

hydrogen with heavy water in the native state at its isoelectric point or in acidic solutions, but which readily exchanges its hydrogen in alkaline media or during the changes of structure accompanying heat denaturation.

Thus from the infra-red spectra of proteins in heavy water solutions at various pH's, we can conclude that the protein absorption band noted in the region of 1,550  $\text{cm}^{-1}$  is a complex absorption band associated in part with  $\text{—COO}^\ominus$  groups (at 1,575  $\text{cm}^{-1}$ ) and in part with two kinds of peptide linkages: one type of peptide grouping is easily deuterated at room temperature, the other type of peptide group being deuterated at elevated temperatures or in alkaline solutions.

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<sup>1</sup> For an excellent discussion, see Sutherland, G. B. B. M., in "Advances in Protein Chemistry", 7, 291 (1952).

<sup>2</sup> Lenormant, H., *Ann. Chim.*, (12), 5, 459 (1950).

<sup>3</sup> cf. Blout, E. R., and Lenormant, H., *J. Opt. Soc. Amer.* (in the press).

<sup>4</sup> Edsall, J. T., Otvos, J. W., and Rich, A., *J. Amer. Chem. Soc.*, 72, 474 (1950).

<sup>5</sup> Blout, E. R., and Linsley, S. G., *J. Amer. Chem. Soc.*, 74, 1946 (1952).

unusual among hydrocarbons in having an appreciable electric dipole moment. We expect to detect spectra of  $\text{H}_3\text{CCCCCD}$ , and it seems reasonably probable that lines due to molecules containing carbon-13 will be detected in a Stark modulation spectrometer now available, and so permit evaluation of a considerable part of the molecular structure.

We are indebted to Prof. E. R. H. Jones and Dr. M. C. Whiting for the gift of a sample of 1 : 4-dichlorobut-2-yne, from which the penta-1 : 3-diyne was made. This work was carried out in collaboration with the Physics Department of the Telecommunications Research Establishment, Malvern, and made possible by the loan of microwave equipment from that Establishment.

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<sup>1</sup> Armitage, J. B., Jones, E. R. H., and Whiting, M. C., *J. Chem. Soc.*, 1993 (1952).

<sup>2</sup> Jones, E. R. H., and Whiting, M. C. *J. Chem. Soc.* (in the press).

<sup>3</sup> Nielsen, H. H., *Phys. Rev.*, 77, 130 (1950).

<sup>4</sup> Trambarulo, R., and Gordy, W., *J. Chem. Phys.*, 18, 1613 (1950).

<sup>5</sup> Anderson, W. E., Trambarulo, R., Sheridan, J., and Gordy, W., *Phys. Rev.*, 82, 58 (1951).

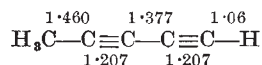
<sup>6</sup> Jeffrey, G. A., and Rollett, J. S., *Proc. Roy. Soc., A*, 213, 86 (1952).

### Microwave Spectrum of Penta-1 : 3-diyne

THE preparation of penta-1 : 3-diyne was reported by Armitage, Jones and Whiting<sup>1</sup>, and it has recently been emphasized<sup>2</sup> that chemical and ultra-violet spectroscopic evidence supports strongly the attributed structure. In confirmation, we have measured the microwave pure rotation spectrum of the substance made by this method, as observed in a video sweep spectrometer, and find it to be that of a symmetric-top molecule of structure  $\text{H}_3\text{C—C}\equiv\text{C—C}\equiv\text{C—H}$ , all five carbon atoms lying on the molecular axis.

Measurements have been made on the  $J = 4 \rightarrow 5$ ,  $5 \rightarrow 6$ ,  $7 \rightarrow 8$  and  $8 \rightarrow 9$  transitions, in all of which the expected  $K$ -splitting is well resolved. The spectroscopic constant  $B_0$  is 2,035.73<sub>3</sub> Mc./s., and the distortion coefficient  $D_{JK}$  is 20.0 kc./s. The distortion coefficient  $D_J$  is very small, not more than 0.2 kc./s. Lines due to molecules in excited bending vibrational states are also observed and show the characteristic type of pattern predicted theoretically<sup>3</sup> and found for similar molecules<sup>4,5</sup>. Measurements on the fine structures are being extended, and will be given in a fuller report later.

The moment of inertia,  $I_B$ , derived from  $B_0$ , is  $412.09 \times 10^{-40}$  gm./cm.<sup>2</sup>, in good agreement with the most probable interatomic distances. Thus the structure



(lengths in Å.), with a tetrahedral methyl group in which  $d_{CH}$  is 1.10 Å., is in accord with  $I_B$ . These bond-lengths are all close to values found for analogous bonds in related molecules, that for the central 'single' C—C bond being close to the 1.375 Å. found for similar bonds in dimethyl triacetylene by Jeffrey and Rollett<sup>6</sup>. The spectrum is reasonably intense, showing that penta-1 : 3-diyne, like methyl acetylene, is

### A New Isomer of Chlorogenic Acid from Peaches

NEOCHLOROGENIC acid, a new isomer of chlorogenic acid<sup>1</sup>, has been isolated from Elberta and Halford peaches by the use of counter-current distribution. It differs from the isochlorogenic acid<sup>2</sup> isolated from coffee and it may be readily separated from chlorogenic acid which is present in somewhat larger amounts. Chlorogenic acid has been found in pears and apples<sup>3</sup> and its presence indicated in peaches<sup>4</sup>.

An aqueous solution, freed of lipids, prepared from a water-saturated butanol extract of lyophilized peach *purée* was subjected to a 100-tube counter-current distribution<sup>5</sup> using the solvent pair ethyl acetate and 2M phosphate, pH 3.0. Analysis of the phenolic content of the tubes with Folin-Denis reagent<sup>6</sup> showed the presence of four bands. The first,  $K \sim 0.05$ , consists of anthocyanins, polymeric and unknown materials. The second,  $K = 0.39$ , is neochlorogenic acid. The third,  $K = 1.40$ , is chlorogenic acid, which may be readily crystallized, and the fourth,  $K > 10$ , consists also of polymeric and unknown materials. ( $K$ , the distribution constant, is the ratio of concentration in the lighter phase to that in the heavier phase.) Isochlorogenic acid would be in the fourth band were it present.

The tubes containing the neochlorogenic acid were collected, ethanol was added (one-fifth the volume of the ethyl acetate layer) and the phases separated. Several further extractions of the aqueous layer with 80 per cent ethyl acetate—20 per cent ethanol were made. These extracts were combined, concentrated, chilled and the precipitated sodium phosphate removed by filtration. The remaining sodium ions were removed by passing a 50 per cent alcohol solution through a column of 'Dowex-50'. Serious losses of neochlorogenic acid attended this operation. The eluate was concentrated *in vacuo*, whereupon crystallization occurred. Recrystallization could be effected from water or ethanol.