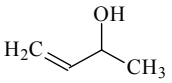
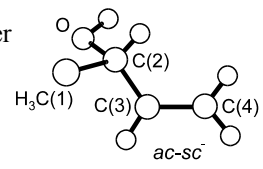
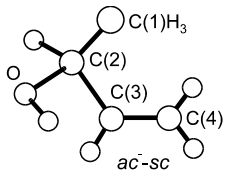
**560** **$C_4H_8O$** **3-Buten-2-ol** **$C_1$** (*ac-sc*$^-$)
ED, DFT **$C_1$** (*sp-sc*)
calculations **$C_1$** (*sp-sc*$^-$)
**$C_1$** (*ac*$^-$*-sc*)

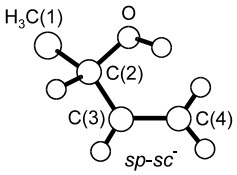
| $r_g$ | Å [a]) | $\theta_\alpha$ | deg [a]) |
|---|---|---|---|
| C(2)–C(1) [b]) | 1.504(9) | C(4)=C(3)–C(2) | 126(1) |
| C(3)–C(2) [b]) | 1.484(9) | C(3)–C(2)–C(1) | 110(1) |
| C(4)=C(3) | 1.327(9) | C(3)–C(2)–O | 109(1) |
| O–C(2) | 1.421(9) | C(1)–C(2)–O | 110(1) |
| O–H | 0.982(21) | H–C(4)–H | 116.9 [c]) |
| C(1)–H [d]) | 1.117(15) | C(4)=C(3)–H | 120.0 [c]) |
| C(4)–H [d]) | 1.088 [c]) | C(2)–O–H | 107.0 [c]) |
| C(2)–H | 1.100 [c]) | C(2)–C(1)–H | 110.0 [c]) |
| | | C(3)–C(2)–H | 108.3 [c]) |
| | | C(1)–C(2)–H | 110.5 [c]) |

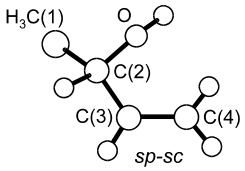



The molecule was found to exist as a mixture of *ac-sc*$^-$ (58(23)%), *sp-sc* and *sp-sc*$^-$ (together 32(23)%) and *ac*$^-$*-sc* (10(23)%) conformers governed by $\tau_1$[O–C(2)–C(3)=C(4)] and $\tau_2$[H–O–C(2)–C(3)] torsional angles ($\tau = 0°$ for *sp* fragment, $\tau = \pm 60°$ for $sc^{\pm}$ fragments and $\tau = \pm 120°$ for $ac^{\pm}$ fragments). The listed values represent effective average values of these conformers.
The nozzle temperature was 300 K.




[a]) Five times the estimated standard errors.
[b]) [C(2)–C(1)] – [C(3)–C(2)] was assumed to be 0.02 Å.
[c]) Constrained to the value from B3LYP/6-31G** calculations.
[d]) Average value.

Shishkov, I.F., Shlykov, S., Rousseau, B., Peng, Z.H., Van Alsenoy, C., Geise, H.J., Kataeva, O.N., Herrebout, W.A., Van der Veken, B.: J. Phys. Chem. A **105** (2001) 1039.
II/25C (**3**, 1734)