

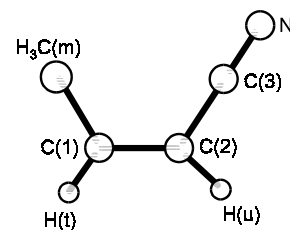
1588  
MW

**C<sub>4</sub>H<sub>5</sub>N**

**(Z)-2-Butenenitrile**  
Isocrotononitrile

**C<sub>s</sub>**  
**H<sub>3</sub>C–CH=CH–C≡N**

$r_e^a)$	$\text{\AA}^b)$	$\theta_e^a)$	deg <sup>b)</sup>
C(3)≡N	1.158(3)	C(1)=C(2)–C(3)	122.4(3)
C(1)=C(2)	1.341(5)	C(2)=C(1)–C(m)	125.6(5)
C(2)–C(3)	1.431(3)	C(1)=C(2)–H(u)	121.0(3)
C(1)–C(m)	1.490(5)	C(2)=C(1)–H(t)	117.1(5)
C(2)–H(u)	1.081(5)	C(1)–C(m)–H(s)	111.7(5)
C(1)–H(t)	1.084(5)	C(1)–C(m)–H(a)	110.2(5)
C(m)–H(s)	1.088(5)	C(2)–C(3)≡N	179.6(5)
C(m)–H(a)	1.091(5)	C(2)=C(1)–C(m)–H(a)	121.0(5)



<sup>a)</sup> A near-equilibrium structure was estimated using offsets derived empirically.

<sup>b)</sup> Uncertainties were not estimated in the original paper.

Lesarri, A.G., Cosleou, J., Li, X., Wlodarczak, G., Demaison, J.: J. Mol. Spectrosc. **172** (1995) 520.