

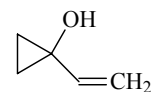
648
MW $\text{C}_3\text{H}_8\text{O}$

1-Ethenylcyclopropan-1-ol

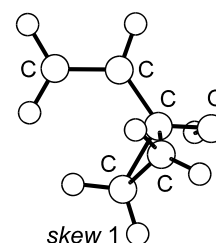
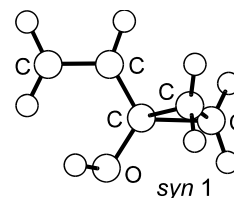
1-Vinylcyclopropan-1-ol

 C_1 (*syn* 1) C_1 (*skew* 1)

θ_0	deg ^{a)}	
	<i>syn</i> 1	<i>skew</i> 1
$\text{C}=\text{C}-\text{O}-\text{C}^{\text{b)}$	-2.6(5)	132.1(5)
$\text{H}-\text{O}-\text{C}-\text{C}^{\text{b)}$	-67.2(5)	-67.1(5)



Two conformers, (*ac-ap*) denoted as *syn* 1 and (*ac-sc*1) as *skew* 1, were assigned. Each of these forms is stabilized with an intramolecular hydrogen bond formed between the H atom of the OH group and the π electrons of the double bond. *Syn* 1 is more stable than *skew* 1 by 4.9(6) kJ mol^{-1} . The spectrum of *syn* 1 is perturbed by tunneling of the OH group. An analysis yielded 2280.184(60) MHz for the tunneling frequency and 39.82(19) MHz for the Coriolis coupling term for the normal species. The corresponding values were 72.401(27) and 5.2(10) MHz for the OD species. A potential function for the tunneling motion consisting of three cosine terms gave the following constants: $V_1 = -918.2 \text{ cm}^{-1}$, $V_2 = -900.0 \text{ cm}^{-1}$, and $V_3 = 418.0 \text{ cm}^{-1}$. The double-minimum function yielded barriers of 16.6(50) kJ mol^{-1} at the *anti* position and 10.6(30) kJ mol^{-1} at *syn*.



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

^{b)} Dihedral angle, measured from *syn*.

Leonov, A., Marstokk, K.-M., de Meijere, A., Møllendal, M.: J. Phys. Chem. A **104** (2000) 4421.