

1653
MW

C₄H₆O

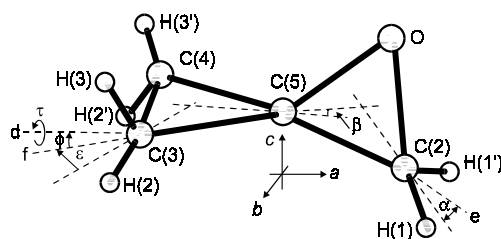
1-Oxaspiro[2.2]pentane

C_s

r_s	Å	θ_s	deg
C(2)–C(5)	1.447(6)	H–C(2)–H	117.0(1)
C(2)–H	1.806(1)	H–C(3)–H	115.0(1)
C(2)–O	1.460(4)	C(2)–O–C(5)	60.4(3)
C(3)–C(4)	1.550(2)	C(2)–C(5)–O	61.3(5)
C(3)–H(2)	1.080(1)	C(3)–C(5)–C(4)	63.6(3)
C(3)–H(3)	1.075(2)	C(5)–C(2)–O	58.3(4)
C(5)–C(3)	1.470(9)	C(5)–C(3)–C(4)	58.2(2)
C(5)–O	1.416(10)	H–C(2)–C(5)	119.5(1)
		H–C(2)–O	114.1(1)
		H(2)–C(3)–H(5)	118.9(2)
		H(2)–C(3)–C(4)	116.9(1)
		H(3)–C(3)–C(5)	118.0(3)
		H(3)–C(3)–C(4)	116.9(1)
		C(2)–C(5)–C(3)	142.5(2)
		C(4)–C(5)–O	130.3(3)
		α^a	9.61(32)
		β^b	9.75(45)
		ε^c	1.57(9)
		ϕ^d	0.68(17)
		τ^e	0.24(24)



Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(5)	–0.0174	0.0	–0.0943
C(2)	1.3032	0.0	–0.6859
H(1)	1.7140	0.9259	–1.0778
H(1')	1.7140	–0.9259	–1.0778
O	1.1100	0.0	0.7616
C(3)	–1.2646	0.7751	–0.0242
H(3)	–1.5051	1.2607	0.9039
H(2)	–1.6132	1.2857	–0.9104
C(4)	–1.2646	–0.7751	–0.0242
H(3')	–1.5051	–1.2607	0.9039
H(2')	–1.6132	–1.2857	–0.9104



Lines “d” and “e” are the bisectors of the HC(3)H and HC(2)H methylene groups, respectively. Line “f” is the projection of the line “d” onto the C(3)C(4)C(5) plane.

- ^a) Angle between plane HC(2)H [C(2)–e on the HC(2)H plane] and bisector of angle C(5)–C(2)–O. Methylene group moved toward oxygen.
- ^b) Angle between plane C(3)C(4)C(5) and bisector of angle C(2)–C(5)–O.
- ^c) Angle formed by projection [C(3)–f] of angle H–C(3)–H bisector [C(3)–d] onto the C(3)C(4)C(5) plane and bisector of angle C(5)–C(3)–C(4). Methylene groups moved toward each other.
- ^d) Angle between bisector of angle H–C(3)–H and its projection onto the C(3)C(4)C(5) plane. Methylene bisectors moved toward oxygen.
- ^e) Twist angle about angle H–C(3)–H bisector, defined as angle between the normal to the HC(3)H plane and the projection of the normal onto the C(3)C(4)C(5) plane.

Slafer, W.D., English, A.D., Harris, D.O., Shellhamer, D.F., Meshishnek, M.J., Aue, D.H.:
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