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OPTIMAL DESIGN CRITERIA FOR MILLIMETER-WAVE SPECTROMETERS

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Publication Date

1975-03-01

To be presented at the 5th European
Microwave Conference, Hamburg,
West Germany, September 1 - 4, 1975

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SPECTROMETERS

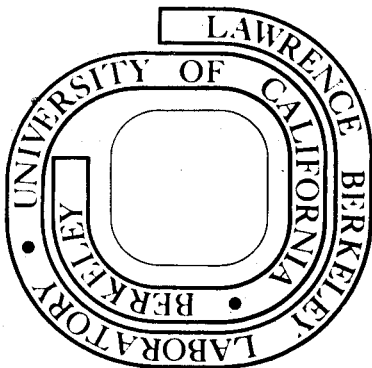
B. Leskovar, D. B. Hopkins, and W. F. Kolbe

March 15, 1975

Prepared for the U. S. Energy Research and
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OPTIMAL DESIGN CRITERIA FOR MILLIMETER-WAVE SPECTROMETERS

B. Leskovar, D. B. Hopkins, W. F. Kolbe

ABSTRACT - Optimal design criteria for millimeter-wave cavity-type spectrometers, used in the measurement of molecular spectra, have been derived. Using an optimally designed spectrometer, the technique of molecular spectroscopy offers a highly sensitive and specific experimental research method for studying chemical kinetics and for monitoring gaseous pollutants and constituents of interest in pollution research. The method is also suitable for the study of the molecular properties of short-lived transient chemical species with lifetimes as short as one millisecond or less. Since the sensitivity of the spectrometer is determined by the total noise introduced during the processes of microwave generation, absorption in the resonant cavity, and the detection and amplification of a spectral line signal, the spectrometer has been analyzed and optimized in detail with respect to the equivalent noise temperatures associated with these processes. The conclusions drawn from the optimum design criteria are applied in the design of a tunable high-Q resonant cavity spectrometer operating at 70 GHz.

1. INTRODUCTION - Millimeter-wave rotational spectroscopy measures the absorption in the millimeter region of the electromagnetic spectrum, caused primarily by transitions between pure rotational states of gaseous molecules possessing permanent dipole moments. The physical process leading to absorption is a coupling of the electrical vector of the incident microwave radiation with the permanent dipole moment of the rotating molecule. Using an optimally designed measuring system, this technique is a highly specific and sensitive experimental research method for studying chemical kinetics and for monitoring gaseous pollutants and constituents of interest in pollution research. Our investigations show that in addition to the detection and measurement of ordinary gases and vapors, the method is suitable for the study of the molecular properties of short-lived transient chemical species with lifetimes down to a millisecond or less. The technique supplements and may replace gas chromatography, mass spectroscopy, and various laser methods in the identification of trace-gas chemicals, and also makes possible fast, highly specific and sensitive measurements in the laboratory.

The intensity of an absorption is determined primarily by the magnitude of the molecular dipole moment and the number of molecules in the lower energy state of the transition. The absorption intensity is considerably stronger at millimeter-wave frequencies than at lower frequencies. This is due to the (frequency)² increase of the absorption coefficient γ_{\max} with increasing frequency, and also partly due to the fact that the higher frequency transitions usually involve states of higher rotational quantum number having larger population differences at ordinary temperatures. Our calculations and measurements of the sulfur dioxide molecule show that the $^{32}\text{S}^{16}\text{O}_2$ transition at 68.9721 GHz, between the 6(0,6) and 6(1,5) levels, has a coefficient peak value of $\gamma_{\max} = 4.5 \times 10^{-4} \text{ cm}^{-1}$, [1]. This amount is a factor of ten greater than for any transition between 8 GHz and 40 GHz. The pattern of absorption frequencies is a sensitive function of the exact structure and isotopic composition of a molecule. As molecules generally

have different structural configurations, their rotational spectra offer distinctive information on their existence in a mixture.

2. NOISE CONSIDERATION IN THE SPECTROMETER SYSTEM - The millimeter-wave high resolution spectrometer under consideration consists of a mechanically and electrically tunable microwave generator (energy source), a high-Q cavity absorption cell, a low-noise microwave receiver with an automatic frequency control device, and a data processing system. A simplified diagram of the system with all relevant noise sources is shown in Fig. 1. Since the sensitivity of the tunable high-Q resonant cavity spectrometer is essentially determined by the total noise introduced during generation of the microwave radiation, by the absorption process in the resonant cavity, and by the detection and amplification of a spectral line signal, the spectrometer has been analyzed and optimized in detail with respect to these various sources. The total noise system includes the AM and FM noise sidebands of the microwave oscillator, thermal radiation noise of the sample absorption cavity, and noise of the microwave receiver.

2.1 AM AND FM NOISE OF THE MICROWAVE OSCILLATOR - A typical microwave source has, in addition to the desired monochromatic output signal, a concentration of noise power surrounding the carrier, due to the thermal, shot noise, and flicker noise perturbations of the oscillator. Generally the noise sidebands are separated into AM and FM components. The AM noise characteristic of the carrier is usually defined by the double-sideband AM noise power to carrier power ratio in a bandwidth B, measured at a distance f_m from the carrier, $(N/C)_{DSB}^{AM}$. Similarly the FM noise of the carrier is defined by the rms noise deviation, Δf_{rms} , that would be measured in a bandwidth B at the output of an FM discriminator with a microwave oscillator at its input. Generally, accurate measurements of AM and FM source noise at carrier frequencies above about 18 GHz are rarely made [2]. From device manufacturers' comments and limited measurements [2-5], and our calculations and measurements, at 10, 28 and 35 GHz, an estimate of source noise to be expected at higher frequencies can be made. The AM and FM noise performance of microwave sources were averaged, normalized, and extrapolated to frequencies of 100 GHz for klystron sources and to 90 GHz for a Gunn oscillator. (Because of a finite intervalley transfer time, the GaAs Gunn oscillator loses its differential negative mobility at about 90 GHz.) The source AM noise characteristics were normalized and extrapolated according to the expression:

$(N/C)_{DSB}^{AM} = (kTB/P_o) / [(S/2)^2 + (Q_{ext} f_m / f_o)^2]$, where k is Boltzmann's constant, T is the effective temperature of the device, B is the bandwidth, P_o is the device output power, S is the saturation factor given by Edson [6], and Q_{ext} is the external circuit quality factor. The source FM noise characteristics were normalized, and extrapolated according to equation: $\Delta f_{rms} = (f_o / Q_{ext}) [kTB/P_o]^{1/2}$. The results are presented in Fig. 2 for free running oscillators, without external stabilization. On the basis of AM and FM noise alone, solid-state Gunn oscillators presently appear to be superior to reflex klystrons, up to frequencies of approximately 35 GHz. Above this frequency the reflex klystrons, and particularly the two-cavity klystrons, are superior to Gunn devices.

The equivalent noise temperature contribution of the microwave source to the total noise temperature of the spectrometer at the input of the detector has been calculated by means of equation (1) derived from the consideration in Ref. [7].

$$T_{eq} = (P_o / KB_s) \left[\tau (N/C)_{DSB}^{AM} + \eta (\Delta f_{rms} / f_m)^2 \right], \quad (1)$$

where P_o is the carrier power level, B_s is the spectrometer bandwidth, f_m is the modulation frequency, and S_τ and η are AM transmission and FM-AM conversion factors, respectively. For the reflection cavity the transmission factor is determined by the expression $\tau = r_o^2 + (Q_o f_m / f_{co})^2$, where f_{co} is the cavity resonant frequency, Q_o is the unloaded quality factor of the cavity, and $r_o^2 = (1 - \beta^2) / (1 + \beta^2)$ is the cavity reflection coefficient, defined by $\beta_o = Q_{ext} / Q_o$. For minimum noise, it is desirable to have $\beta \approx 1$. The reflection coefficient value is then $r_o^2 = (1 - \beta^2) / 4$. The FM-AM conversion factor is defined by the equation $\eta = Q_o^2 S^2 \cos^2 \xi + \tau \sin^2 \xi$, where $S = (f_o - f_{co}) / f_{co}$ is the long term frequency stability, f_o is the oscillator frequency, ξ is the phase difference between the signal and the reference wave at the demodulator, and Q_o , Q_{ext} , and τ are terms defined previously.

Using a 100 mW reflex klystron source in the spectrometer, with $f_o = 70$ GHz, $Q_o = 2 \times 10^4$, $f_m = 10$ KHz, it can be seen from Fig. 2 that $\Delta f_{rms} = 18$ Hz and $(N/C)_{DSB}^{AM} = -125$ dB = 3.16×10^{-13} . Equation (1) gives, for $S = 10^{-9}$, $\xi = 10^{-2}$ rad, $B_s = 100$ Hz, $P_o = 10^{-4}$ W, and $r_o^2 = (Q_o f_m / f_{co})^2$, the value of the equivalent noise temperature $T_{eq} \approx 382^\circ\text{K}$.

2.2 THERMAL RADIATION NOISE OF THE ABSORPTION CELL is characterized by the effective noise temperature of the resonant cavity, which is typically $T_a \approx 300^\circ\text{K}$ for a high sensitivity spectrometer.

2.3 MICROWAVE RECEIVER NOISE is characterized by the effective input noise temperature T_e , defined as $T_e = P_n / KB_r$, where P_n is the available noise power. Figure 3 shows the measured overall effective input noise temperature and noise figure as functions of input signal frequency for the microwave receiver, using as the front end the traveling wave tube amplifier, the SSB mixer, the field-effect transistor, noncryogenic and cryogenic parametric amplifiers, and a traveling wave maser [8]. It can be seen from the figure that at 70 GHz the receiver has effective noise temperatures of 500°K and 700°K , achieved with the double-sideband parametric amplifier and the single-sideband mixer front ends, respectively.

For the detection of very weak absorption lines, or for a reduction in the measuring system response time, the spectrometer sensitivity is considerably increased by the use of Stark or Zeeman modulation of the electromagnetic field, followed by phase-sensitive detection. A phase-sensitive detector, as a cross-correlator, utilizes amplitude and phase information of an input signal, offering a considerable gain in the output signal-to-noise ratio, compared with a conventional envelope detector.

With properly optimized operating conditions, a phase-sensitive detector has excellent performance concerning low nonlinearity, wide dynamic range, and bandwidth under almost any signal-to-noise ratio conditions, [9].

3. CONCLUSIONS - A comparison of the microwave source noise with the absorption cell noise and the microwave receiver noise shows that the microwave source noise contributes significantly to the total spectrometer noise and ultimately limits the achievable spectrometer sensitivity. Furthermore, it can be seen from comparison of T_e with the effective noise temperatures of the microwave source and sample absorption cell, T_{eff} and T_a , respectively, that in the case where $T_e \ll T_a$, the sensitivity of the millimeter-wave measuring system cannot be significantly improved, since the sample absorption cell would radiate thermal noise into the receiver, making T_e comparable with the absorption cell temperature T_a . Similarly, for $T_e = T_a \ll T_{eff}$, the source noise temperature would dominate the total noise temperature of the measuring system. Consequently, in millimeter-wave measuring system applications the optimum tradeoff between the sensitivity, complexity, reliability and cost occurs at a level of receiver effective noise temperature T_e comparable to the sample absorption cell noise temperature T_a and the effective microwave source noise temperature T_{eff} ; i.e., $T_{eff} \approx T_a \approx T_e$.

This work was performed as a part of the program of the Electronics Research and Development Group of the Lawrence Berkeley Laboratory, University of California, Berkeley, and was supported by the U.S. Energy Research and Development Administration, Contract No. W-7405-eng-48.

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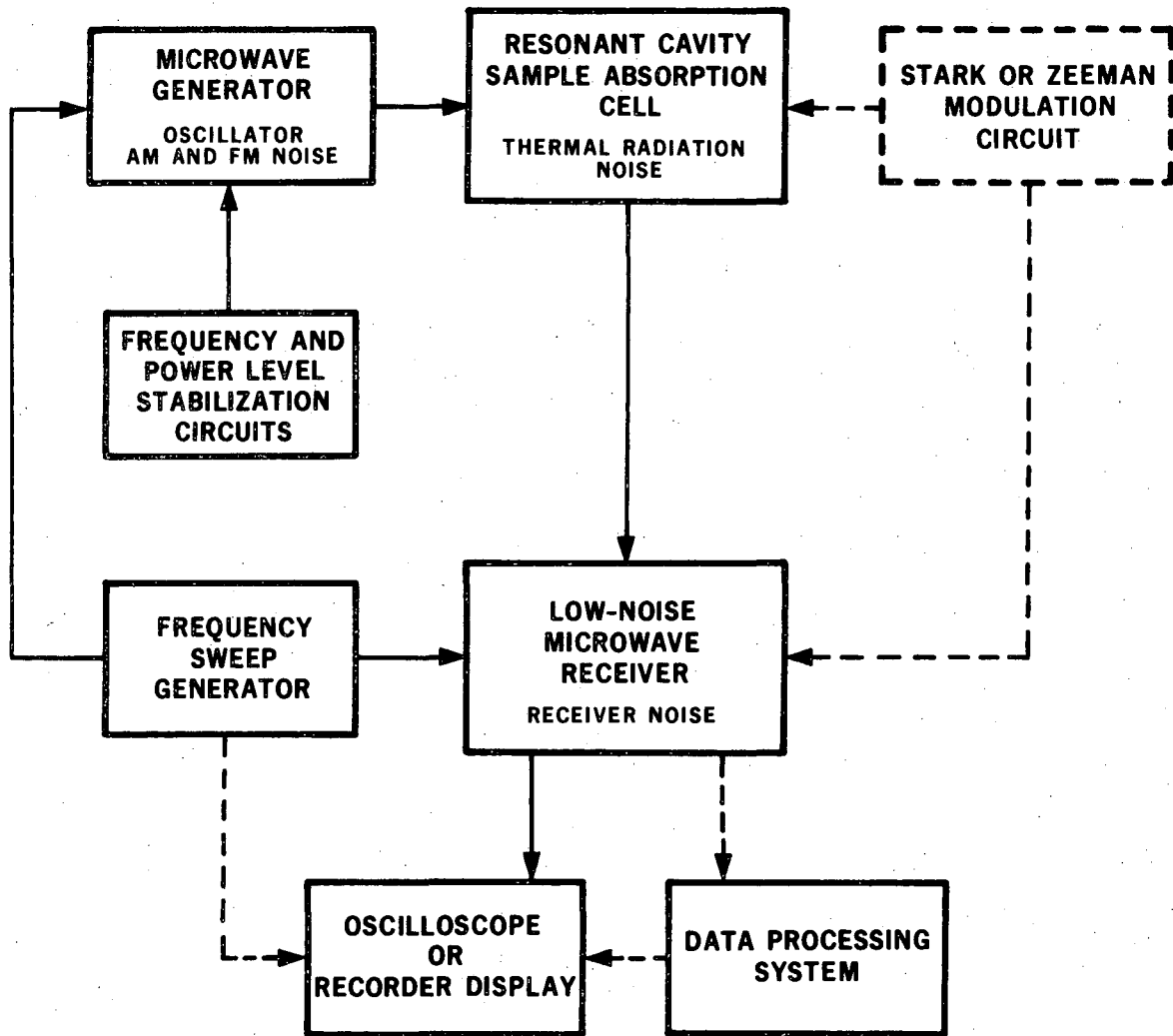
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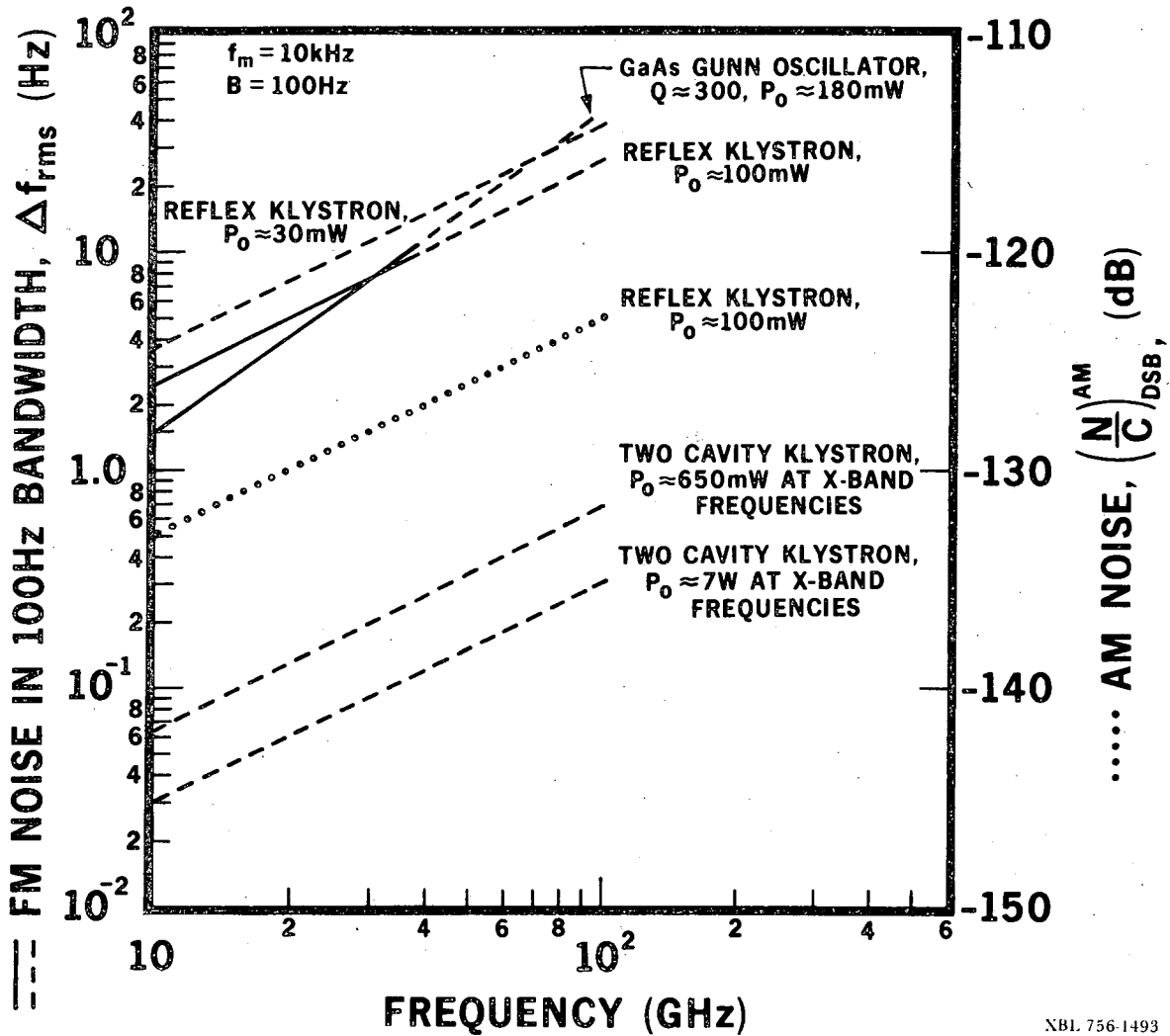
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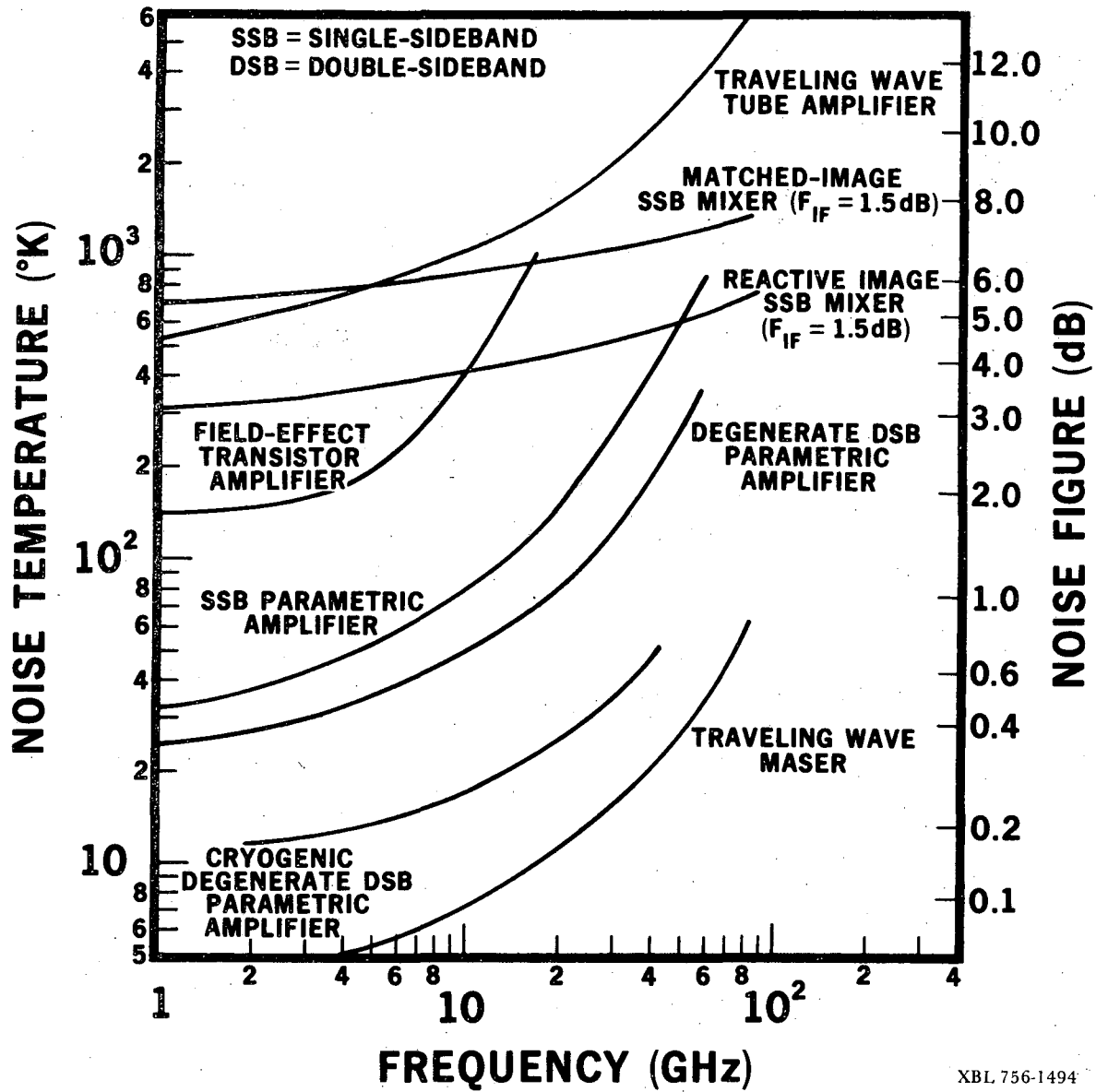
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Fig. 1 - Typical millimeter-wave spectrometer system with noise sources.



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Fig. 2 - AM and FM noise of the microwave source as a function of frequency.



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Fig. 3 - Effective noise temperature and noise figure as a function of frequency.

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