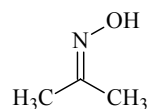


431  
ED $\text{C}_3\text{H}_7\text{NO}$ **Propanone oxime**  
Acetone oxime $\text{C}_s$ 

$r_g$	$\text{\AA}^a)$	$\theta_u$	$\text{deg}^a)$
C(1)–C(2)	1.490(3)	C(1)–C(2)=N	116.4(2)
C(2)–C(3)	1.521(5)	C(3)–C(2)=N	123.4(3)
C(2)=N	1.289(1)	C(2)=N–O	111.2(2)
N–O	1.423(2)	H–C–H (mean)	107.8(4)
C–H (mean)	1.116(2)	N–O–H	102.7 <sup>b)</sup>
O–H	0.993(6)	$\tau_1^c)$	0.0 <sup>d)</sup>
		$\tau_2^e)$	60.0 <sup>d)</sup>
		tilt(CH <sub>3</sub> ) <sup>f)</sup>	0 <sup>d)</sup>



Local  $\text{C}_{3v}$  symmetry was assumed for the methyl group.  
The sample was vaporized at about 47 °C.

<sup>a)</sup> 2.6 times the estimated standard errors including a systematic error.

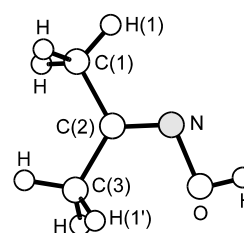
<sup>b)</sup> Assumed according to literature data for similar molecules.

<sup>c)</sup> N=C(2)–C(1)–H(1) torsional angle.

<sup>d)</sup> Fixed in the final refinement.

<sup>e)</sup> N=C(2)–C(3)–H(1') torsional angle from the *syn* position.

<sup>f)</sup> Tilt angle between the  $\text{C}_3$  axis of the  $\text{CH}_3$  group and the C–C bond direction.



Iijima, K., Suzuki, M., Sakaizumi, T., Ohashi, O.: J. Mol. Struct. **413–414** (1997) 327.