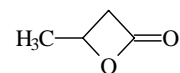


1663 **C₄H₆O₂**
 MW, *ab initio* calculations
 (HF/3-21G, 4-31G)

4-Methyl-2-oxetanone

C₁

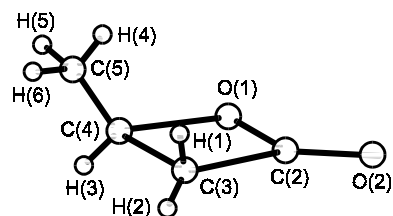


r_0	Å ^{a)}	θ_0	deg ^{a)}
C(2)=O(2)	1.169(50)	O(1)-C(2)-C(3)	92.4(50)
C(3)-C(2)	1.520(50)	O(1)-C(4)-C(3)	92.4(50)
C(2)-O(1)	1.430(50)	C(4)-O(1)-C(2)	91.0(50)
C(4)-O(1)	1.430(50)	C(4)-C(3)-C(2)	84.3(50)
C(4)-C(3)	1.520(50)	O(1)-C(2)=O(2)	133.8(50)
C(4)-C(5)	1.520(50)	C(3)-C(2)=O(2)	133.8(50)
C(3)-H(1,2)	1.095(50)	O(1)-C(4)-C(5)	108.7(50)
C(4)-H(3)	1.095(50)	C(2)-C(4)-C(5)	117.7(50)
C(5)-H(4,5,6)	1.090(50)	H(3)-C(4)-O(1)	113.6(50)
		H(3)-C(4)-C(2)	113.6(50)
		H(1,2)-C(3)-C(4)	115.3(50)
		H(1,2)-C(3)-C(2)	115.3(50)
		H(4,5,6)-C(5)-C(4)	109.5(50)
		H(4)-C(5)-C(4)-O(1)	54.3 ^{b)}
		H(4)-C(5)-C(4)-C(3)	45.5 ^{b)}

The structure was estimated using the assumptions that the ring structure could be transferable from 2-oxetanone [1] and a standard methyl group.

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Fixed at the *ab initio* (HF/4-31G) value.



González, E., López, J.C., Alonso, J.L.: J. Mol. Struct. **223** (1990) 365.

[1] Boggia, L.M., Sorriarain, O.M., Fornes, J.A., Villani, M.C.: Z. Phys. Chem. (Leipzig) **255** (1974) 44.