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Network Analyzer Tests of Equivalent Circuits of Vibrating Polyatomic Molecules

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To illustrate the use of the equivalent circuits derived in the companion paper for vibrating polyatomic molecules, this paper describes network-analyzer tests of circuits for three successively more complicated molecules. The first is the symmetrical linear CO₂ molecule; the second is the unsymmetrical linear OCS molecule; and the third is the unsymmetrical nonlinear CH₂CH₂OH molecule. In each case, starting from given constants of the molecular structure, the normal frequencies and modes are measured by means of the equivalent circuit. It is shown that for these cases the analyzer measurements agree satisfactorily with the known normal-frequency characteristics.

NETWORK ANALYZER

HE alternating-current network analyzer¹ consists of a set of adjustable resistance, inductance, and capacitance units, each connected to a pair of flexible cords and plugs. Connections between units to form any desired network are made by inserting the plugs in adjacent jacks in a jack panel. As many units as desired can be connected to a common point. Alternating-current electric power is supplied by a motor-generator set to individual generator units so that several different voltages, independently adjustable, can be inserted into different parts of the network. A centrally located set of measuring instruments can be connected to any unit or circuit by means of a set of key switches.

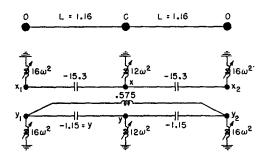


Fig. 1. Equivalent circuit of the CO₂ molecule.

¹ H. P. Kuehni and R. G. Lorraine, "A New A-C Network Analyzer," Trans. A.I.E.E. 57, 67 (1938).

Procedure

The equivalent circuits for the CO₂, OCS, and CH₃CH₂OH molecules are shown in Figs. 1–3, respectively. These circuits were obtained by methods described in the companion paper,² using the molecular constants listed in Table I; the

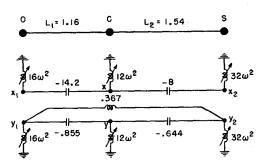


Fig. 2. Equivalent circuit of the OCS molecule.

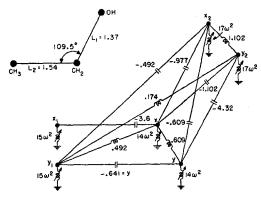


Fig. 3. Equivalent circuit of the ehtyl-alcohol molecule.

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² G. Kron, "Electric Circuit Models for the Vibration Spectrum of Polyatomic Molecules," J. Chem. Phys. 14, 19 (1945).

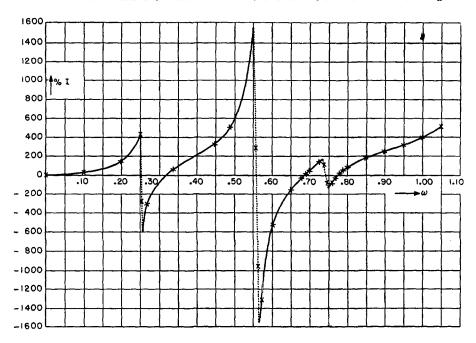


Fig. 4. Variation of generator current with frequency.

constants are based on previous data,^{3,4} with the angular spring constants of the former reference corrected by a factor of one-fourth.

The process of locating the normal frequencies from these circuits is similar to that already described in connection with the study of the Schrödinger equation.⁵ The circuits specify both

TABLE I. Molecular constants.

CO_2	L = 1.16	k = 15.3	$m_c = 12$
		$k_{\alpha} = 0.772$	$m_o = 16$
ocs	$L_{oc} = 1.16$	$k_{oc} = 14.2$	$m_c = 12$
	$L_{cs} = 1.54$	$k_{cs} = 8$	$m_0 = 16$
		$k_{\alpha} = 0.655$	$m_s = 32$
CH₃CH₂OH	$L_1 = 1.37$	$k_1 = 4.1$	$m_{\text{CH}_3} = 15$
	$L_2 = 1.54$	$k_2 = 3.6$	$m_{\text{CH}_2} = 14$
	$\alpha = 109.5^{\circ}$	$k_{\alpha} = 1.102$	$m_{\rm OH} \approx 17$

The stretching force-constants k are expressed in 10⁵ dyne/cm, the bending force-constants k_{α} in 10⁻¹¹ dyne-cm/radian; m is the atomic weight (O=16); and the wave-length $\nu=1303\omega$.

⁵ G. Kron and G. K. Carter, "A-C Network Analyzer

positive and negative admittances; since negative-resistance units are difficult to work with, positive and negative reactive admittances are used, with a.c. excitation. The circuit is excited by applying a generator at any junction point, and the forced-vibration frequency is varied by varying the admittances of the units expressed in terms of ω . For any given ω , the generator current represents the applied force required to force vibration at that frequency; so that when this current is plotted as a function of ω , as in Fig. 4, the points at which the resulting curve passes through zero should correspond to frequencies at which no external force is required to sustain the

TABLE II. Measured and calculated normal frequencies.

		= = = = = =		
CO_2	Test theory	ν ₁ 1273 1274	ν ₂ 670 668	2447 2440
ocs	Test	860	526	2072
	theory	859	527	2079
CH₃CH₂OH	Test	897	1009	421
	theory	910	1020	430

Study of the Schrödinger Equation," Phys. Rev. 67, 44-49 (1945).

³ W. G. Penney and G. B. B. M. Sutherland, "On the Relation Between the Form, Force Constants, and Vibration Frequencies of Triatomic Systems," Proc. Roy. Soc. 156, 654–678 (1936).

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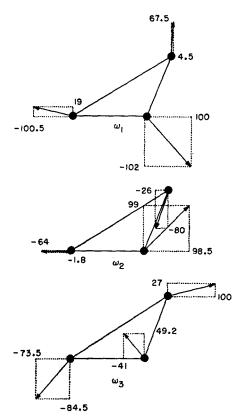


Fig. 5. Measured normal modes of vibration of the ethyl-alcohol.

vibration, that is, to the natural frequencies of the circuit and of the molecule which it represents. Ideally, the curve shown should be a continuously increasing function with increasing ω , passing through a series of infinite discontinuities; these discontinuities represent frequencies for which the point of excitation is a nodal point; practically, of course, the current supplied is incapable of increasing without limit, and instead it changes very rapidly from positive through zero to negative before once more taking the upward course. These extra zero points are generally obvious; and in any case the true natural frequencies can and should be checked by using the exciting generator at more than one junction of the network.

For the three molecules being considered, Table II shows how the natural frequencies measured on the network analyzer compare with those calculated from the constants in Table I (omitting the obvious case of zero frequency). It is seen that the check is very good; in fact, the discrepancies generally are less than might have been expected from uncorrected readings with the equipment used.

Not only the natural frequencies, but also the natural modes, can be read from the circuits by means of the analyzer. The latter are given simply by the voltages of the several junction points at the natural frequencies. Figure 5 shows, for example, the natural modes of the CH₃CH₂OH molecule as measured in this way; these are similar to the corresponding modes shown in reference 4.