Provisional Computation of the Plane Vibration Frequencies of Symmetrical Deuteroethylenes

SEVERAL workers[1],[2] have developed the theory of the vibration spectrum of ethylene and have deduced from the experimental data values for some of the force constants occurring in the potential energy function of the molecule. A recent investigation by Bonner[3] has improved our knowledge of the vibration spectrum of ethylene.

The most general potential function for plane deformations which is compatible with the admitted symmetry of that molecule contains 15 constants. On the other hand, as there are 9 plane normal modes, it seems at first that only 9 constants of force can be determined from the present data. However, in order to reach a precision in accord with the accuracy of some data (1 cm.$^{-1}$), 11 constants are necessary, owing to reality conditions to be satisfied. Such a numerical potential function has been calculated for ethylene from Bonner's experimental data and checked by recomputation of the vibration frequencies with less than 0·15 per cent error.

Assuming that the potential function is not altered when 'heavy' hydrogens are present in the molecule, the vibration spectrum of C_2D_4 was readily obtained. The spectrum of each of the three isomers $C_2D_2H_2$ was calculated from two secular equations, one of the fifth degree, the other of the fourth. Each of them results from coupling together two families of normal modes of different symmetries in the completely symmetrical molecule C_2X_4, in such a way that a mode of the isomer of lower symmetry is produced. The coupling occurs through the kinetic energy function only, which has a lesser symmetry for the isomeres than for C_2X_4.

	C_2H_4		C_2D_4		HDC : CDH cis	HDC : CDH trans		$H_2C : CD_2$
1	S_1	1621·3	S_1	1428·8	π' 1516·5	S 1514·2	π	1555·3
2		3019·0		2283·9	3065·0	3049·2		3004·3
3		1343·9		1008·9	2304·2	2291·2		2221·0
4	A_1	2988·0	A_1	2152·5	1247·9	1240·2		1357·8
5		1444·0		1072·8	752·7	807·9		1043·1
6	S_2	3069·0	S_2	2308·0	σ' 3031·1	A 3053·2	σ	3088·1
7		950·0		758·3	2228·9	2233·4		2316·3
8	A_2	3107·0	A_2	2325·0	1295·4	1308·4		945·6
9		949·7		678·1	820·2	765·3		724·8

The horizontal lines separate the frequencies in different symmetry families. S and A, respectively, mean symmetric and antisymmetric with respect to the centre of the molecule. S frequencies are Raman active and infra-red inactive ; the reverse is true for A frequencies. π and σ respectively mean symmetric and antisymmetric with respect to the carbon axis and π' and σ' the same with respect to the perpendicular axis in the plane of the molecule. They are all active in Raman effect and in infra-red absorption, but may be of widely different intensities. The π and π' frequencies are polarized and expected strong Raman lines, whereas the σ and σ' are depolarized and weaker. As is well known, for C_2H_4 and C_2D_4, S frequencies divide into two separate families $S_1(\pi\pi')$ and $S_2(\sigma\sigma')$ and also $A_1(\pi\sigma')$ and $A_2(\pi'\sigma)$. The π frequencies show a marked Q branch in the infra-red absorption. The four fundamental symmetry families of the totally symmetric molecule combine in the following way to form the normal modes of the three isomers : $\pi'(S_1A_2)$; $\sigma'(S_2A_1)$; $\pi(S_1A_1)$; $\sigma(S_2A_2)$; $S(S_1S_2)$; $A(A_1A_2)$.

Owing to the uncertainty resting upon some data and also the neglect of the anharmonicity, no too close fit with the experiment can be hoped. However, it is expected that the obvious qualitative relationships existing between the spectra of heavy ethylenes will hold.

C. MANNEBACK.
A. VERLEYSEN.

Institute of Physics,
Louvain.
July 27.

[1] Sutherland and Dennison, *Proc. Roy. Soc.*, A, **148**, 250 (1935).
[2] Delfosse, *Ann. Soc. Sci. Bruxelles*, B, **45**, 114 (1935).
[3] Bonner, *J. Amer. Chem. Soc.*, **58**, 34 (1936).

Some Properties of Pentadeuterobenzoic Acid, C_6D_5COOH

THE acid was obtained by the reaction between pentadeuterophenyl magnesium bromide and carbon dioxide[1]. The following details enable a comparison to be made between this acid and benzoic acid :

	C_6H_5COOH	C_6D_5COOH
Melting point :	121·7° C.	120·9° C.
Solubility in 100 c.c. water at 18° C :	0·28 gm.	0·34 gm.
Molecular heat of combustion :	771400 cal.	761380 cal.
Dissociation constant at 25° C. :	$6·6 \times 10^{-5}$	$6·6 \times 10^{-5}$

A detailed account of this work will shortly appear in *Helvetica Chimica Acta*.

H. ERLENMEYER.
A. EPPRECHT.

Chemical Institute,
University of Basle.
July 29.

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Nuclear Reactions due to Neutrons of 2 m.e.v. Energy

MOST neutron workers hitherto have used Ra-Be, Ra-B or Ra-F as sources ; these yield neutrons with continuous ranges of energies extending up to several m.e.v. The D$-$D nuclear reaction is considered to yield a homogeneous group of neutrons of about 2 m.e.v. energy. It is of interest, therefore, to know whether or not D$-$D neutrons can excite the nuclear reactions of the non-capture type reported by investigators using the radioactive sources.

We have been working in the Clarendon Laboratory with the neutrons obtained by bombarding heavy hydrogen with heavy hydrogen ions. The source of ions was a low-voltage arc of a modified Tuve and Dahl type. The total ion currents used have been of the order of 100 microamps. The accelerating voltage was 225 kv. Heavy phosphoric acid has proved to possess reasonably good lasting qualities as a target material. The yield of neutrons, as measured by the 2·3 min. induced activity of silver, has been checked at intervals over fifty hours' intermittent use, and has shown a constancy well within 10 per cent. Continuous runs of up to six hours' duration have been made.

With the exceptions of silicon and iron, the element under investigation was itself exposed to the 2 m.e.v. neutrons and then tested for induced radioactivity by means of a thin-walled Geiger-Müller counter. Silicon and iron were irradiated as SiO_2 and FeS respectively.