AMD 2 in conformational defects of DNA, no specificity should be expected in this latter case. This is regardless of the similar optical changes which were observed when actinomycin and AMD 1 or AMD 2 interact with DNA.

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[1] Reich, E., and Goldberg, I. H., in *Progress in Nucleic Acid Research and Molecular Biology* (edit. by Davidson, J. N., and Cohn, W. E.), 184 (Academic Press, 1964).

[2] Goldberg, I. H., Rabinowitz, M., and Reich, E., *Proc. US Nat. Acad. Sci.*, **48**, 2094 (1962).

[3] Kahan, E., Kahan, F. M., and Hurwitz, J., *J. Biol. Chem.*, **238**, 2491 (1963).

[4] Cerami, A., Reich, E., Ward, D. C., and Goldberg, I. H., *Proc. US Nat. Acad. Sci.*, **57**, 1036 (1967).

[5] Liquori, A. M., De Lerma, B., Ascoli, F., Botrè, C., and Trasciatti, M., *J. Mol. Biol.*, **5**, 521 (1962).

[6] Liquori, A. M., Ascoli, F., and De Santis Savino, M., *J. Mol. Biol.*, **24**, 123 (1967).

[7] Brockmann, H., and Muxfeldt, H., *Chem. Ber.*, **91**, 1242 (1958).

[8] Mauger, A. B., and Wade, R., *J. Chem. Soc.*, 3126 (1965).

[9] Weinstein, B., Crews, O. P., Leaffer, M. A., Baker, B. R., and Goodmann, L., *J. Org. Chem.*, **27**. 1389 (1962).

[10] Gellert, M., Smith, C. E., Neville, D., and Felsenfeld, G., *J. Mol. Biol.*, **11**, 445 (1965).

[11] De Santis, P., Giglio, E., Liquori, A. M., and Ripamonti, A., *Nature*, **191**, 900 (1961).

[12] Damiani, A., De Santis, P., Giglio, E., Liquori, A. M., Puliti, R., and Ripamonti, A., *Acta Cryst.*, **19**, 340 (1965).

[13] Damiani, A., Giglio, E., Liquori, A. M., Puliti, R., and Ripamonti, A., *J. Mol. Biol.*, **20**, 211 (1966).

[14] Liquori, A. M., Costantino, L., Crescenzi, V., Elia, V., Giglio, E., Puliti, R., De Santis Savino, M., and Vitagliano, V., *J. Mol. Biol.*, **24**, 113 (1967).

Molecular Structures of Propargyl Alcohol and Propargyl Amine from Microwave Spectra

PROPARGYL alcohol and propargyl amine are of particular structural interest, because they belong to the rare class of substituted derivatives of methanol and methylamine in which the only possibilities of rotational isomerism are those associated with the COH or CNH_2 groups. We have assigned microwave spectra for six isotopic forms of propargyl alcohol and for the normal form of propargyl amine. The moments of inertia show that the rotamers concerned are those in which the OH and both NH bonds occupy gauche positions, that is, subtend dihedral angles in the region of 60° with respect to the acetylenic group. In the alcohol, the properties of the potential function for internal rotation are reflected in the occurrence of spectra of molecules in a very low-lying excited state and in the occurrence of series of spectral lines with first-order Stark effects.

Table 1. ROTATIONAL CONSTANTS

Molecule and state		A (MHz)	B ($\pm 0{\cdot}1$) MHz	C ($\pm 0{\cdot}1$) MHz
$HCC.CH_2OH$	state 1	33,000	4,700·23	4,232·25
	state 2	—	4,684·19	4,227·99
$HCC.CH_2OD$	state 1	—	4,612·73	4,130·68
	state 2	—	4,600·74	4,127·71
$DCC.CH_2OH$	state 1	—	4,360·65	3,944·66
	state 2	—	4,345·77	3,940·89
$HCC.CD_2OH$	state 1	—	4,578·71	4,087·81
	state 2	—	4,564·15	4,084·25
$DCC.CH_2OD$	state 1	—	4,282·04	3,852·89
	state 2	—	4,271·32	3,850·08
$H.CC.CD_2OD$	state 1	—	4,500·08	3,992·13
	state 2	—	4,489·53	3,989·81
$HCC.CH_2NH_2$		29,619·46 ± 0·1	4,595·12	4,160·62

The spectroscopic constants are shown in Table 1. For the alcohol, observed transitions are all caused by the component of the dipole moment in the A-axis of inertia; a total of some hundred lines were assigned on a rigid-rotor basis. For the amine, lines caused by components of the dipole in both the A- and B- axes were assigned.

The spectrum of the alcohol consists of two chief series of lines, the intensities of one series being only slightly greater than those of the corresponding members of the second. For convenience, we have distinguished the constants for the stronger series as those of the ground state (state 1) and those for the other series as belonging to a very low-lying excited state (state 2). A number of lines caused by other states of the molecules are also present. With any reasonable set of structure parameters the constants of all forms correspond convincingly only with those expected for the gauche rotamer. In particular, the changes in B and C accompanying deuteration can be accounted for only with this geometry, which is that expected by analogy with the conformation found for allyl alcohol[1]. Since beginning this work, we have learnt of similar measurements on propargyl alcohol by Dr. E. Hirota[2], at the University of Tokyo, and we are grateful to him for allowing a comparison of the data obtained by our two groups. Agreement of the rotational constants is very good, and Dr Hirota has made a considerably deeper study of the internal rotation problem, which we shall accordingly not discuss in detail here. The suggestion that the low-lying excited states arise from a rather easy tunnelling of the OH proton from one of the two equivalent gauche positions to the other fits well with Dr. Hirota's theoretical analysis of the spectra, including the series of lines with first-order Stark effects.

The rotational constants for propargyl amine, all of which can be evaluated with high accuracy, show that four hydrogen atoms are outside the HCCCN plane, and thus the spectra are those of the form in which the NH_2 group straddles the acetylenic bond. In accordance with this we have not found lines at the accurately predicted frequencies where absorption caused by any C-component of the dipole moment would lie. Support is also found in the nuclear quadrupole coupling constants for nitrogen, which have the values:

$$eQ_a = -3{\cdot}00\ \text{MHz};\ eQ_b = 1{\cdot}34\ \text{MHz};\ eQ_c = 1{\cdot}66\ \text{MHz}$$

The coupling tensor is thus roughly symmetrical about the A-axis of inertia and the constants are approximately consistent with the lone-pair electrons on the nitrogen being directed roughly along the A-axis. This would be expected for the proposed rotamer, but not for the other rotamer in which the lone pair is adjacent to the carbon-carbon triple bond. No intense satellite spectra have been observed for the amine, in contrast with the alcohol, and this, too, conforms with the proposed geometry.

We are continuing to seek spectra of the alternative rotamers of both these substances, and it is hoped that evidence of the importance, or otherwise, of these will be obtained from high resolution infrared studies of both molecules, over a range of temperatures, which are in progress. Work on the microwave spectra is also being extended in order to obtain more detailed structural information.

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[1] Murty, A. N., and Curl, R. F., *J. Chem. Phys.*, **46**, 4176 (1967).

[2] Hirota, E., *J. Mol. Spectrosc.* (in the press).