Microwave Spectrum, Conformation and Internal Hydrogen Bonding in *N*-Methylallylamine

K.-M. Marstokk and Harald Møllendal*

Department of Chemistry, The University of Oslo, P.O. Box 1033, Blindern, N-0315 Oslo 3, Norway

Marstokk, K.-M. and Møllendal, H., 1986. Microwave Spectrum, Conformation and Internal Hydrogen Bonding in *N*-Methylallylamine. – Acta Chem. Scand. A 40: 615–621.

The microwave spectra of $CH_3NHCH_2CH=CH_2$ and $CH_3NDCH_2CH=CH_2$ have been investigated at dry-ice temperature. Only one *skew* conformation was assigned and shown to be at least 3 kJ mol^{-1} more stable than any other possible rotameric form. The assigned conformation has a $N-C-C=C$ dihedral angle which is 123(3)° from *syn*. The methyl group is *anti* to the CH_2-CH bond. A weak intramolecular hydrogen bond is formed between the methylamino group hydrogen atom and the π electrons of the double bond. Four vibrationally excited states belonging to three different normal modes were assigned and their vibrational frequencies determined by relative intensity measurements. Extensive centrifugal distortion analyses were made for the ground state and the vibrationally excited states.

Allyl derivatives of the general form $X-CH_2-CH=CH_2$ normally adopt *syn* or *skew* conformations, as discussed in a recent paper.[1] In the *syn* form, the $X-C-C=C$ skeleton is planar and the $C-X$ bond eclipses the double bond, whereas in the *skew* form, the $C-X$ bond is rotated 120° out of this plane. If additional rotational isomerism around the $C-X$ bond is possible, several *syn* or *skew* forms may exist. Allylamine, $H_2NCH_2CH=CH_2$, is one such example. Five rotameric forms, two *syn* and three *skew*, are conceivable for this molecule. The two *syn* conformations and two of the three possible *skew* rotamers have indeed been assigned by microwave (MW) spectroscopy by Botskor and co-workers.[2] There are small energy differences between the four different rotamers of allylamine. In the related molecule *N*-methylallylamine, $CH_3NHCH_2CH=CH_2$, the total number of possible *syn* and *skew* rotamers is, in fact, no less than nine. These nine forms are drawn in Fig. 1.

Many factors may determine the conformational preferences of a compound. Steric repulsion, intramolecular hydrogen (H) bonding, and repulsion between the lone electron pair of the nitrogen atom and the double bond π electrons may be of importance in the case of *N*-methylallylamine. In conformation I of Fig. 1, there is no steric crowding since the methyl group is *anti* to the CH_2-CH bond. An internal H bond may be formed between the hydrogen atom of the methylamino group and the double bond π electrons. Moreover, the lone electron pair of the nitrogen atom is oriented in such a way that the repulsion between this electron pair and the π-electrons is minimized. Inspection of Fig. 1 reveals that similar favourable intramolecular interactions are not simultaneously present in any other of the remaining 8 possible conformations denoted by Roman numerals II through IX. For example, an intramolecular H bond is not present in rotamers II, III, VI, VII, and IX. Steric repulsion may be of importance in conformer V, while repulsion between the nitrogen lone pair and the double bond π electrons is presumably present in forms III, IV, VI, and VII.

This work was undertaken in the hope of obtaining insight into what determines the conformational properties of the title compound. It was found that conformation I, having optimal intra-

---

*To whom correspondence should be addressed.

molecular interactions, is the most stable form of the molecule. This rotamer, which was the only one that was assigned, is at least 3 kJ mol^{-1} more stable than any other form of N-methylallylamine.

Experimental

N-Methylallylamine was purchased from Fluka A.G., Buchs, Switzerland. The compound was purified by gas chromatography before use. The spectrum was investigated extensively in the 12.4–26.7 GHz spectral range. Many measurements were also made in the 28.0–38.0 GHz region. The cell was cooled to dry-ice temperature during the measurements, which were made at a pressure of roughly 1 Pa. The spectrometer used was a modified version of the one described briefly in Ref. 3 with free-running klystrons. The deuterated species was produced by direct exchange with heavy water in the wave-guide.

Results

Spectrum and assignment of the ground vibrational state. The microwave spectrum of N-methylallylamine is rich and of moderate intensity. The strongest lines, which turned out to be high-J b- and c-type Q-branch transitions of the ground vibrational state, have peak absorption coefficients of roughly 4×10^{-7} cm^{-1} at dry-ice temperature.

Preliminary rotational constants were calculated for many of the conformations shown in Fig. 1. A search was first made for conformation I because it was presumed that stabilizing conditions in this rotamer were favourable, as mentioned above. The dipole moment components along the principal axes were calculated to be μ_a = 0.6×10^{-30} C m, μ_b = 0.9×10^{-30} C m, and μ_c = 3.3×10^{-30} C m using the bond-moment method.[4] Strong c-type $K_{-1} = 1 \leftarrow 0$ Q-branch transitions were thus predicted to occur for this rotamer in the region below about 18 GHz. The quadrupole coupling constants were predicted to be roughly χ_{aa} = 2.0 MHz and χ_{bb} = -2.0 MHz, using the procedure of Ref. 5 and assuming the principal quadrupole coupling constant of the ^{14}N nucleus to be χ_z = -4.1 MHz, the value found for NH$_3$,[6] and to be oriented 109.47° with respect to the three bonds to the nitrogen atom. Very small splittings caused by quadrupole coupling of the
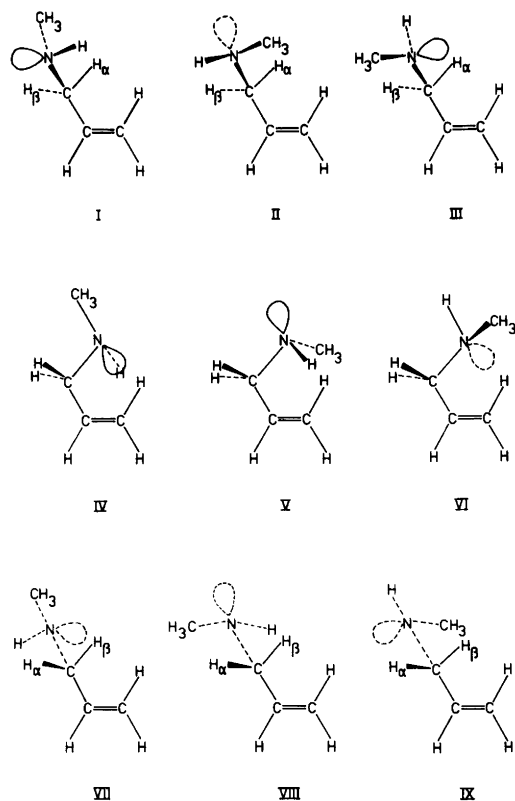

Fig. 1. The nine possible rotameric forms of N-methylallylamine. The lobe indicates the probable direction of the lone electron pair of the nitrogen atom. Conformations IV, V and VI are heavy-atom *syn* forms, while the remaining six are *skew* forms. Conformation I was the only one which was assigned. This rotamer is at least 3 kJ mol^{-1} more stable than any other hypothetical form.

^{14}N nucleus with the molecular rotation were thus predicted for these c-type transitions. This strong Q-branch series was soon found, because these lines were among the most prominent ones below 18 GHz. Q-branch lines belonging to the b-type $K_{-1} = 1 \leftarrow 0$ series and to the c-type $K_{-1} = 2 \leftarrow 1$ were next identified with ease. None of these transitions are resolvably split by quadrupole coupling, although some of them are definitely broadened by this effect. There are few low-J R-branch lines in this spectrum and they are comparatively weak. It therefore took some time to find these transitions. Extension of the R-branch assignments to include high values of J was then

Table 1. Selected transitions of the ground state of $CH_3NHCH_2CH=CH_2$.

Transition	Observed frequency[a] (MHz)	Obs.-Calc. frequency (MHz)	Centrifugal distortion	
			Total (MHz)	Sextic (MHz)
b-type				
$6_{1,5} \leftarrow 6_{0,6}$	18122.36	−0.11	−0.94	
$8_{1,7} \leftarrow 8_{0,8}$	18371.43	−0.07	−1.08	
$11_{1,10} \leftarrow 11_{0,11}$	18877.46	−0.15	−0.82	−0.01
$15_{1,14} \leftarrow 15_{0,15}$	19815.64	0.02	1.57	−0.04
$20_{1,19} \leftarrow 20_{0,20}$	21455.53	−0.08	11.68	−0.13
$25_{1,24} \leftarrow 25_{0,25}$	23687.90	0.00	37.33	−0.41
$30_{1,29} \leftarrow 30_{0,30}$	26604.17	0.16	90.72	−1.06
$35_{1,34} \leftarrow 35_{0,35}$	30300.17	0.17	188.85	−2.45
$40_{1,39} \leftarrow 40_{0,40}$	34862.06	0.07	353.08	−5.16
$43_{1,42} \leftarrow 43_{0,43}$	38040.99	−0.16	493.23	−7.76
$3_{1,3} \leftarrow 2_{0,2}$	30997.86	−0.06	0.21	
$4_{1,4} \leftarrow 3_{0,3}$	35372.13	0.03	0.58	
$7_{1,6} \leftarrow 7_{0,7}$	18238.40	0.05	−1.02	
$16_{1,15} \leftarrow 15_{2,14}$	19861.27	−0.17	−22.66	−0.05
$23_{2,21} \leftarrow 22_{3,20}$	13556.37	−0.22	−56.40	−0.07
$28_{2,27} \leftarrow 27_{3,24}$	34941.60	−0.06	−104.69	0.13
c-type				
$4_{1,4} \leftarrow 4_{0,4}$	17617.14	−0.02	0.74	
$8_{1,8} \leftarrow 8_{0,8}$	17202.94	0.02	3.40	
$13_{1,13} \leftarrow 13_{0,13}$	16349.81	0.07	7.11	0.02
$17_{1,17} \leftarrow 17_{0,17}$	15425.95	0.08	8.41	0.06
$23_{1,23} \leftarrow 23_{0,23}$	13712.42	−0.07	3.46	0.20
$27_{1,27} \leftarrow 27_{0,27}$	12411.18	−0.18	−6.51	0.38
$44_{2,43} \leftarrow 44_{1,43}$	37898.75	−0.08	− 136.55	6.24
$48_{2,47} \leftarrow 48_{1,47}$	35179.48	0.07	222.70	9.55
$56_{2,55} \leftarrow 56_{1,55}$	29365.32	0.05	− 456.03	19.83
$63_{2,62} \leftarrow 63_{1,62}$	24096.57	0.02	− 707.39	33.18
$71_{2,70} \leftarrow 71_{1,70}$	18256.85	−0.01	− 991.25	52.04
$75_{2,74} \leftarrow 75_{1,74}$	15545.64	0.19	−1106.49	61.69
$3_{1,2} \leftarrow 2_{0,2}$	31192.53	0.00	− 0.69	
$4_{1,3} \leftarrow 3_{0,3}$	35696.43	−0.06	− 0.88	
$9_{0,9} \leftarrow 8_{1,7}$	21571.13	−0.16	− 0.72	
$16_{1,15} \leftarrow 15_{2,13}$	19756.24	−0.12	− 21.28	−0.04
$23_{2,21} \leftarrow 22_{3,20}$	13556.37	−0.22	− 56.40	−0.07
$36_{3,34} \leftarrow 35_{4,32}$	35283.91	−0.07	−219.63	−0.02
Coalescing b- and c-type[b]				
$12_3 \leftarrow 13_2$	31195.41	−0.09	−8.61	−0.01
$20_4 \leftarrow 21_3$	31207.76	0.00	3.32	−0.04
$20_4 \leftarrow 21_3$	31212.77	0.00	3.13	−0.04
$36_6 \leftarrow 37_5$	31385.86	0.10	115.64	−0.17
$43_7 \leftarrow 44_6$	35947.03	−0.01	200.07	−0.40
$62_9 \leftarrow 63_8$	23293.80	−0.02	806.27	−1.00
$71_{10} \leftarrow 72_9$	19343.14	0.00	1250.26	−2.38
$56_6 \leftarrow 55_7$	16876.39	−0.14	−739.36	−0.28
$66_7 \leftarrow 65_8$	25252.35	−0.01	−1219.07	0.02
$74_8 \leftarrow 73_9$	24738.28	0.06	− 1679.52	1.19

[a] ±0.10 MHz. [b] The K_{-1} energy levels coalesce for high values of K_{-1}. Subscripts of J quantum number refer to K_{-1}, and not to K_{+1}.

easily made. None of the R-branch transitions are detectably split by quadrupole coupling. A portion of the ground state spectrum is shown in Table 1, and the spectroscopic constants derived using 227 selected transitions are listed in Table 2. Six of the seven sextic centrifugal distortion constants were employed in order to get a good fit since high-J transitions (up to $J = 75$) were available for fitting. Ray's asymmetry parameter, $\varkappa$, is -0.996.[7] In spite of this, no problems were encountered using the A reduction and I^r representation[8] in the fitting procedure. The hypothetical frequencies of the a- type transitions can be very accurately predicted using the spectroscopic constants of Table 2. However, none of them were identified with certainty. It was therefore concluded that the dipole moment component along the a inertial axis is very small. The dipole moment is of interest. Attempts to make quantitative Stark effect measurements on several low-J transitions proved unsuccessful due to insufficient intensities of these lines.

Vibrationally excited states. The ground state spectrum is accompanied by a strong satellite spectrum presumably arising from vibrationally

excited states. Four excited states belonging to three different normal modes were ultimately assigned as shown in Table 3. The strongest of these satellites has about 50 % of the ground state intensity at dry-ice temperature. Relative intensity measurements performed largely as described in Ref. 9 yielded 96(20) cm^{-1} for this vibration, which is assumed to be the torsion around the CH_2-CH bond because this frequency is so similar to those found for the corresponding vibration in several other allylic compounds. For example, this frequency is 93(3) cm^{-1} in 1-butene,[10] 84(20) cm^{-1} in 3-buten-1-ol,[11] 91(19) cm^{-1} in 3-buten-2-ol,[1] and 90(30) cm^{-1} in 2,3-butadien-1-ol.[12] The rather large changes that occur for the rotational constants upon excitation of this mode (see Tables 2 and 3) are also typical for a vibration involving heavy atoms.

The Q-branch transitions of the second excited state of this torsional mode were also assigned, as shown in Table 3. However, due to low intensities, only tentative assignments could be obtained for a few low-J R-branch lines. For this excited state, the values $A-C=16958.410(53)$ MHz and $\varkappa=-0.996779$ are certain.

The second most prominent vibrationally ex-

Table 2. Spectroscopic constants[a] of the ground vibrational states of $CH_3NHCH_2CH=CH_2$ and $CH_3NDCH_2CH=CH_2$.

Species	$CH_3NHCH_2CH=CH_2$[b]	$CH_3NDCH_2CH=CH_2$[b]
N.o.t.[c]	227	54
R.m.s.[d]/MHz	0.0087	0.103
A_0/MHz	19998.241(12)	18687.038(52)
B_0/MHz	2235.7349(14)	2220.8662(46)
C_0/MHz	2203.1495(16)	2189.5416(47)
Δ_J/kHz	0.6441(16)	0.560(14)
Δ_{JK}/kHz	$-23.329(33)$	$-19.774(69)$
Δ_K/kHz	452.69(25)	429 (11)
δ_J/kHz	$-0.104872(76)$	$-0.093241(75)$
δ_K/kHz	38.65(27)	12.58(37)
Φ_J/Hz	0.00079(69)	$-0.178(14)$
Φ_{JK}/Hz	0.029(27)	$-$[e]
Φ_{KJ}/Hz	1.18(37)	$-$[e]
Φ_K/Hz	$-37.3(65)$	$-$[e]
φ_J/Hz	$-0.000547(18)$	$-0.000377(15)$
φ_{JK}/Hz	$-0.462(53)$	$-$[e]

[a]Uncertainties represent one standard deviation. [b]φ_K preset at zero. [c]Number of transitions. [d]Root-mean-square deviation. [e]Preset at the value found for the parent species shown in adjacent column.

Table 3. Spectroscopic constants[a] of vibrationally excited states of $CH_3NHCH_2CH=CH_2$.

Vib. state	1st ex. lowest tors.[b,e]	2nd ex. lowest tors.[f]	1st ex. second lowest tors.[g]	1st ex. lowest bending[h]
N.o.t.[c]	184	50[i]	82[i]	48[i]
R.m.s.[d]	0.103	0.141	0.079	0.137
A_v/MHz	19562.514(17)	19172.209(44)	20276.487(21)	19771.396(51)
B_v/MHz	2239.0896(24)	2241.106(28)	2223.4341(98)	2253.000(15)
C_v/MHz	2209.2618(23)	2213.799(29)	2192.571(10)	2224.823(16)
Δ_J/kHz	0.6482(23)	$-^j$	$-^j$	$-^j$
Δ_{JK}/kHz	$-20.439(44)$	$-19.52(16)$	$-26.581(46)$	$-21.95(19)$
Δ_K/kHz	163.72(28)	$-^j$	780 (16)	$-^j$
δ_J/kHz	$-0.11306(11)$	$-0.12196(37)$	$-0.105334(30)$	$-0.11332(33)$
δ_K/kHz	43.44(51)	83.9(39)	43.58(25)	56.6(35)
Φ_J/Hz	$-0.0121(11)$	$-^j$	$-^j$	$-^j$
Φ_{JK}/Hz	$-0.439(39)$	$-2.46(22)$	$-^j$	$-0.54(23)$
Φ_{KJ}/Hz	7.68(63)	$-^j$	$-^j$	$-^j$
Φ_K/Hz	-314 (12)	$-^j$	$-^j$	$-^j$
φ_J/Hz	$-0.000812(26)$	$-0.00213(16)$	$-0.0005497(52)$	$-0.00077(15)$
φ_{JK}/Hz	$-1.372(77)$	$-^j$	$-^j$	$-^j$

[a,b,c,d]Comments as for Table 2. [e]Presumably first excited state of the $-CH_2-CH=$ torsion. [f]Second excited state of the $-CH_2-CH=$ torsion. [g]Presumably the first excited state of the $-NH-CH_2-$ torsion. [h]First excited state of lowest bending vibration. [i]Tentative assignments of low-J R-branch lines. A_v-C_v and $\varkappa$ are certain, see text. [j]Fixed at ground state value shown in Table 2.

cited state has about 40 % of the ground state intensity at dry-ice temperature. This translates into a vibrational frequency of 124(30) cm^{-1}. It is again seen from Tables 2 and 3 that rather large changes in the rotational constants occur, which is typical for a mode involving heavy atoms. It is therefore presumed that this is the first excited state of the CH_2-N torsional vibration. The frequency of this vibration is rather close to 152(20) cm^{-1} found for the corresponding vibration in $CH_3NHCH_2C\equiv CH$,[13] and 151(30) cm^{-1} found for $CH_3NHCH_2C\equiv N$.[14] The R-branch lines found in this case are considered only as tentative. However, the values $A-C=18083.916(23)$ MHz and $\varkappa=-0.996587$ are certain.

The last entry of Table 3 is tentatively assigned as the first excited state of the lowest bending vibration. A frequency of 198(40) cm^{-1} was determined for this vibration which has roughly 23 % of the ground state intensity at dry-ice temperature. The reason for assigning this as a bending mode is the comparatively large change in the rotational constants upon excitation, which indicates that heavy atoms are involved. Its frequency is also typical for this kind of vibration.

Again, only tentative assignments of R-branch lines could be made; $A-C=17546.573(53)$ MHz and $\varkappa=-0.996788$ were determined in this case.

The methyl group torsion has a frequency of 225 cm^{-1} in $CH_3NHCH_2C\equiv CH$.[13] A similar frequency was expected for the corresponding vibration in the title compound. An intensity of about 19 % of the intensity of the ground state was thus predicted for the first excited state of this torsional vibration at dry-ice temperature. The rotational transitions of this state were furthermore expected to occur rather close to the corresponding ground state lines, because relatively small changes of the rotational constants were expected since little reduced mass is involved in this vibration. However, searches for this excited state were not successful. Apart from low intensity, non-rigid rotor behaviour or splitting caused by tunneling of the methyl group with consequent splitting and intensity reduction could be the cause of this.

Searches for further conformations. The assignments reported above include almost 600 transitions. All the strongest lines in the spectrum,

Table 4. Plausible molecular structure[a] (bond lengths in pm, angles in degrees) of $CH_3NHCH_2CH=CH_2$.

Structural parameters held fixed

C–N	146.4	∠CNC	112.0
C=C	133.1	∠CCN	110.0
C–C	149.6	∠CCC	124.3
N–H	101.7	∠HC=C	121.5
–C–H	109.3	∠NCH	109.47
=C–H	109.0	∠CCH	109.47
		∠HCH	109.47

Fitted structural parameter

∠NCCC   123(3)   from *syn*

Rotational constants/MHz

Species	$CH_3NHCH_2CH=CH_2$			$CH_3NDCH_2CH=CH_2$		
	Obs.	Obs.-Calc.	Diff./%	Obs.	Obs.-Calc.	Diff./%
A_O	19998.24	−22.27	0.11	18687.04	−37.67	0.20
B_O	2235.73	−7.09	0.32	2220.87	−6.22	0.28
C_O	2203.15	−12.83	0.58	2189.54	−11.30	0.52

Kraitchman's coordinates[b] for methylamino group hydrogen atom

From rotational constants	76.31(22)	78.41(22)	108.51(16)
From plausible structure	84.1	76.8	108.5

Hydrogen bond parameters

$H\cdots C_H$	263	∠N–H$\cdots C_H$	67
$H\cdots C_{H_2}$	344	∠N–H,C=C[c]	57

[a]See text. [b]Ref. 15. [c]Angle between N–H and C=C bonds.

most of the lines of intermediate intensity and many weak ones also have been assigned. Stark effect studies were made for the remaining lines of intermediate intensity, but none of them were found to have a resolved Stark effect. No obvious quadrupole splittings were noted for the unidentified lines. It is, in fact, believed that most of them are high-*J* Q- or R-branch lines belonging to vibrationally excited states of the identified conformation. It is also very likely that the hypothetical rotamers II–IX shown in Fig. 1 would possess sizable dipole moments. The strongest unidentified lines have less than roughly 20 % of the intensity of the strongest assigned ones. Maximum possible intensity could thus be 20 % for any hypothetical unassigned rotamer. It was therefore conservatively estimated that conformation I is at least 3 kJ mol⁻¹ more stable than any other form.

Deuterated species. The deuterated species was studied in order to determine beyond doubt the position of the methylamino group hydrogen atom position. To determine the spectroscopic constants listed in Table 1, 54 transitions with *J* ⩽ 62 were used. The substitution coordinates[15] of this atom are shown in Table 4, and they clearly show that conformation I has not been confused with any of the other eight rotamers shown in Fig. 1.

Structure. Only two isotopic species were studied for *N*-methylallylamine. A complete geometric structure could not, therefore, be determined for the compound. Some assumptions had to be made. Only the C=C–C–N dihedral angle was fitted in steps of 1°, all the remaining structural parameters being taken from recent accurate structural studies and held fixed at the values

shown in Table 4. The C=C−C−N dihedral angle was found to be 123° from *syn*, and a liberal uncertainty limit, corresponding approximately to three standard deviations, is 3°. The two *skew* conformations found for allylamine[2] also have dihedral angles close to 120°.

The distance between the hydrogen atom of the methylamino group and the nearest carbon atom of the double bond is 263 pm. This is about 30 pm shorter than the sum of the van der Waals distances[16] between an aromatic carbon atom (170 pm) and hydrogen (120 pm), and is indicative of a weak H bond.

Discussion

This study shows that substitution of a hydrogen atom in the amino group of allylamine with a methyl group has rather great conformational consequences. Instead of four rotameric forms with rather similar energies,[2] one conformation predominates for N-methylallylamine. This rotamer is the N−C−C=C *skew* form denoted I in Fig. 1. The introduction of the methyl group means that only one amino group hydrogen atom is available for H bonding in N-methylallylamine, while two such atoms are available in allylamine. The conditions for forming what we prefer to call weak internal H bonds are thus much better in allylamine than in the title compound. Indeed, intramolecular H bonds are present in all four assigned forms of allylamine.[2] Moreover, the greater size of the methyl group than that of the hydrogen atom means that steric repulsion is possible in some forms of N-methylallylamine, whereas this effect is not present in allylamine. In addition, several of the conformations of Fig. 1 may suffer from repulsion between the double bond π electrons and the nitrogen atom lone electron pair. Conformation I of Fig. 1 is therefore preferred by the title compound since this rotamer has ideal steric conditions in that the methyl group avoids close proximity with neighbouring groups. The presumed repulsion between the nitrogen atom lone electron pair and the π electrons of the double bond is also minimal in this conformer, and a weak intramolecular hydrogen bond is presumably formed between the methylamino group hydrogen atom and the double bond. It is difficult to give quantitative values for the individual interactions, but their sum must be at least 3 kJ mol^{-1} more favourable than for any other possible rotameric form.

References

1. Smith, Z., Carballo, N., Wilson, E. B., Marstokk, K.-M. and Møllendal, H. *J. Am. Chem. Soc. 107* (1985) 1951.
2. (a) Roussy, G., Demaison, J., Botskor, I. and Rudolph, H. D. *J. Mol. Spectrosc. 38* (1971) 535; (b) Botskor, I., Rudolph, H. D. and Roussy, G. *J. Mol. Spectrosc. 52* (1974) 457; (c) Botskor, I., Rudolph, H. D. and Roussy, G. *J. Mol. Spectrosc. 53* (1974) 15; (d) Botskor, I., Rudolph, H. D. *J. Mol. Spectrosc. 71* (1978) 430.
3. Marstokk, K.-M. and Møllendal, H. *J. Mol. Struct. 5* (1970) 205.
4. Smyth, C. P. *Dielectric Behavior and Structure,* McGraw-Hill, New York 1955, p. 244.
5. Gordy, W. and Cook, R. L. *Microwave Molecular Spectra,* Wiley, New York 1984, p. 419.
6. Gordy, W. and Cook, R. L. *Microwave Molecular Spectra,* Wiley, New York 1984, p. 415.
7. Gordy, W. and Cook, R. L. *Microwave Molecular Spectra,* Wiley, New York 1984, p. 229.
8. Gordy, W. and Cook, R. L. *Microwave Molecular Spectra,* Wiley, New York 1984, p. 329.
9. Esbitt, A. S. and Wilson, E. B. *Rev. Sci. Instrum. 34* (1963) 901.
10. Kondo, S., Hirota, E. and Morino, Y. *J. Mol. Spectrosc. 28* (1968) 471.
11. Marstokk, K.-M. and Møllendal, H. *Acta Chem. Scand. Ser. A 35* (1981) 395.
12. Horn, A., Marstokk, K.-M., Møllendal, H. and Priebe, H. *Acta Chem. Scand. Ser. A 37* (1983) 679.
13. Marstokk, K.-M. and Møllendal, H. *Acta Chem. Scand. Ser. A 39* (1985) 483.
14. Braathen, O.-A., Marstokk, K.-M. and Møllendal, H. *Acta Chem. Scand. Ser. A 39* (1985) 605.
15. Kraitchman, J. *Am. J. Phys. 21* (1953) 17.
16. Pauling, L. *The Nature of the Chemical Bond,* 3rd ed., Cornell University Press, New York 1960, p. 260.