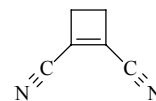


702
MW $C_6H_4N_2$ **1-Cyclobutene-1,2-dicarbonitrile**
1,2-Dicyanocyclobutene C_{2v} 

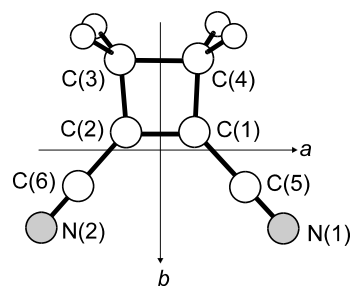
r_s	Å
C(1)=C(2)	1.326(2) ^{a)}
C(1)–C(4)	1.522(3)
C(3)–C(4)	1.578(2)
C(1)–C(5)	1.426(2)
C(5)≡N(1)	1.159(1)

θ_s	deg
C(2)=C(1)–C(4)	94.7(2)
C(1)–C(4)–C(3)	85.3(1)
C(1)–C(5)≡N(1) ^{b)}	178.6(12)

r_0	Å ^{c)}
C(1)=C(2)	1.361(4)
C(1)–C(4)	1.515(5)
C(3)–C(4)	1.567(4)
C(1)–C(5)	1.420(4)
C(5)≡N(1)	1.157(2)
C(4)–H	1.088(5)

θ_0	deg ^{c)}
C(2)=C(1)–C(4)	93.9(4)
C(1)–C(4)–C(3)	86.1(2)
C(4)–C(1)–C(5)	133.3(5)
C(1)–C(5)≡N(1) ^{b)}	178.2(15)
C(1)–C(4)–H	114.7(10)
C(2)=C(1)–C(4)–H ^{d)}	115.8(10)

Atom	a_s [Å]	b_s [Å]
C(1,2)	±0.6633	−0.3057
C(4,3)	±0.7888	−1.8222
C(5,6)	±1.6522	0.7214
N(1,2)	±2.4763	1.5360



^{a)} This bond length was commented by the authors to be unreliable.

^{b)} Bent outwards.

^{c)} Uncertainties were not estimated in the original paper.

^{d)} Dihedral angle.

Petitprez, D., Wlodarczak, G., Lignier, H., Demaison, J., de Meijere, A., Steinig, A.G., Møllendal, H.: J. Mol. Struct. **612** (2002) 315; Erratum: J. Mol. Struct. **649** (2003) 69.