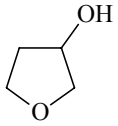
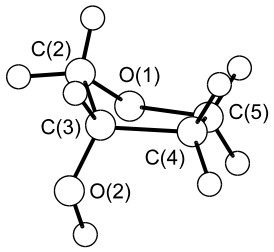
**567** **$C_4H_8O_2$** **3-Hydroxytetrahydrofuran** **$C_1$**
MW Tetrahydro-3-furanol




| $r_0$ | Å |
|---|---|
| C–H | 1.100 [a]) |
| O(1)–C(5) | 1.434(20) |
| C(4)–C(5) | 1.566(30) |
| C(3)–C(4) | 1.526(31) |
| C(2)–C(3) | 1.521(23) |
| C(2)–O(1) | 1.438(65) |
| C(3)–O(2) | 1.418 [a]) |
| O(2)–H | 0.965 [a]) |

| $\theta_0$ | deg |
|---|---|
| H–C–H | 109.0 [a]) |
| O–C(5)–C(4) | 106.1(11) |
| C(3)–C(4)–C(5) | 103.1(5) |
| C(2)–C(3)–C(4) | 101.9(23) |
| C(3)–C(2)–O | 102.9(28) |
| C(2)–O–C(5) | 105.5(26) |
| H–C(3)–O(2) | 106.9 [a]) |
| C(3)–O(2)–H | 104.5 [a]) |
| C(2)–O–C(5)–C(4) [b]) | 28.6(20) |
| O–C(5)–C(4)–C(3) [b]) | –1.3(16) |
| C(5)–C(4)–C(3)–C(2) [b]) | –24.4(10) |
| C(4)–C(3)–C(2)–O [b]) | 42.6(20) |
| C(3)–C(2)–O–C(5) [b]) | –44.9(20) |
| H–C(5)–O–C(2) [b]) | 152.6 [a]) |
| H–C(4)–C(5)–O [b]) | 117.5 [a]) |
| O–C(3)–C(4)–C(5) [b]) | 94.8(20) |
| H–C(2)–C(3)–C(4) [b]) | 161.6 [a]) |
| H–C(3)–O(2)–H [b]) | 169.2 [a]) |

| Atom | $a_0$ [Å] | $b_0$ [Å] | $c_0$ [Å] |
|---|---|---|---|
| C(5) | –1.391 | –0.590 | 0.285 |
| C(4) | –0.122 | –1.277 | –0.325 |
| C(3) | 0.847 | –0.113 | –0.510 |
| C(2) | –0.103 | 1.071 | –0.611 |
| O(1) | –1.065 | 0.799 | 0.422 |
| O(2) | 1.736 | 0.030 | 0.586 |




The best-fit structure is a $C_4$-*endo* envelope ring conformation shown in the figure.

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

Lavrich, R.J., Rhea, R.L., McCargar, J.W., Tubergen, M.J.: J. Mol. Spectrosc. **199** (2000) 138.