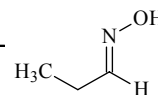


430
ED, MW $\text{C}_3\text{H}_7\text{NO}$ **(E)-Propionaldehyde oxime**
(E)-Propanal oxime C_1 (*ac*)
 C_s (*sp*)

r_g	\AA^a		θ_α^0	deg^a	
	<i>ac</i>	<i>sp</i>		<i>ac</i>	<i>sp</i>
C(1)–C(2)	1.552(3)		C(3)=N–O	109.4(2)	
C(2)–C(3)	1.493(2)		C(1)–C(2)–C(3)	111.5(1)	112.6(6)
N–O	1.429(2)		C(2)–C(3)=N	119.0(3)	122.6(6)
C(3)=N	1.284(2)	1.291(3)	τ^b	60	180

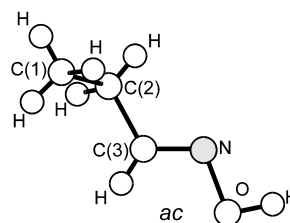


E- and *Z*-isomers exist in the gas phase. The geometrical parameters for the *antiperiplanar* (*ap*) form of the *Z*-isomer were taken from [1]. *E*-isomer exists as a mixture of *anticlinal* (*ac*) and *synperiplanar* (*sp*) conformers. The *ac* conformer was found to be more stable by 0.15(10) kcal mol^{−1} than the *sp* conformer. The ratio of *E-ac*, *E-sp* and *Z-ap* forms was determined to be 56:23:21. The torsional motion around the C(2)–C(3) bond was treated as a large-amplitude motion.

The nozzle was at about 323 K.

^a) Estimated limits of error.

^b) C–C–C=N torsional angle, $\tau = 0^\circ$ for the *anti* position.



Iijima, K., Matsuoka, M., Sakaizumi, T., Ohashi, O.: Bull. Chem. Soc. Jpn. **69** (1996) 2481.

[1] Iijima, K., Ohashi, O.: J. Mol. Struct. **291** (1993) 159.

[II/25C \(3, 1325\)](#)