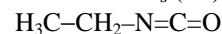


1216  
ED, MW

**C<sub>3</sub>H<sub>5</sub>NO**

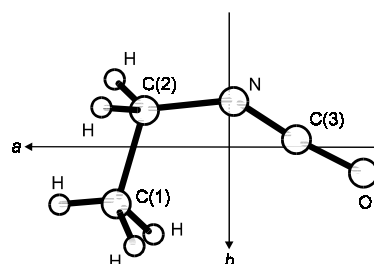
**Ethyl isocyanate**

**C<sub>s</sub> (*cis*)**



$r_{av}$	$\text{\AA}^a$
C-N	1.448(9)
C-H	1.084(7)
C-C	1.524(11)
N=C	1.218(5)
C=O	1.174(4)

$\theta_{av}$	deg <sup>a)</sup>
C-C-N	114.7(16)
C-N=C	132.2(22)
N=C=O <sup>b)</sup>	192.2(25)
C(2)-C(1)-H	111.4(19)



A *cis* conformation is compatible with the ED and MW data, but the MW spectrum contains many more lines than can be explained on the basis of a single *cis* conformer. Thus the conformation about the C(2)-N axis seems to remain uncertain. The rotational constants were extrapolated to remove the zero-point effect of the torsion about the C(2)-N axis.

The temperature was not stated, probably room temperature.

<sup>a)</sup> Uncertainties were unidentified, possibly estimated standard errors.

<sup>b)</sup> The direction of the bend was not defined in the original paper, possibly bent away from the CH<sub>3</sub> group.

Cradock, S., Durig, J.R., Sullivan, J.F.: J. Mol. Struct. **131** (1985) 121.

MW

$r_s$	$\text{\AA}$	$\theta_s$	deg
C-N	1.439(8)	C-C-N	113.5(5)
C-H	1.10 <sup>a)</sup>	C-N=C	138.8(12)
C-C	1.531(11)	N=C=O	175.6(26)
N=C	1.188(19)	C-C-H	109 <sup>a)</sup>
C=O	1.194(19)	H-C-H <sup>b)</sup>	110 <sup>a)</sup>

$r_0$	$\text{\AA}$	$\theta_0$	deg
C-N	1.441(6)	C-C-N	113.7(4)
C-H	1.1018(8)	C-N=C	138.2(8)
C-C	1.523(8)	N=C=O	175.7(17)
N=C	1.189(13)	C-C-H	109 <sup>a)</sup>
C=O	1.184(12)	H-C-H <sup>b)</sup>	110 <sup>a)</sup>

Oxygen atom is *trans* to the ethyl group.

<sup>a)</sup> Parameter held fixed during the fit.

<sup>b)</sup> The HCH-bisector of the CH<sub>2</sub> group was assumed to be collinear to the CCN-bisector.

Heineking, N., Grabow, J.-U., Stahl, W.: Mol. Phys. **81** (1994) 1177.