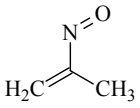
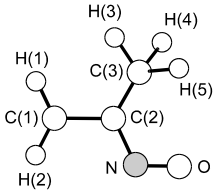
382 **C_3H_5NO** **2-Nitroso-1-propene** **C_s**
MW



r_0	Å
C(1)=C(2)	1.344 [a])
C(2)–N	1.438 [a])
N=O	1.248 [a])
C(3)–H(3)	1.084 [a])
C(3)–H(4,5)	1.084 [a])
C(1)–H(1,2)	1.090 [a])
C(2)–C(3)	1.494(5)

θ_0	deg
C(1)=C(2)–N	112.8 [a])
C(2)=C(1)–H(1,2)	121.3 [a])
C(2)–C(3)–H(3)	111.8 [a])
C(2)–C(3)–H(4,5)	109.6 [a])
C(1)=C(2)–C(3)	126.0(5)
C(2)–N=O	111.8(5)

Atom	$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]
N	0.7208	0.7393



The effect of nitrogen isotopic substitution suggests that the N atom lies in or close to the *ab* inertial plane of the molecule and shows that only two H atoms are located symmetrically out of the symmetry plane. The molecule was determined to have *syn*-eclipsed conformation shown in the figure. The barrier heights to CH_3 torsion in the ground and first excited torsional states were determined to be 7.32(21) and 7.28(21) kJ mol^{-1}, respectively, and wavenumbers of the C–N and C–C torsions to be 160(40) and 175(40) cm^{-1}, respectively.

[a]) Assumed.

Sakaizumi, T., Imajo, H., Yamasaki, R., Usami, T., Kawaji, S., Abe, S., Haraga, T., Morii, H., Kuze, N., Ohashi, O.: J. Mol. Spectrosc. **204** (2000) 26.