Microwave Spectrum, Conformation, Dipole Moment, and Quantum Chemical Calculations of 1-Amino-1-ethenylcyclopropane[†]

Karl-Magnus Marstokk,[‡] Armin de Meijere,[§] Harald Møllendal,*[,‡,||] and Karsten Wagner-Gillen[§]

Department of Chemistry, The University of Oslo, P.O. Box 1033 Blindern, N-0315 Oslo, Norway, and Institut für Organische Chemie, Georg-August-Universität Göttingen, Tammannstrasse 2, D-37077 Göttingen, Germany

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The microwave spectrum of 1-amino-1-ethenylcyclopropane has been investigated in the 13−40 GHz spectral region at about −45 °C. The prevailing *(ap)*-rotamer (*sp* with respect to the cyclopropyl and amino, *ap* with respect to cyclopropyl and the vinyl group) was assigned. This rotamer is virtually a hybrid of the most stable conformer of unsubstituted ethenylcyclopropane and unsubstituted cyclopropylamine, each in its preferred orientation; it has a symmetry plane (C_s symmetry) with the C−N bond and the C═C double bond syn to each another. In this conformation, both of the hydrogen atoms of the amino group may be involved in weak intramolecular hydrogen bonds with the π electrons of the double bond. The dipole moment components and the total dipole moment are (in units of 10^{-30} C m): $\mu_a = 2.00(1)$, $\mu_b = 0.89(14)$, $\mu_c = 0.0$ (for symmetry reasons), and $\mu_{tot} = 2.19(9)$. Four vibrationally excited states belonging to three different normal modes were assigned and their frequencies determined by relative intensity measurements. The microwave work has been assisted by quantum chemical computations at the elaborate MP2/cc-pVTZ, as well as at the B3LYP/6-31G* levels of theory.

Introduction

The laboratory in Oslo has for a long time been interested in intramolecular hydrogen (H) bonding.[1] The amino group often takes part in this kind of interaction. In the majority of cases it acts as a proton *acceptor* ("base"). Much fewer examples of the amino group acting as proton *donor* ("acid") have been reported. However, in recent years the amino group has indeed been found to be a proton *donor* toward a number of different acceptors in molecules possessing weak internal H bonds. This has been seen in ethylamines, $H_2NCH_2CH_2X$, where the acceptor atom or group X = F,[2] NH_2,[3] C≡N,[4] C≡CH,[5] OCH_3,[6] CH═CH_2,[7] as well as in $H_2NCH_2CHF_2$.[8] Further examples include $H_2NCH_2C{\equiv}CH$,[9] $H_2NCH_2C{\equiv}N$,[10] $H_2NCH_2C{=}CH_2$,[11] aminomethylcyclopropane,[12] and 1-amino-1-ethynylcyclopropane.[13]

Allylamine, $H_2NCH_2C{=}CH_2$, is of special relevance to the present work on 1-amino-1-ethenylcyclopropane (AECP). Microwave (MW) studies[11] have shown that four conformers exist for allylamine within a narrow energy range. In two of these rotamers the C−N bond is synclinal (sp) to the double bond (N−C−C═C dihedral angle = 0°); in the other two forms it is anticlinal (ac) (N−C−C═C dihedral angle about 120° from syn).[11] The syn conformer, which has a symmetry plane (C_s symmetry), is the most stable rotameric form of allylamine.[11,14] In this conformer *both* H atoms of the amino group are simultaneously involved in intramolecular H bonding with the double bond.

Formally, AECP can be thought of as a *derivative* of allylamine in which the H atoms of the methylene group have been replaced by two *methylene* groups that form a cyclopropyl ring. This replacement introduces steric and electronic interactions between the amino and the cyclopropyl group of a kind that is not present in the simpler allylamine molecule. AECP can also be considered as a hybrid between cyclopropylamine and ethenylcyclopropane (vinylcyclopropane). The conformation of the former has been determined by microwave spectroscopy to be solely synperiplanar (sp) with respect to the lone pair on nitrogen and the axis bisecting the cyclopropyl group.[15,16] Ethenylcyclopropane, on the other hand, exists in the gas phase as an equilibrium mixture of approximately 75% antiperiplanar (ap or s-trans) and 25% synclinal (sc or gauche) conformer.[17] The structural and conformational consequences of this increased complexity were an additional motivation to carry out the present investigation.

Five rotameric forms, two syn and three skew, can be envisaged for AECP in analogy with the findings made for allylamine (see Figure 1).[11] In syn I both H atoms of the amino group are involved in H bonding with the π electrons of the double bond. This rotamer has a symmetry plane (C_s symmetry). In syn II the amino group is rotated 120° around the N−C bond from the position it had in syn I. Only *one* of the H atoms of the amino group can interact with the π electrons of the double bond in this case.

In the three skew rotamers shown in Figure 1, a 120° rotation about the C1−C2 bond from syn has been made. No rotation around the N1−C1 bond has been made for skew I as compared to syn I, whereas rotation of 120° and 240° has been made for skew II and skew III, respectively. H bonding with the said π electrons would only be possible for skew I and II, and not for skew III. Only one of the H atoms of the amino group can be involved in H bonding in skew I and II.

[†] Dedicated to Professor Wolfgang Lüttke on the occasion of his 80th birthday.

* To whom correspondence should be addressed.

[‡] Department of Chemistry, The University of Oslo.

[§] Institut für Organische Chemie, Georg-August-Universität Göttingen.

[||] E-mail; harald.mollendal@kjemi.uio.no.

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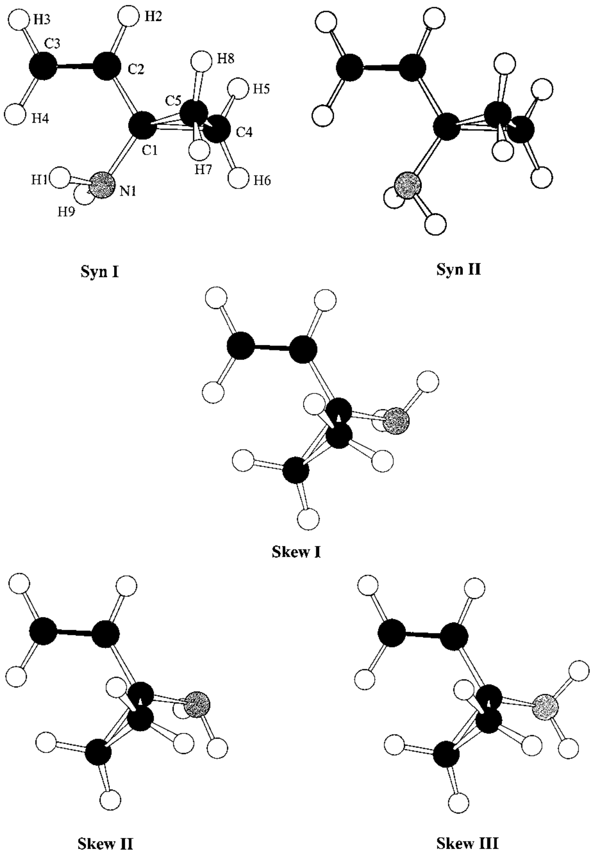

Syn I **Syn II**

Skew I

Skew II **Skew III**

Figure 1. Five conformations of 1-amino-1-ethenylcyclopropane (AECP). The first denominator stands for the conformation of the cyclopropylamine subunit with respect to the lone pair on nitrogen and the plane bisecting the cyclopropane ring; the second, for that of the ethenylcyclopropane subunit. Atom numbering is shown for the sp,ap conformer denoted syn I, the MW spectrum of which was assigned in this work.

No experimental studies of the conformational properties of the title compound have been reported. MW spectroscopy is ideal for investigating conformational properties in cases where dipolar forms are present because of its high selectivity and specificity. All conceivable rotamers would each possess a sizable dipole moment, which is a prerequisite for a MW spectrum. AECP is therefore very well suited for a MW conformational investigation.

Advanced quantum chemical computations are often found to be useful in predicting rotational constants, dipole moments, and energy differences for the various conformers that are sufficiently close to the experimental ones to be really helpful starting points in the spectral analysis. In addition, they may give important information about rotamers that for whatever reason have not been assigned by MW spectroscopy. Such calculations are therefore of interest in their own right as well.

Experimental Section

The sample used in this work was synthesized and purified as described in ref 18. The MW spectrum was studied using the Oslo spectrometer, which is briefly described in ref 19. Measurements were made in the 13−40 GHz spectral region. The X-band brass Stark absorption cell was cooled to about −45 °C during the experiments. Lower temperatures that would have enhanced the intensity of the spectrum could not be used owing to the limited vapor pressure of the compound. Radio frequency MW double resonance (RFMWDR) experiments were carried out as described in ref 20 using the equipment mentioned in ref 7. The spectra were recorded at a pressure of a few Pa and stored electronically using the computer programs written by Waal.[21] The accuracy of the frequency measurements is presumed to be better than ±0.10 MHz. The spectral resolution was approximately 0.5 MHz. The noise level was roughly 3×10^{-9} cm^{-1}. The weakest absorption lines used in the least-squares fits had intesities exceeding 1.5×10^{-8} cm^{-1}.

Results and Discussion

Quantum Chemical Calculations. The Gaussian 94 program package[22] running on the IBM RS6000 cluster in Oslo was employed in all the quantum chemical calculations. The 6-31G* basis set[22] as well as the correlation-consistent polarized triple-ζ basis set,[23] cc-pVTZ, provided with the program[22] were employed. Two different computational schemes, the elaborate MP2/cc-pVTZ procedure and the much less demanding B3LYP/6-31G* method, were employed in the majority of the computations. In the first of these procedures, electron correlation was included using the second-order Møller−Plesset (MP2) perturbation theory.[24] In the second procedure, density functional theory (DFT) calculations were carried out by employing the B3LYP procedure.[25] Full geometry optimization was made in both the MP2 and in the B3LYP computations.

The reason for selecting these two computational schemes is that the MP2/cc-pVTZ procedure is assumed to produce accurate structures[26] for the conformations in question. Rather accurate rotational constants are thus expected from such calculations. This, of course, facilitates the spectral assignments.

It is assumed that the B3LYP/6-31G* structures, dipole moments, and vibrational frequencies[25] are also rather accurate. Calculations of the structures and vibrational frequencies were first made with the B3LYP procedure, allowing for full geometry optimization. The B3LYP structures thus obtained were then used as input in the MP2 computations. MP2 vibrational frequencies were not computed because of lack of resources.

Of the five possible conformations in Figure 1, only four, syn I and II as well as skew I and II, were found to be *stable* (i.e. minima on the potential energy hypersurface) in the B3LYP calculations, because no negative vibrational frequencies[27] were computed for any of them. No stable skew III form was identified in these computations. The computations in fact refined to another structural isomer in this case, and *not* to the skew III conformation. Because the MP2/cc-pVTZ calculations are so comprehensive, no calculations for an assumed starting geometry of the hypothetical skew III rotamer were carried out. Instead, computations using a third computational scheme, i.e. the HF/6-31G* procedure, were made only in this particular case. These computations yielded the same result as found in the B3LYP procedure above. It is believed on the basis of the B3LYP and HF calculations that skew III indeed does not exist as a minimum energy conformation of the molecule and that the other four conformers (syn I and II, and skew I and II) are the *only* stable forms of this compound.

The MP2 geometries are given in Table 1 (atom numbering in Figure 1) together with some other parameters of interest. The B3LYP geometries that are not included in this table for economic reasons, were very similar to the MP2 geometries. This was also the case for the dipole moments and energy differences between the conformers.

Some of the results in Table 1 deserve comment. It is noted that syn I is favored by more than 9 kJ mol^{-1} relative to the other three stable forms. Several factors are presumed to be of importance for the stability of this rotamer.

TABLE 1: Structure, Rotational Constants, Dipole Moment, and Energy Differences between the Syn and Skew Rotamers of 1-Amino-1-ethenylcyclopropane As Calculated at the MP2/cc-pVTZ Level of Theory[a]

	conformer[b]			
	syn I	syn II	skew I	skew II
	Bond Distance/pm			
N1−H1	101.4	101.2	101.4	101.3
C1−N1	143.8	144.1	144.7	144.7
C1−C2	147.7	147.5	148.4	148.1
C2−C3	133.7	133.6	133.6	133.5
C2−H2	108.5	108.4	108.7	108.4
C3−H3	107.9	108.0	108.0	108.0
C3−H4	108.1	108.0	108.1	108.1
C1−C4	151.2	151.9	150.0	150.7
C1−C5	151.2	150.4	150.6	150.2
C4−C5	150.1	150.8	151.1	151.5
C4−H5	107.9	108.0	107.8	107.9
C4−H6	107.9	108.0	107.8	108.0
C5−H7	107.9	108.1	107.9	108.1
C5−H8	107.9	107.9	107.9	107.9
N1−H9	101.4	101.5	101.4	101.4
	Angle/deg			
H1−N1−C1	109.7	110.0	109.6	110.0
N1−C1−C2	120.0	114.6	117.0	111.8
C1−C2−C3	125.0	124.6	126.0	125.8
C1−C2−H2	115.8	115.6	115.0	114.3
C2−C3−H3	121.0	120.7	121.0	120.8
C2−C3−H4	121.4	120.6	121.4	121.6
N1−C1−C4	114.7	120.7	114.8	120.9
N1−C1−C5	114.7	118.5	113.9	116.2
C1−C4−H5	117.6	116.3	118.7	119.6
C1−C5−H6	115.5	116.3	115.8	116.3
C1−C5−H7	115.5	116.7	116.2	117.1
C1−C5−H8	117.6	117.8	117.4	117.6
H9−N1−C1	109.7	109.4	109.2	109.3
	Dihedral Angle[c]/deg			
H1−N1−C1−C2	−58.4	169.0	−60.4	168.6
N1−C1−C2−C3	0.0	3.4	125.1	132.4
N1−C1−C2−H2	180.0	−175.7	−53.8	−46.9
C1−C2−C3−H3	180.0	−179.3	179.9	−179.0
C1−C2−C3−H4	0.0	1.8	−0.1	1.1
H1−N1−C1−C4	154.6	−43.7	150.9	−40.9
H1−N1−C1−C5	88.4	−25.7	84.0	−28.8
N1−C1−C4−H5	146.3	146.5	148.5	149.0
N1−C1−C4−H6	2.9	2.0	3.2	3.0
N1−C1−C5−H7	−2.8	3.1	−1.9	4.0
N1−C1−C5−H8	−146.3	−140.0	−146.8	−140.4
H9−N1−C1−C2	58.4	−74.1	56.1	−74.7
	Rotational Constants/MHz			
A	6175.4	6199.0	5381.5	5377.2
B	2952.2	2960.9	3151.1	3183.2
C	2399.1	2403.1	2501.9	2495.1
$(I_a + I_b - I_c)^d/10^{-20}$ m^2 u	42.38	41.91	50.29	50.20
	Dipole Moment Components and Total Dipole Moment/10^{-30} C m			
μ_a	2.19	4.39	2.95	2.11
μ_b	1.14	0.01	1.86	2.13
μ_c	0.00[e]	2.82	1.13	3.06
μ_{tot}	2.46	5.21	3.67	4.29
	Energy Difference[f]/kJ mol^{-1}			
	0.0	10.6	9.3	16.2

[a] Atom numbering is given in Figure 1. [b] syn I has C_s symmetry (see text). [c] Measured from syn = 0°. Clockwise rotation corresponds to positive dihedral angle. [d] Principal moments of inertia. Conversion factor: 505379.05 × 10^{-20} m^2 u MHz. [e] For symmetry reasons. [f] Relative to syn I. Total energy of syn I: −656 645.51 kJ mol^{-1}.

The two most important effects are most probably the repulsion between the π electrons of the double bond and the lone pair of the nitrogen nucleus as well as the interaction of the electrons of the cyclopropyl group with the same lone pair. The amino group in syn I has the same orientation relative to the cyclopropyl group as it has in cyclopropylamine[15] and in tricyclopropylamine.[16] This latter preference has been explained as a result of the interaction of the electrons of the cyclopropyl ring with the lone electron pair of the amino group.[15,16] The third effect is the conjugative interaction between the ethenyl and the cyclopropyl group, which favors the ap orientation[17] of the two as in syn I. The fourth effect, finally, may be the H bond interaction, which is optimal here because *both* H atoms of the amino group can interact with the π electrons of the double bond. This interaction is definitely not strong since the distances between the H1 and H9 atoms and C2 and C3 atoms are 276 and 291 pm, respectively. The sum of the van der Waals distances for hydrogen (120 pm[28]) and aromatic carbon (170 pm[28]) is 290 pm.

MW Spectrum and Assignment of the Ground Vibrational State of Syn I. The quantum chemical computations above indicate that there is a comparatively large energy difference between syn I and the remaining three stable forms. The dipole moment components along the *a* and *b* inertial axes are not large (see Table 1 and below). μ_c is identical to zero for symmetry reasons for this rotamer. The relatively weak survey spectrum that was first observed is compatible with a small dipole moment.

The dipole moment is predicted (Table 1) to have its largest component along the *a* inertial axis. Searches were therefore first made for the relatively strong ^aR branch transitions using the rotational constants obtained in the MP2 computations as the starting point. These *R*-branch transitions were soon identified close to their predicted frequencies. Stark effect studies as well as RFMWDR experiments[20] were carried out to confirm the assignments.

A preliminary set of rotational constants was obtained from the ^aR transitions and used to predict medium- and high-*J* ^bQ-branch lines that are the strongest *b*-type transitions. These lines were readily found. Many weak high-*J* ^bR lines were then assigned. A few selected transitions are listed in Table 1S in the Supporting Information.

A total of about 250 transitions were ultimately assigned for the ground vibrational state, 237 of which were used to determine the spectroscopic constants (*A* reduction, I^r representation[29]) shown in Table 2. The maximum value of *J* was 40. Only quartic centrifugal distortion constants were employed in the least-squares fit. Inclusion of sextic constants yielded no significant improvement of the fit and insignificant sextic constants.

Comparison of the experimental rotational constants (Table 2) with the MP2 rotational constants (Table 1) shows agreement to within better than 1%. This is as good as one can expect because the experimental and MP2 constants are defined differently. The experimental rotational constants are derived from the r_o structure, whereas the MP2 constants reflect an approximate equilibrium structure.

There is also good agreement between the calculated (42.38 × 10^{-20} m^2 u) and experimental value (42.82 (same units)) of $I_a + I_b - I_c$ (I_a, I_b, and I_c are the principal moments of inertia) as seen from the same two tables. The corresponding number is 43.09 (same units) in cyclopropylamine,[15] which has a symmetry plane and the same out-of-plane atoms and groups as syn I.

The nitrogen nucleus is known to produce a quadrupole fine structure. These splittings are usually larger for the ^bQ-branch lines than for the ^aR-branch transitions. However, no well-resolved splittings were observed in the present case. It was

TABLE 2: Spectroscopic Constants[a,b] of the Ground and Vibrationally Excited States of Syn I of 1-Amino-1 ethenylcyclopropane

	ground vibrational state	1st ex state of the C1-C2 torsion	2nd ex state of the C1-C2 torsion	1st ex lowest bending vibration	1st ex lowest C1-N1 torsional vibration
no. of transitions	237	134	89	29	30
rms dev[c]/MHz	0.072	0.078	0.071	0.073	0.081
A_v/MHz	6112.8583(18)	6090.3907(41)	6067.4127(50)	6127.48(18)	6098.95(239
B_v/MHz	2925.869 55(88)	2927.0770(32)	2927.9630(38)	2925.657(11)	2923.465(12)
C_v/MHz	2377.319 88(78)	2380.8257(32)	2382.3721(38)	2374.8877(83)	2375.253(11)
Δ_J/kHz	0.2970(15)	0.382(35)	0.337(43)	0.214(51)	0.540(59)
Δ_{JK}/kHz	1.8225(86)	1.834(16)	1.805(22)	1.55(10)	0.91(13)
Δ_K/kHz	0.5370 (62)	0.472(91)	0.83(11)	0.537[d]	0.537[d]
δ_J/kHz	0.051 69(68)	0.051 84(88)	0.0451(12)	0.113(45)	0.205(53)
δ_K/kHz	0.022(15)	0.016(20)	0.097(29)	0.023[d]	0.023[d]
$(I_a + I_b - I_c)^e/10^{-20}$ m^2 u	42.819 037(48)	43.365 805(89)	43.642 231(99)	42.4166(34)	42.9646(44)

[a] *A* reduction, I^r- representation.[29] [b] Uncertainties represent one standard deviation. [c] Root-mean-square deviation. [d] Kept constant at this value in the least-squares fit. [e] Principal axis moments of inertia. Conversion factor: 505 379.05 m^2 u MHz.

therefore not possible to determine the nuclear quadrupole coupling constants of the nitrogen nucleus.

Vibrationally Excited States. The ground state transitions were accompanied by series of transitions presumably belonging to vibrationally excited states of syn I. Four excited states belonging to three different vibrational normal modes were assigned in the same manner as described for the ground vibrational state lines. The spectroscopic constants obtained for these excited states are listed in Table 2; the full spectra are found in Tables 2S−5S.

The most intense excited state (Table 2) has about 49% of the intensity of the ground vibrational state at 228 K. Its frequency was determined to be 113(20) cm^{-1} by relative intensity measurements made largely as described in ref 28. This should be compared with 137 cm^{-1} found in the B3LYP calculations (not given in Table 1) for the lowest torsional mode, i.e., the torsion around the C1−C2 bond. The second excited state of this mode was also identified, as shown in the same table. It is seen that the rotational constants change quite significantly, but not completely linearly upon excitation, as would have been typical for a harmonic vibration.[31] It is also noted that $I_a + I_b - I_c$ increases from the ground-state value upon excitation. This is typical for an out-of-symmetry-plane vibration.[31]

The first excited state of another fundamental (Table 2) was found to have about 20% of the intensity of the ground vibrational state. A frequency of 255(25) cm^{-1} was determined by relative intensity measurements.[30] This mode is assumed to be the lowest heavy-atom bending vibration. The B3LYP value for this fundamental was 268 cm^{-1}. The decrease of $I_a + I_b - I_c$ upon excitation is typical for bending vibrations of a molecule possessing a symmetry plane.[31]

The first excited state of the torsional vibration of the amino group (torsion around the N1−C1 bond) was also found (approximately 17% of the intensity of the ground vibrational state), and a frequency of 280(30) cm^{-1} determined by relative intensity measurements,[30] compared to 280 cm^{-1} calculated in the B3LYP procedure. A small increase of $I_a + I_b - I_c$ from the ground-state value was seen in this case, as expected.[31]

The fourth lowest fundamental vibration was calculated at the B3LYP level to have a frequency of 362 cm^{-1}. This corresponds to a Boltzmann factor of about 10% at 228 K. This rather small value can explain why this weak excited state was not found.

Dipole Moment. The dipole moment of syn I was determined in the standard way[8] by employing Stark voltages in the 1000−2000 V cm^{-1} range. The results are shown in Table 3.

TABLE 3: Stark Coefficients[a] and Dipole Moment[a] of Syn I of 1-Amino-1-ethenylcyclopropane

		$\Delta\nu E^{-2}/10^{-6}$ MHz V^{-2} cm^2	
transition	$\|M\|$	obs	calc
$5_{2,4} \leftarrow 4_{2,3}$	1	0.726(9)	0.756
	2	3.07(3)	3.06
	3	7.02(7)	6.87
	4	12.3(2)	12.2
$3_{1,2} \leftarrow 2_{1,1}$	1	−1.38(2)	−1.40
$3_{1,3} \leftarrow 2_{1,2}$	1	1.52(2)	1.50

dipole moment/10^{-30} C m

$\mu_a = 2.004(11)$ $\mu_b = 0.88(14)$ $\mu_c = 0.0^b$ $\mu_{tot} = 2.191(88)$

[a] Uncertainties represent one standard deviation. 1 D = 3.335 64 × 10^{-30} C m. [b] For symmetry reasons; see text.

The MP2 values (Table 1) for μ_a and μ_b were (in units of 10^{-30} C m) 2.19 and 1.14, respectively. The corresponding B3LYP values were (same units) 2.13 and 0.95, respectively. Comparison with the results in Table 3 reveals that the B3LYP predictions are slightly closer to the experimental values than the MP2 calculations are.

The total dipole moment of the corresponding conformer of $H_2NCH_2C{=}CH_2$ is 2.99(2) × 10^{-30} C m,[11a] a little larger than 2.191(88) (same units) seen for the title compound (Table 3).

The calculated rotational constants (Table 1) of syn I and II are rather similar and close to the experimental rotational constants (Table 2). A distinction between syn I and II cannot therefore be made solely on the basis of the rotational constants. Additional evidence, e.g., the dipole moment, is needed. The dipole moment is predicted (Table 1) to be rather different in the two cases. The experimental dipole moment is close to that predicted for I. This makes us conclude beyond doubt that syn I has indeed been assigned and not confused with II.

Searches for Further Conformations. The three other rotamers (syn II, skew I and II) are predicted to be at least 9 kJ mol^{-1} less stable than syn I in the MP2 computations above (Table 1). If this energy difference were correct, any one of the other three forms would each be present in a concentration below approximately 5% of the concentration of syn I. Each of these three conformers are predicted to have a sizable dipole moment (same table). It should therefore be possible to assign them provided they would exist in relatively large fractions.

All the strongest lines of the spectrum could be assigned to syn I. Attempts to find the other three rotamers were unsuccessful. The starting points in these searches were the spectra predicted using the MP2 rotational constants and the dipole moment components given in Table 1. Ordinary Stark spectroscopy and RFMWDR searches were made among the weak unassigned absorption lines. These searches were unsuccessful. It is concluded that any other rotameric form would have been identified provided the energy difference between it and syn I was less than 3 kJ mol^{-1}. This value is consistent with the MP2 predictions (more than 9 kJ mol^{-1}; Table 1).

Structure. The observed (Table 2) and the calculated (Table 1) rotational constants of syn I agree to within better than 1%. The B3LYP rotational constants (not given in Table 1) also agree to within better than 1%. There is in addition good agreement for the calculated (Table 1) and the observed (Table 3) values of $I_a + I_b - I_c$. It is believed that this agreement is not fortuitous, but in fact reflects that both the elaborate MP2 and as well as the much less expensive B3LYP structures are accurate in this case. The MP2 structure (Table 1) is therefore suggested as a *plausible* structure for syn I. It is expected that any full experimental structure that is determined in the future will be very close to this structure.

Conclusions

This study has demonstrated that gaseous 1-amino-1-ethenylcyclopropane (AECP) consists almost exclusively of the rotamer syn I (Figure 1) at −45 °C. The prevalence of this conformer is undoubtedly a consequence of several factors: Two weak internal H bonds formed between the H atoms of the amino group and the π electrons of the double bond probably help to stabilize the said rotamer. Repulsion between the lone pair of the amino group and the same π electrons as well as interaction between this lone pair and the electrons of the cyclopropyl group are presumed to have the major effect on the stability of this conformer. The conjugative interaction between the ethenyl and the cyclopropyl group is likely to also contribute to the stability of this rotamer. Essentially, the preferred conformer of AECP is the ideal hybrid of the most favorable conformations of all three of its subunits, i.e., allylamine, cyclopropylamine, and ethenylcyclopropane.

Accurate predictions of the structure and dipole moment is found in the elaborate MP2/cc-pVTZ calculations as well as in the cost-efficient B3LYP/6-31G* computations.

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Supporting Information Available: Tables 1S−5S contain the MW transitions used to determine the spectroscopic constants shown in Table 2. This material is available free of charge via the Internet at http://pubs.acs.org.

References and Notes

(1) Recent examples include: (a) (3,3,3-trifluoropropanol) Marstokk, K.-M.; Møllendal, H. *Acta Chem. Scand.* **1999**, *53*, 202. (b) (dicyclopropyl carbinol) Marstokk, K.-M.; Møllendal, H. *Acta Chem. Scand.* **1997**, *51*, 800. (c) (1,2-diphosphinoethane) Marstokk, K.-M.; Møllendal, H. *Acta Chem. Scand.* **1997**, *51*, 875. (d) (1,2-ethanedithiol) Marstokk, K.-M.; Møllendal, H. *Acta Chem. Scand.* **1997**, *51*, 653. (e) (2-nitroethanol) Marstokk, K.-M.; Møllendal, K.-M. *Acta Chem. Scand.* **1996**, *50*, 505. (f) (1-cyclopropylcyclopropanol) Chaplinski, V.; Marstokk, K.-M.; de Meijere, A.; Møllendal, H. *Acta Chem. Scand.* **1996**, *50*, 486. See also reviews: (g) Wilson, E. B.; Smith, Z. *Acc. Chem. Res.* **1987**, *20*, 257. (h) Møllendal, H. In *Structures and Conformations of Non-Rigid Molecules*; Laane, J., Dakkouri, M., van der Veken, B., Oberhammer, Eds.; H. Kluwer Academic Publishers: Dordrecht, The Netherlands, 1993; p 277.

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