

1832 **C₄H₁₁N**
ED, *ab initio*
calculations (HF/4-21G)

Diethylamine

C_s (without H in NH) (TT)
C₁ (TG)
H₃C–CH₂–NH–CH₂–CH₃

<i>r</i> _g	Å ^{a)}	Å ^{a)}	Å ^{a)}
	TT	TG	GG
N–C(1)	1.460(1)	1.464(1)	1.464(1)
N–C(3)	1.460(1)	1.462(1)	1.462(1)
C(1)–C(2)	1.527(1)	1.529(1)	1.528(1)
C(3)–C(4)	1.527(1)	1.528(1)	1.534(1)
C–H(average)	1.114(3)	1.114(3)	1.113(3)
N–H	1.036 ^{b)}	1.035 ^{b)}	1.034 ^{b)}

<i>θ</i> _α	deg ^{a)}	deg ^{a)}	deg ^{a)}
	TT	TG	GG
C(1)–N–C(3)	112.7 ^{b)}	113.7 ^{b)}	115.6 ^{b)}
N–C(1)–C(2)	111.1(6)	112.7(6)	112.5(6)
N–C(3)–C(4)	111.2(6)	110.9(6)	116.0(6)
N–C–H(average)	110.0 ^{c)}	110.0 ^{c)}	108.8 ^{c)}
C–C–H(average)	109.6(8)	109.5(8)	109.6(8)
C–N–H(average)	108.1 ^{b)}	107.9 ^{b)}	108.5 ^{b)}
∠(C(3)–N–C(1)–C(2))	175.3 ^{c)}	71(12)	69.7 ^{c)}
∠(C(1)–N–C(3)–C(4))	178.4 ^{c)}	180(18)	67.9 ^{c)}

The molecule exists as a mixture of TT (42(16)%), TG (53(24)%) and GG (5(20)%) conformers. Another possibility of the conformational composition is TT 42(16)%, TG 58(27)% and G'G 0(19)%.

The differences between the structural parameter values of conformers were assumed at the *ab initio* values. The measurements were made at room temperature.

^{a)} Three times the estimated standard errors.

^{b)} Estimated by adding the empirical correction to the *ab initio* value.

^{c)} Assumed at the *ab initio* value.

Takeuchi, H., Kojima, T., Egawa, T., Konaka, S.: J. Phys. Chem. **96** (1992) 4389.

