

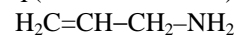
1317 C₃H₇N

ED, MW, *ab initio*

calculation (HF/4-31G(N*))

Allylamine

C_s (CT)

C₁ (other conformers)


r_g	\AA^a		
	CT	ST	S ⁺ G ⁺
C=C	1.334(7)	1.337 ^b	1.336(7) ^b
C-C	1.501(3)	1.501 ^b	1.495 ^b
C-N	1.463 ^c	1.475 ^c	1.473 ^c
N-H	1.045 ^c	1.046 ^c	1.046 ^c
C-H	1.106(3)	1.106 ^b	1.106(2) ^b

θ_z	deg^a		
	CT	ST	S ⁺ G ⁺
C=C-C	127.5(6)	126.3 ^b	125.6(6) ^b
C-C-N	117.1 ^d	114.7(7)	109.6 ^b
C-N-H(3)	110.3 ^d	109.8 ^d	110.4 ^d
C=C-H(1)	121.9 ^d	122.2 ^d	122.2 ^d
C-C-H(2)	108.9 ^d	109.8 ^d	109.3 ^d
C=C-C-N	0.0 ^d	-118.2(13)	-124.7(12)
C=C-C-H(2)	122.7 ^d	1.6 ^d	-1.8 ^d
C-C-N-H(3)	58.7 ^d	58.5 ^d	-178.6 ^d

The relative abundances of the *cis*

(CT + CG, CG being predicted by

ab initio calculation to be less

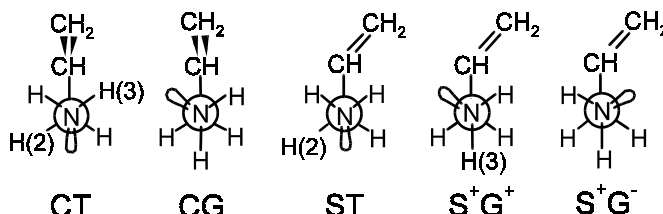
abundant than CT) and the *skew*

(ST + S⁺G⁺ + S⁺G⁻, S⁺G⁻ being

predicted to be the least abundant)

conformers were estimated to be 25(6) and 75(6)%, respectively, at room temperature.

The nozzle was at room temperature.


^a) 2.5 times the estimated standard errors.

^b) The differences among the conformers were assumed to be those estimated by *ab initio* calculation.

^c) Assumed.

^d) Estimated by *ab initio* calculation.

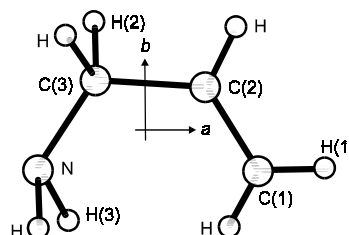
Hamada, Y., Tsuboi, M., Yamanouchi, K., Matsuzawa, T., Kuchitsu, K.: J. Mol. Struct. **224** (1990) 345.

MW

C_s (CT)

r_s	\AA	θ_s	deg
C(1)=C(2)	1.336(13)	C=C-C	125.9(7)
C(2)-C(3)	1.498(11)	C-C-N	118.0(6)
C-N	1.455(10)	C-N-H	110.2(7)
N-H	1.018(5)	C-C-N-H	58.5(6)

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$	$c_s [\text{\AA}]$
C(1)	1.515	-0.577	0.0
C(2)	0.818	0.563	0.0
C(3)	-0.675	0.680	0.0
H (NH)	-1.225	-1.112	± 0.814


Wiedenmann, K.-H., Botskor, I., Rudolph, H.D., Stiefvater, O.L.: J. Mol. Struct. **190** (1988) 173.

