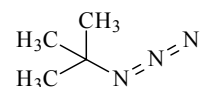


**591** **C<sub>4</sub>H<sub>9</sub>N<sub>3</sub>**  
ED, *ab initio* and DFT  
calculations

**2-Azido-2-methylpropane**  
*t*-Butyl azide

essentially C<sub>s</sub>



$r_g$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C–H	1.111(5)	C(1)–C(2)–N(1)	102.5(6)
N(2)=N(3)	1.143(4)	C(3,4)–C(2)–N(1)	110.5(4)
C(2)–C(3,4)	1.536(3)	C(2)–C(1)–H	111.2(4)
N(1)=N(2) <sup>b)</sup>	1.240(5)	C(2)–N(1)=N(2)	118.6(10)
C(1)–C(2) <sup>c)</sup>	1.531(3)	N(1)=N(2)=N(3)	171.8(20)
C(2)–N(1) <sup>c)</sup>	1.508(5)	C(1)–C(2)–C(3) <sup>b)</sup>	110.2(7)
		C(3)–C(2)–C(4) <sup>b)</sup>	112.6(7)
		C(4)–C(2)–C(1) <sup>b)</sup>	110.2(7)
		$\tau_1$ <sup>d)</sup>	167.5(12)
		$\tau_2$ <sup>e)</sup>	50.1(6)
		$\tau_3$ <sup>b) f)</sup>	–75.2(6)

The NC(CH<sub>3</sub>)<sub>3</sub> and CH<sub>3</sub> groups were assumed to have C<sub>s</sub> and C<sub>3v</sub> symmetry, respectively. One of the C–H bonds of each methyl group was assumed to be in the *anti* position with respect to the C–N bond. According to HF/6-31G\* and B3LYP/6-31G\*\* calculations, the rotation around the N(1)=N(2) bond is essentially free; the energy difference between the *syn* and *anti* conformations of the C–N=N=N moiety was estimated to be 0.34 kcal mol<sup>–1</sup> (*anti* is more stable form). The rotational potential from quantum chemical calculations was used for the modelling a mixture of pseudoconformers in the ED analysis. The nozzle was at room temperature.

<sup>a)</sup> Estimated total errors.

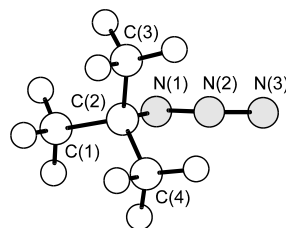
<sup>b)</sup> Dependent parameter.

<sup>c)</sup> Differences in the C–C bond lengths and between C–N and C–C bond lengths were assumed at the values from B3LYP/6-31G\*\* calculations.

<sup>d)</sup> Torsional angle N(2)=N(1)–C(2)–C(1).

<sup>e)</sup> Torsional angle N(2)=N(1)–C(2)–C(3).

<sup>f)</sup> Torsional angle N(2)=N(1)–C(2)–C(4).



MacKenzie, A., Klapötke, T.M., Schultz, G., Hargittai, M.: Struct. Chem. **10** (1999) 59.