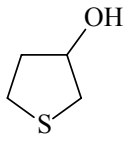
564 **C_4H_8OS** **3-Hydroxytetrahydrothiophene** **C_1**

MW, *ab initio* calculations

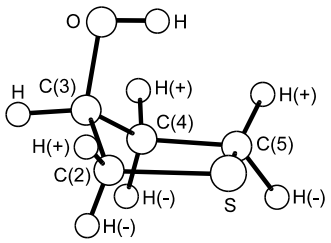
Tetrahydrothiophene-3-ol



r_0	Å
S–C(2)	1.826(7)
C(2)–C(3)	1.531(26)
C(3)–C(4)	1.521(15)
C(4)–C(5)	1.544(8)
C(2)–H	1.095 [a])
C(3)–H	1.097 [a])
C(3)–O	1.428(9)
C(4)–H	1.096 [a])
C(5)–H	1.094 [a])
O–H	0.965 [a])

θ_0	deg
S–C(2)–C(3)	104.6(8)
C(2)–C(3)–C(4)	105.4(12)
C(3)–C(4)–C(5)	107.1(3)
C(4)–C(5)–S	106.6(3)
S–C(2)–H(+)	109.4 [a])
S–C(2)–H(–)	110.9 [a])
H–C(2)–H	109.3 [a])
C(2)–C(3)–H	110.9(11)
C(2)–C(3)–O	111.0(18)
H–C(3)–O	106.2 [a])
C(3)–O–H	105.8 [a])
C(3)–C(4)–H(+)	110.8 [a])
C(3)–C(4)–H(–)	109.2 [a])
H–C(4)–H	108.7 [a])
C(4)–C(5)–H(+)	111.1 [a])
C(4)–C(5)–H(–)	112.1 [a])
H–C(5)–H	108.2 [a])
C(4)–C(5)–S–C(2) [b])	–2.3(7)
C(3)–C(4)–C(5)–S [b])	29.3(10)
C(2)–C(3)–C(4)–C(5) [b])	–48.8(10)
S–C(2)–C(3)–C(4) [b])	45.5(10)
C(5)–S–C(2)–C(3) [b])	–24.7(10)
S–C(2)–C(3)–H [b])	166.4(10)
S–C(2)–C(3)–O [b])	–75.8(10)
C(2)–C(3)–O–H [b])	43.8 [a])
C(2)–C(3)–C(4)–H(+) [b])	–170.7(10)
C(2)–C(3)–C(4)–H(–) [b])	69.6(10)
C(3)–C(4)–C(5)–H(+) [b])	–88.0 [a])
C(3)–C(4)–C(5)–H(–) [b])	150.8 [a])
C(5)–S–C(2)–H(+) [b])	–144.4 [a])
C(5)–S–C(2)–H(–) [b])	94.9 [a])

The structure was found to have C(3) puckered out of plane, and it is stabilized by a 2.634 Å hydrogen bond from the hydroxyl group to the thioether.



[a]) Assumed.
[b]) Dihedral angle.

Torok, C.R., Lavrich, R.J., Tubergen, M. J.: Chem. Phys. **283** (2002) 125.