

559
MW $\text{C}_4\text{H}_8\text{O}$

3-Buten-1-ol

 C_1 (conformer I) C_1 (conformer II)

θ_0	deg ^{a)}	
	conformer I	conformer II
$\text{C}(1)-\text{C}(2)-\text{C}(3)=\text{C}(4)$ ^{b)}	-107.4(5)	-113.9(5)
$\text{C}(3)-\text{C}(2)-\text{C}(1)-\text{O}$ ^{b)}	64.3(5)	183.1(5)
$\text{C}(2)-\text{C}(1)-\text{O}-\text{H}$ ^{b)}	-49.7(5)	181.5(5)

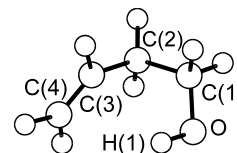
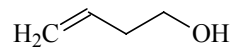
Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_0 $ [Å]
conformer I			
H(1)	0.4148	1.4228	0.2555
conformer II			
H(1)	2.955	0.355	0.405

Conformer I (CMG) and conformer II (CAA) were detected. Relaxation of the extended conformers including conformer II to the more stable *gauche* (CMG) is precluded by high intervening energy barriers.

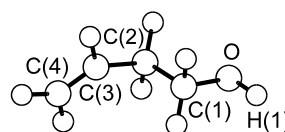
^{a)} Uncertainties were not estimated in the original paper.

^{b)} Dihedral angle.

Crofts, J.G., Brown, R.D., Godfrey, P.D.: J. Phys. Chem. A **103** (1999) 3629.



conformer I (CMG)



conformer II (CAA)

[II/25C \(3, 1740\)](#)