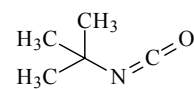


**657 C<sub>5</sub>H<sub>9</sub>NO**ED, MW, *ab initio* and DFT calculations***t*-Butyl isocyanate**

2-Isocyanato-2-methylpropane

**C<sub>s</sub>**

$r_a$	$\text{\AA}^a$	$\theta_a$	deg <sup>a)</sup>
C–H	1.103(5)	C=N–C	137.0(20)
C=O	1.163(7)	N=C=O	173.1 <sup>b)</sup>
N=C	1.225(6)	C–C–C	110.1(13)
N–C	1.440(6)	H–C–H	108.6(9)
C–C	1.535(2)	tilt(CH <sub>3</sub> ) <sup>c)</sup>	0.0 <sup>b)</sup>
		tilt( <i>t</i> -butyl) <sup>d)</sup>	1.4 <sup>b)</sup>

Local C<sub>3v</sub> symmetry was assumed for the methyl and *t*-butyl groups. The experimental intensities were fitted best with a nonrigid model which possesses a large-amplitude torsional motion of the *t*-butyl group around the N–C bond and an equilibrium structure with staggered orientation of the *t*-butyl group with respect to the N=C=O group, which is only slightly bent *anti* to the N–C bond. The three-fold rotational barrier derived from the MW spectra [1], 118.72 cal mol<sup>−1</sup>, was assumed.

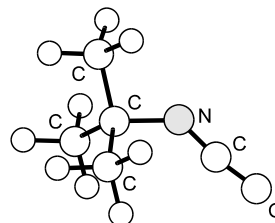
The nozzle was at room temperature.

<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Assumed at the B3PW91 theoretical value.

<sup>c)</sup> Tilt angle between the C<sub>3</sub> axis of methyl group and the C–C bond direction.

<sup>d)</sup> Tilt angle between the C<sub>3</sub> axis of *t*-butyl group and the N–C bond direction towards the nitrogen lone pair.



Knölker, H.-J., Braxmeier, T., Oberhammer, H.: J. Mol. Struct. **413-414** (1997) 211.

[1] Grabow, J.U., Heineking, N., Stahl, W.: J. Mol. Spectrosc. **154** (1992) 129.