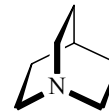


812
MW $C_7H_{13}N$ 1-Azabicyclo[2.2.2]octane
Quinuclidine C_{3v}
(effective symmetry class)

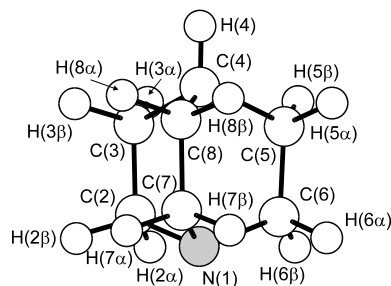
r_0	\AA
C(2)–C(3)	1.565(2)
C(3)–C(4)	1.532(2)
C(2)–N	1.463(2)
C(<i>i</i>)–H(<i>i</i>) ^b	1.118(8)

θ_0	deg
C(4)–C(3)–C(2)	108.04(9)
C(3)–C(2)–N	111.83(9)
C(3)–C(2)–H(2 α)	108.60 ^a
C(2)–C(3)–H(3 α)	109.05 ^a
N–C(2)–H(2 β)	109.14 ^a
C(4)–C(3)–H(3 α)	110.58 ^a

r_s	\AA
C(2)–C(3)	1.552(14)
C(3)–C(4)	1.529(7)
C(2)–N	1.466(7)

θ_s	deg
C(4)–C(3)–C(2)	108.32(55)
C(3)–C(2)–N	111.85(53)

Atom	a_0 [\AA]	b_0 [\AA]	c_0 [\AA]
C(4)	1.3101	0.0	0.0
C(3)	0.7803	–1.4377	0.0
C(5)	0.7803	0.7189	1.2451
C(8)	0.7803	0.7189	–1.2451
C(2)	–0.7832	–1.3780	0.0
C(6)	–0.7832	0.6890	1.1933
C(7)	–0.7832	0.6890	–1.1933
N	–1.2749	0.0	0.0
H(4)	2.4283	0.0	0.0
H(3 α)	1.246	–1.9836	0.9132
H(3 β)	1.246	–1.9836	–0.9132
H(5 α)	1.246	1.7826	1.2612
H(5 β)	1.246	0.2010	2.1744
H(8 α)	1.246	0.2010	–2.1744
H(8 β)	1.246	1.7826	–1.2612
H(2 α)	–1.1601	–1.9018	0.9132
H(2 β)	–1.1601	–1.9018	–0.9132
H(6 α)	–1.1601	1.7417	1.1904
H(6 β)	–1.1601	0.1601	2.1036
H(7 α)	–1.1601	0.1601	–2.1036
H(7 β)	–1.1601	1.7417	–1.1904

^a) Assumed.^b) $i = 2, 3$ and 4 .Consalvo, D., Stahl, W.: J. Mol. Struct. **447** (1998) 119.[II/25D \(3, 2498\)](#)