

1833 **C₄H₁₁N**
ED, *ab initio* calculations
(HF/4-21G)

***t*-Butylamine**

C_s assumed
H₂N–C(CH₃)₃

r_g	Å ^{a)}	θ_α	deg ^{a)}
N–C	1.493(6)	C–N–H	110.0(27)
C(2)–C(3) ^{b)}	1.536(4)	N–C(2)–C(3) ^{c)}	111.8(3)
C(2)–C(4) ^{b)}	1.529(4)	N–C(2)–C(4) ^{c)}	107.0(3)
C–H	1.114(3)	C(3)–C(2)–C(4)	110.5(5) ^{d)}
N–H	1.048(12)	C(4)–C(2)–C(5)	109.9(3)
		C–C–H (average)	111.2(6)
		H–C–H (average)	107.7(6) ^{d)}
		H–N–H	105.2 ^{e)}
		$\tau_4 (= -\tau_5)$ ^{f)}	10(4)
		δ ^{g)}	3.2

The experimental ED intensity reported in [1] was reanalyzed.
The nozzle temperature was 22 °C.

^{a)} Estimated limits of error.

^{b)} The differences in the parameters of C(2)–C(3) and C(2)–C(4) were assumed to be equal to the corresponding values derived from *ab initio* calculations.

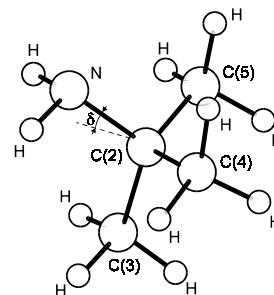
^{c)} The differences in the parameters of N–C(2)–C(3) and N–C(2)–C(4) were assumed to be equal to the corresponding values derived from *ab initio* calculations.

^{d)} Dependent parameter.

^{e)} Assumed at the value given by a molecular mechanics (MM2) calculation.

^{f)} Torsional angle H–C(4)–C(2)–N (= –(H–C(5)–C(2)–N)); $\tau = 0^\circ$ for *anti* position.

^{g)} Tilt angle of the *t*-butyl group; $\delta = (2/3)[(N-C-C(3)) - (N-C-C(4))]$; see figure.



Konaka, S., Takeuchi, H., Siam, K., Ewbank, J.D., Schäfer, L.: J. Mol. Struct. **222** (1990) 503.

[1] Konaka, S., Yanagihara, N.: J. Mol. Struct. **196** (1989) 375.