(10)
C(3)–H	1.101(34)	C(2)–C(3)=N	125.38(20)
C(3)=N	1.286(6)	C(3)=N–H	108.89(60)
N–H	1.039(3)		

$r_0$	Å	$\theta_0$	deg
C(1)–H	1.058(1)	H–C(1)≡C(2)	179.3 <sup>a)</sup>
C(1)≡C(2)	1.208(1)	C(1)≡C(2)–C(3)	180.8 <sup>a)</sup>
C(2)–C(3)	1.431(1)	C(2)–C(3)–H	121.4(17)
C(3)–H	1.126(12)	C(2)–C(3)=N	125.2(2)
C(3)=N	1.293(2)	C(3)=N–H	108.8(2)
N–H	1.034(2)		

Atom	$a_s$ [Å]	$b_s$ [Å]
H(1)	–2.898	–0.450
C(1)	–1.875	–0.180
C(2)	–0.704	0.115
C(3)	0.680	0.482
H(2)	1.027	1.527
N	1.669	–0.341
H(3)	1.299	–1.312



<sup>a)</sup> Assumed.

McNaughton, D., Osman, O.I., Kroto, K.W.: J. Mol. Struct. **190** (1988) 195.

See also: Sugie, M., Takeo, H., Matsumura, C.: J. Mol. Spectrosc. **111** (1985) 83.