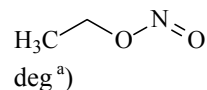
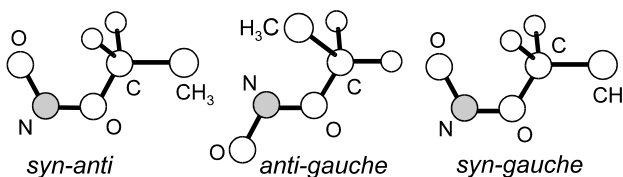


288  
MW $\text{C}_2\text{H}_5\text{NO}_2$ **Ethyl nitrite**  
Nitrous acid ethyl ester $\text{C}_s$  (*syn-anti*)  
 $\text{C}_1$  (*anti-gauche*)  
 $\text{C}_1$  (*syn-gauche*)

$r_0$	$\text{\AA}^{\text{a})}$		$\theta_0$	$\text{deg}^{\text{a})}$	
	<i>syn-anti</i>	<i>anti-gauche</i>		<i>syn-anti</i>	<i>anti-gauche</i>
C–H	1.0933(1)	1.090 <sup>b)</sup>	C–C–O	105.90(7)	109.5 <sup>b)</sup>
C–C	1.5174(8)	1.523 <sup>b)</sup>	C–O–N	114.19(9)	111.2(11)
C–O	1.435(1)	1.429(3)	O–N=O	115.9(2)	110.4(12)
O–N	1.414(3)	1.437(2)	H–C–C		109.5 <sup>b)</sup>
N=O	1.185(1)	1.172 <sup>b)</sup>	C–O–N=O <sup>c)</sup>		96.26(118)

Three rotational conformers, *syn-anti*, *syn-gauche* and *anti-gauche*, were detected. The potential barrier to internal rotation of  $\text{CH}_3$  is 1082 and 918  $\text{cm}^{-1}$  for *syn-anti* and *syn-gauche*, respectively. For *anti-gauche* the *b*- and *c*-type lines showed doubling due to the interconversion between the two equivalent *gauche* conformers through internal rotation about the C–O axis. The difference between the two lowest energy levels of the torsion around the C–O bond is 68 kHz. Based on the observed splittings and the rotational constants, the Fourier coefficients of the potential hindering this internal rotation were determined to be  $V_1 = -1322 \text{ cm}^{-1}$ ,  $V_2 = -1048 \text{ cm}^{-1}$ ,  $V_3 = -412 \text{ cm}^{-1}$  and  $V_4 = -109 \text{ cm}^{-1}$  with a low barrier of 183  $\text{cm}^{-1}$  in the *anti* position and a higher barrier of 1916  $\text{cm}^{-1}$  in the *syn* position.

<sup>a)</sup> Estimated standard errors.<sup>b)</sup> Assumed.<sup>c)</sup> Dihedral angle.Hansen, N., Temps, F., Mäder, H., Larsen, N.W.: Phys. Chem. Chem. Phys. **1** (1999) 3219.[II/25B\(3, 834\)](#)