# Microwave Spectrum of 1-Fluoronaphthalene

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The microwave spectrum of 2-fluoronaphthalene was assigned earlier by Bak *et al.*,[1] and preliminary results for 1-fluoronaphthalene were obtained at the same time.[2] This work is a more detailed investigation of 1-fluoronaphthalene (AFN).

A sample of 1-fluoronaphthalene was purchased from Fluka. Its purity was checked by capillary gas chromatography and used without further purification.

The microwave spectrum was observed in the range 18.0 – 40.0 GHz on a Hewlett-Packard Model 8460 A MRR spectrometer. All measurements were made at room temperature and at Starkfields of 2000 – 3800 V/cm. The transition frequencies were measured with a sample pressure of 0.005 to 0.010 mmHg.

The 1-fluoronaphthalene molecule is quite heavy and its rotational constants are rather small. Reasonable molecular models have values of the asymmetry parameter, $\varkappa$, around −0.3. The approximate orientation of the principal inertial axes are given in Fig. 1.

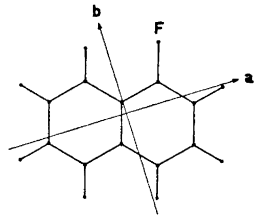


*Fig. 1.* Molecular model of 1-fluoronaphthalene, $C_{10}H_7F$. *a* and *b* are principal inertial axes.

Based on a vector model, the dipole moment of AFN has its main contribution along the C,F bond. This suggests that the molecular dipole moment is directed mainly along the principal *b*-axis, see Fig. 1. Consequently, the microwave spectrum is very rich and the majority of the observed lines could be assigned to be *b*-type transitions. No *a*-type transitions were assigned.

A part of the *b*-type spectrum calculated from a molecular model is given as a FORTRAT-diagram in Fig. 2. The curves in this figure connect transitions with common values of $K_{-1}$. It should be noted, that several lines appear as close doublets, see Fig. 2 and Table 1, although the molecule is quite asymmetric, see above.

*Table 1.* Selected microwave transitions (MHz) of 1-fluoronaphthalene.

| Transition | Obs. frequency[a] | Obs. − calc. |
|---|---|---|
| $12_{0,12}-13_{1,13}$ / $12_{1,12}-13_{0,13}$ | 19129.09 | +0.04 |
| $12_{1,11}-13_{2,12}$ | 20550.66 | +0.02 |
| $12_{2,11}-13_{1,12}$ | 20549.46 | +0.04 |
| $13_{0,13}-14_{1,14}$ / $13_{1,13}-14_{0,14}$ | 20545.97 | +0.04 |
| $15_{11,4}-15_{12,3}$ / $15_{11,5}-15_{12,4}$ | 22328.77 | 0.00 |
| $16_{11,5}-16_{12,4}$ / $16_{11,6}-16_{12,5}$ | 22205.83 | +0.08 |
| $19_{10,9}-19_{11,8}$ | 19203.05 | +0.01 |
| $19_{10,10}-19_{11,9}$ | 19319.09 | −0.04 |

[a] ±0.05 MHz.

The spectrum is dominated by the intense high-*J* *Q*-branch transitions. The characteristic *R*-branch transitions, almost equidistant with differences of 2C, were however assigned first. Some of the 78 measured transitions are marked in Fig. 2. A selection of experimental frequencies are given in Table 1. The list of measured frequencies ($J \leq 20$) is available from the author or from the Microwave Data Center at the National Bureau of Standards, Washington, D.C., U.S.A., where it has been deposited.

A least-squares fit of the measured frequencies in the rigid rotor approximation (using a computer program received from Dr. Stig Ljunggren at the Royal Institute of Technology, Stockholm) was satisfactory and gave the results in Table 2.

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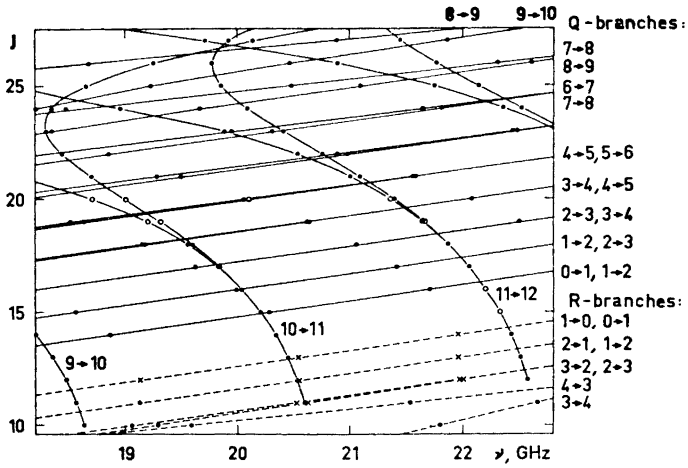


*Fig. 2.* FORTRAT-diagram of 1-fluoronaphthalene. ×, measured $R$-lines. ○, measured $Q$-lines. The $R$-branches (– – –) and $Q$-branches (———) are marked with the $K_{-1}$-values.

*Table 2.* Rotational constants, principal moments of inertia and inertial defect of 1-fluoronaphthalene. Conversion factor 505376 MHz × uÅ².

| | | |
|---|---|---|
| Maximum J | | 20 |
| Number of lines | | 78 |
| $\sigma$ (MHz) [a] | | 0.069 |
| A | (MHz) | 1920.5617 ± 0.0008 |
| B | (MHz) | 1122.2318 ± 0.0010 |
| C | (MHz) | 708.4778 ± 0.0004 |
| $I_a$ | (uÅ²) | 263.1397 ± 0.0001 |
| $I_b$ | (uÅ²) | 450.3312 ± 0.0004 |
| $I_c$ | (uÅ²) | 713.3265 ± 0.0004 |
| I.D. | (uÅ²) | −0.1444 ± 0.0007 |

[a] $\sigma = [\sum(\nu_i(\text{obs}) - \nu_i(\text{calc}))^2/N]^{1/2}$

A fit including centrifugal distortion (using computer programs by Dr. G. O. Sørensen, Copenhagen University) resulted in a decrease of the mean deviation from 0.069 to 0.052 MHz. However, the significance of the distortion constants was doubtful, and the corrections were quite small, less than 0.4 MHz. Centrifugal distortion effects could therefore be neglected for $J$-values less than 20, as was expected for this rather heavy and rigid molecule. Transitions with $J$-values less than 40 could easily be observed (but were not measured exactly). They did not deviate seriously from frequencies calculated in the rigid rotor approximation.

The inertial defect of AFN (Table 2) is small and negative and of the same order of magnitude as was found for the 2-fluoro species, −0.132 uÅ², Ref. 1. This indicates that these molecules are planar.

Since no isotopic species were investigated, a molecular structure of AFN cannot be derived from the present results.

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1. Bak, B., Christensen, D., Hansen-Nygaard, L. and Rastrup-Andersen, J. *Spectrochim. Acta* **18** (1962) 229.
2. Christensen, D. *Spectrochim. Acta* **15** (1959) 767.

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