

1611
MW

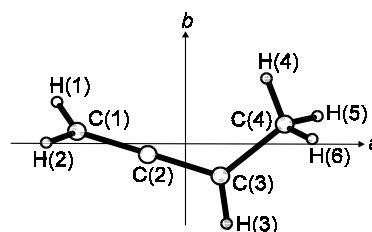
C₄H₆

1,2-Butadiene

C_s
H₃C–CH=C=CH₂

r_s	Å	θ_s	deg
C(1)=C(2)	1.313(11)	C(1)=C(2)=C(3)	179.5(9)
C(2)=C(3)	1.301(11)	C(2)=C(3)–C(4)	124.0(11)
C(3)–C(4)	1.515(10)	C(2)=C(1)–H(1)	120.9(9)
C(1)–H(1,2)	1.083(17)	H(1)–C(1)–H(2)	118.2(19)
C(3)–H(3)	1.088(6)	C(2)=C(3)–H(3)	117.8(11)
C(4)–H(4)	1.089(8)	C(3)–C(4)–H(4)	110.6(4)
C(4)–H(5,6)	1.097(20)	C(3)–C(4)–H(5,6)	110.5(24)
		H(4)–C(4)–H(5,6)	109.0(28)
		H(5)–C(4)–H(6)	107.3(23)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(1)	–1.9009	0.2400	0.0
C(2)	–0.6517	–0.1649	0.0
C(3)	0.5893	–0.5553	0.0
C(4)	1.7751	0.3880	0.0
H(1)	–2.4323	0.4045	0.9290
H(2)	–2.4323	0.4045	–0.9290
H(3)	0.7837	–1.6256	0.0
H(4)	1.4409	1.4242	0.0
H(5)	2.4022	0.2158	0.8832
H(6)	2.4022	0.2158	–0.8832



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