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MW $\text{C}_3\text{H}_6\text{ClNO}$ **(E)-1-Chloro-2-propanone oxime**  
Chloroacetone oxime $\text{C}_1$ 

$$\frac{\theta_0}{\varphi^{b)}} \frac{\text{deg}^a)}{116.8(5)}$$

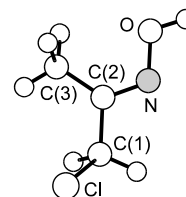
Atom	$ a_s  [\text{\AA}]$	$ b_s  [\text{\AA}]$	$ c_s  [\text{\AA}]$
Cl	2.119	0.0 <sup>c)</sup>	0.255

The observed rotational constants, in particular, the change in  $I_{cc}-I_{aa}-I_{bb}$  upon substitution of  $^{35}\text{Cl}$  by  $^{37}\text{Cl}$  and the  $r_s$ -coordinates of Cl agreed well with those expected for the *anticlinal* form in the *E*-isomer.

<sup>a)</sup> Uncertainty was not estimated in the original paper.

<sup>b)</sup> Dihedral angle  $\text{Cl}-\text{C}(1)-\text{C}(2)=\text{N}$ .

<sup>c)</sup> Assumed.



Sakaizumi, T., Imajo, H., Usami, T., Kuze, N., Ohashi, O., Iijima, K.: J. Mol. Struct. **522** (2000) 243.