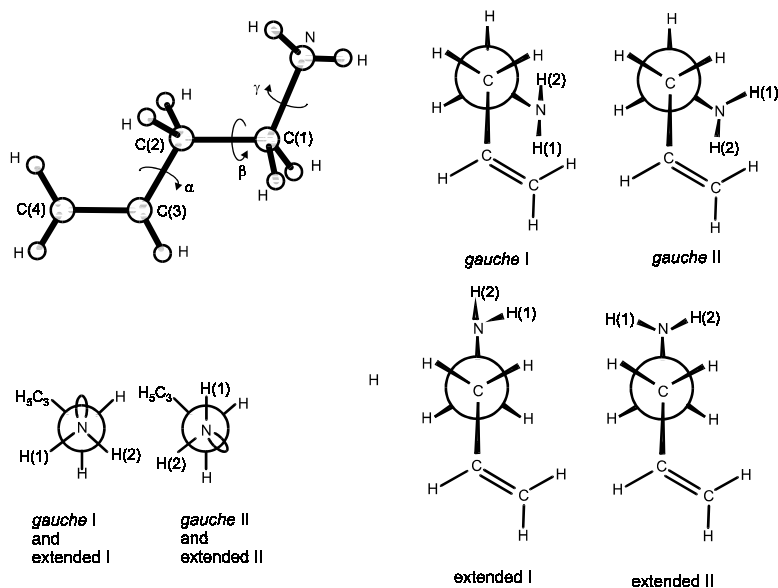


r_0	Å	θ_0	deg
N–C(1)	1.475 ^{a)}	C(2)–C(1)–N	110.0 ^{a)} ^{b)} or 115.0 ^{a)} ^{c)}
C(4)=C(3)	1.331 ^{a)}	C(3)–C(2)–C(1)	111.6 ^{a)}
C(3)–C(2)	1.496 ^{a)}	C(4)=C(3)–C(2)	127.8 ^{a)}
C(2)–C(1)	1.528 ^{a)}	C(1)–N–H	107.0 ^{a)}
C(4)–H	1.090 ^{a)}	C(2)–C(1)–H	109.47 ^{a)}
C(3)–H	1.090 ^{a)}	C(1)–C(2)–H	109.47 ^{a)}
C(2)–H	1.093 ^{a)}	C(3)=C(4)–H	121.5 ^{a)}
C(1)–H	1.093 ^{a)}	C(4)=C(3)–H	121.5 ^{a)}
N–H	1.017 ^{a)}	$\alpha(\text{C}(4)=\text{C}(3)-\text{C}(2)-\text{C}(1))$	60.0 ^{a)} (extended conformers)
		$\beta(\text{C}(3)-\text{C}(2)-\text{C}(1)-\text{N})$	0.0 ^{a)} (extended conformers)
		$\alpha(\text{C}(4)=\text{C}(3)-\text{C}(2)-\text{C}(1))$	66(3) (<i>gauche</i> I and <i>gauche</i> II)
		$\beta(\text{C}(3)-\text{C}(2)-\text{C}(1)-\text{N})$	116(3) (<i>gauche</i> I and <i>gauche</i> II)
			64(3) (from <i>syn</i> position)

The molecule exists in five rotameric forms, of which four were assigned (see figures): *gauche* I, *gauche* II [0.8(3)], extended I [1.9(5)], and extended II [2.1(5)], where the energy differences in brackets are in units of kJ mol^{-1} . The conformation shown has $\alpha(\text{C}(4)=\text{C}(3)-\text{C}(2)-\text{C}(1)) = \beta(\text{C}(3)-\text{C}(2)-\text{C}(1)-\text{N}) = \gamma(\text{C}(2)-\text{C}(1)-\text{N}-\text{H}(2)) = 0^\circ$. Rotation around α by about 60° , β by approximately 120° and γ by about 0° in the direction indicated by the arrows produces the H-bonded *gauche* I conformer. Keeping α and β constant at these values, a further rotation around γ by approximately 120° yields the other H-bonded *gauche* II. Rotation about α by 60° , β by 0° and γ by 0° yields extended I. If a 120° rotation around γ is then made, extended II will result.



^{a)} Assumed.

^{b)} Kept at this value for *gauche* I, *gauche* II, extended I, and extended II.

^{c)} Kept at this value for *gauche* II and extended II.

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