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Abstract

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MICROWAVE SPECTRUM OF 1,2-FLUOROCHLOROETHANE

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In the present work an investigation has been carried out of the microwave spectrum of the molecule 1,2-fluorochloroethane. The study of such molecules is of particular interest because they may occur in several different isomeric states.

In the approximation of a rigid asymmetric top, the rotational spectrum of the 1,2-fluorochloroethane molecule was calculated for various values of the angle between the projections of the CF and CCl bonds onto the plane perpendicular to the C–C bond. In the calculations the following structural data were adopted: interatomic distances C–C 1.54 Å; C–H 1.10 Å; C–F 1.375 Å and C–Cl 1.78 Å; the angles CCF, HCC, and HCH equal to 109°28′ (for the CH_2F group); the angle HCH 110°20′, the angle HCC 109°49′, and the angle CCCl 110°30′ (for the CH_2Cl group).

The calculations showed that a large number of different rotational absorption lines lie in the frequency range from 10,000 to 30,000 Mc/s.

With the aid of a radiospectroscope with Stark modulation, the microwave spectrum of the 1,2-fluorochloroethane molecule was investigated in the range 10,000-20,000 Mc/s, and a large number of absorption lines was found.

It was established that the general pattern of the arrangement of the observed lines agrees well with the calculated pattern at (= 70^{ }). According to the calculations, for (= 70^{ }) in the range 10,000-20,000 Mc/s, groups of lines belonging to the (Q)-branch with (K_{-1} = -1) and (K_1 = 1), from (J = 1) to (J = 8), should have been observed. Absorption lines corresponding to the transitions (1_{01}–1_{10}), (2_{02}–2_{11}), (3_{03}–3_{12}), (4_{04} –4_{13}), and (5_{05}–5_{14}) of the molecule $FH_2C–CH_2Cl^{35}$ were found and identified. The identification was made by studying the hyperfine splittings of the lines of the indicated transitions.

Table 1

Transitions (J_{K_{-1},K_1} –J_{K' _{-1},K' _1})	Frequencies in Mc/s, calculation	Frequencies in Mc/s, experiment
(1_{01}–1_{10})	–	10729.7
(2_{02}–2_{11})	–	11155.0
(3_{03}–3_{12})	11815.5	11815.4
(4_{04}–4_{13})	12737.6	12736.4
(5_{05}–5_{14})	13954.8	13952.1

Table 1 gives the values of the experimentally measured and theoretically calculated frequencies of the indicated lines. In the calculations it was assumed that (A - C = 10729.6) Mc/s and (= -0.923), which were determined by us on the basis of the measured frequencies for the transitions (1_{01}–1_{10}) and (2_{02}–2_{11}). From analysis of the hyperfine structure of these lines the values of the quadrupole-coupling constants in the directions of the principal axes of inertia of the molecule $FH_2C–CH_2Cl^{35}$ were determined: (_a = -23.5) Mc/s, (_b = -8.8) Mc/s.

The discrepancy between the experimental and theoretical values of the frequency (see Table 1) increases with increasing (J), which is apparently connected with the presence of centrifugal perturbation not taken into account in the calculations, owing to the "nonrigidity" of the molecule.

Thus, from the analysis of the spectrum of the 1,2-fluorochloroethane molecule it has been established that for this molecule there exists a stable configuration with a val–

with $\alpha = 70^\circ$, i.e., the so-called gauche isomers. For the gauche isomer, on symmetry grounds one would expect an angle $\alpha = 60^\circ$. The deviation of the angle α by 10° is apparently connected with the strong repulsion of the fluorine and chlorine atoms.

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Note: Figure translations are in progress. See original paper for figures.