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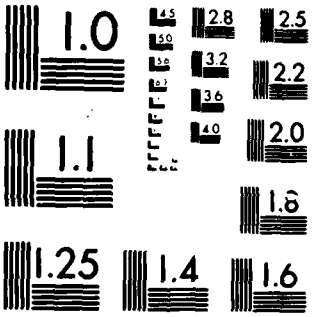

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER ARO 21756.1-PH	2. GOVT ACCESSION NO. N/A	3. RECIPIENT'S CATALOG NUMBER N/A
4. TITLE (and Subtitle) Molecular Absorption of Atmospheric Species		5. TYPE OF REPORT & PERIOD COVERED Final 7 May 84 - 1 Sep 85 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Frank C. De Lucia		8. CONTRACT OR GRANT NUMBER(s) DAAG29-84-K-0073
9. PERFORMING ORGANIZATION NAME AND ADDRESS Duke University Durham, NC 27706		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS U. S. Army Research Office Post Office Box 12211 Research Triangle Park, NC 27709		12. REPORT DATE 12/17/85 13. NUMBER OF PAGES 11
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

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17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

NA

18. SUPPLEMENTARY NOTES

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Microwaves
Millimeterwaves
Propagation

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

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ARO 21756.1-PH

MOLECULAR ABSORPTION OF ATMOSPHERIC SPECIES

Final Report

Frank C. De Lucia

December 15, 1985

U. S. Army Research Office

DAAG29-84-K-0073

Duke University

ABSTRACT

The propagation of microwaves and millimeterwaves through the disturbed atmosphere is affected by molecular absorption that can be significantly different than the absorption in the ambient atmosphere. This is due to two factors. First, the constituents of the ambient atmosphere will exhibit significantly different electromagnetic properties at elevated temperatures. Second, many additional species that are strong absorbers of microwaves, such as HNO_3, HNO_2, O_3, NO_2, H_2O_2, OH, and N_2O, are present in the disturbed atmosphere. This work addressed both of these issues. A preliminary version of a code that utilized the previously available molecular data base was written in a form that would be compatible with NORSE. This code was turned over to PRi (the keeper of the NORSE code) and is currently being integrated into it. In addition, measurements to 1000K were made on one transition of H_2O as a check on the extrapolation to higher temperature that was used in this code.

The propagation of microwaves and millimeterwaves (mw/mmw) through the disturbed atmosphere is affected by molecular absorption. The small molecules present in the ambient atmosphere (excluding N_2) absorb microwaves because their rotational energy level spacing correspond to microwave frequencies. In addition, theoretical calculations show that most of the small molecules that can be made by rearranging the atoms in O_2, N_2, and H_2O are present in the disturbed atmosphere. In general, these molecules are much stronger absorbers of mw/mmw radiation than the normal constituents, but their much lower abundance significantly reduces this effect.

In order to test system and other concepts, large codes have been written that simulate the disturbed atmosphere. These codes include pressure and shock wave effects, the extinction due to dust, calculate chemical effects and temperature profiles, etc. However, the current version, NORSE, does not include any effects due to molecular absorption, including effects due to the constituents of the ambient atmosphere, which are known to be large in the millimeter wave region. As a result, it is our understanding that the NORSE code is currently "locked" against use above 10 GHz.

In the first part of our work we have written a preliminary version of a code that can be integrated into NORSE to account for these effects. We have designed it so that as additional molecular parameters become available, no significant changes will be required, especially in its interface with NORSE. There are substantial amount of molecular physics involved in these calculation that will not be detailed here. We refer the interested reader to the literature and note that much of the work on which these

calculations are based resulted from earlier support of our laboratory by the Army Research Office.

Figure 1 shows a block diagram of the code in its stand alone form in which the output is set directly to a plotter rather than returned to a larger code. The scenario inputs required from the main code are the temperature and the molecular abundances. This is required to specify the physical and chemical conditions. It should be noted that this is a very small amount of information and can be easily passed from the larger code. For technical reasons the ambient atmosphere is calculated separately from the contributions due to the trace species, but both require the input from the molecular data files. These store the molecular information at the most fundamental level (i. e. transition frequency, transition strength, and absolute energy) and as a result a wide variety of scenarios can be calculated from them. These files suffer from two short comings. First, there are many scenarios, especially at higher temperatures that require information about states and collision processes that is not currently known. This is primarily because the rather large effort that has been put into understanding mw/mmw propagation has been directed almost entirely to understanding the temperature region between 200 - 300 K. Secondly, they are rather large, although by no means prohibitive by the standards of codes like NORSE. This is because the information at the most fundamental level must literally deal with ~100,000+ transitions. It would be possible to preprocess this data to very significantly reduce the size of both the calculation and storage at the expense of generality. If the basic physics and spectroscopy of the situation were carefully considered, it should be possible to do this and to not have this compression be a significant contributor to the error budget of the

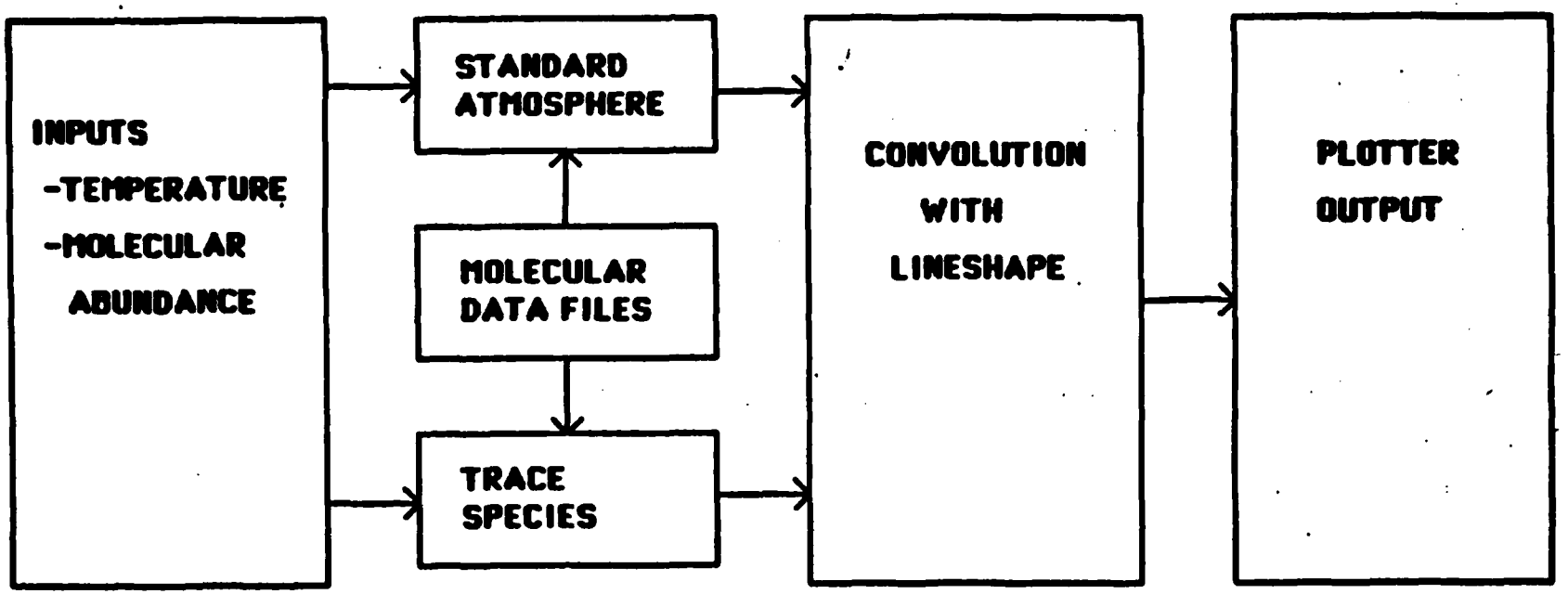

Figure 1. Block diagram of code in its stand alone configuration.

calculation. This information is then convoluted with lineshape functions in a procedure that in many cases uses an estimate of the lineshape parameter. This estimate is necessary because at present many of these are poorly known in this spectral region. Finally, the output is sent to a plotter. When this code is used as a subroutine in a larger code, this calculation is done many times along the sight path and contributes an additional term at each point to the overall attenuation.

A tape that contains both the code and the molecular parameters has been turned over to Physical Research Incorporated of Huntsville, Alabama for integration into the NORSE code. Although this is a preliminary version, its form will require little or no modification to its interface with NORSE as it is updated. Examples of its output in graphical form are shown in Figs. 2-4. It should be emphasized that the code is still preliminary and that as soon as the first cut integration into NORSE is completed, a number of straightforward "tunings" should be done before it is used.

It is our judgment that the most significant uncertainty in the code (except for the possibilities of "blunders" that still must be checked for as part of a verification process) are the effects of temperature on the molecular parameters. This is especially true for linewidth parameters because the theory of collisions is too complex to allow reliable "first principle" calculations. As a result we have carried out a check of the temperature dependence used for the width of the H_2O absorption at 183 GHz over the temperature range 300 - 1000K. The code uses

$$\Delta\nu(\text{MHz}) = 3.76\, P_a\, [T/300]^{0.8},$$

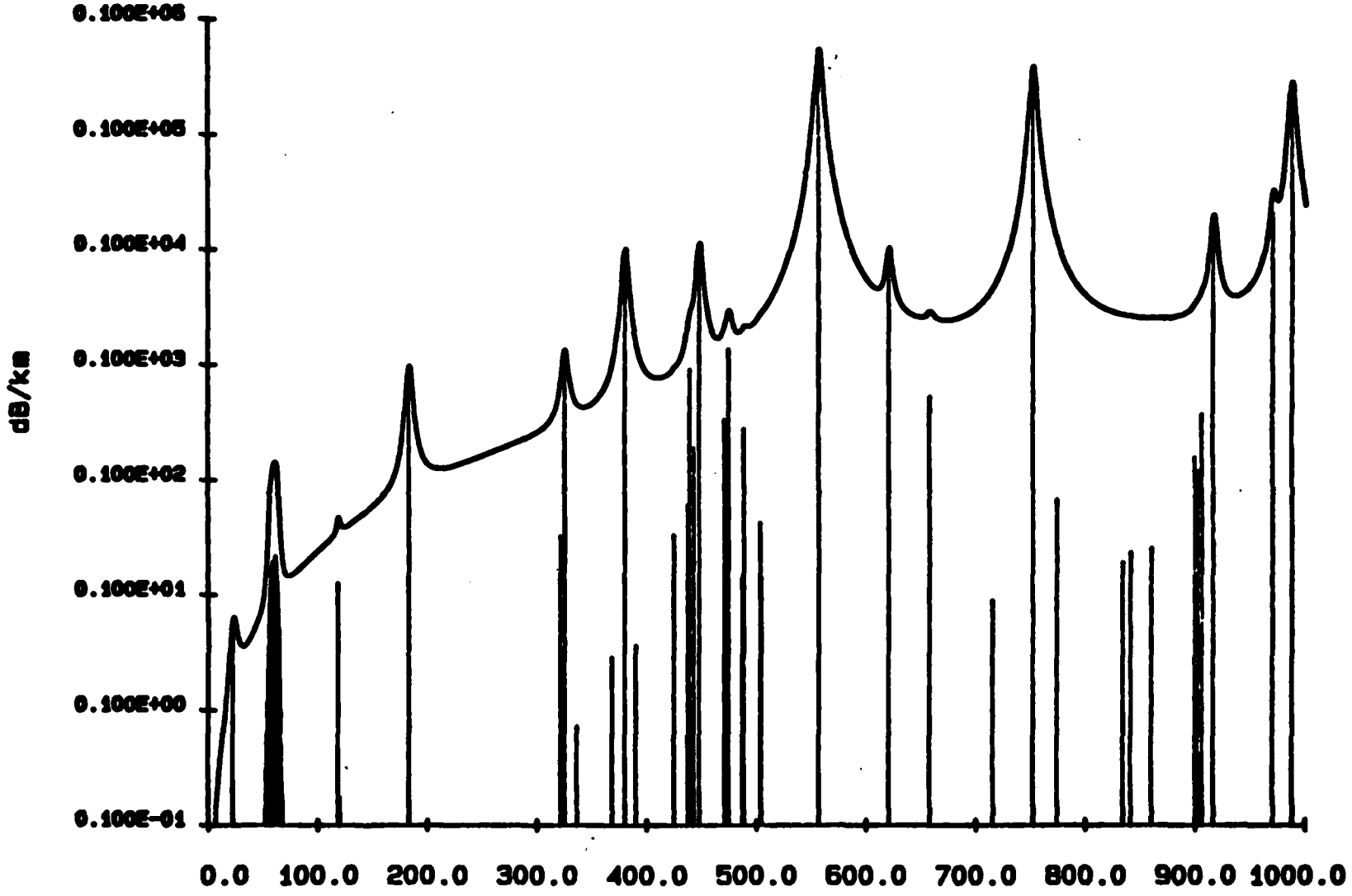

Figure 2. Atmospheric attenuation for ambient atmosphere at sea level.

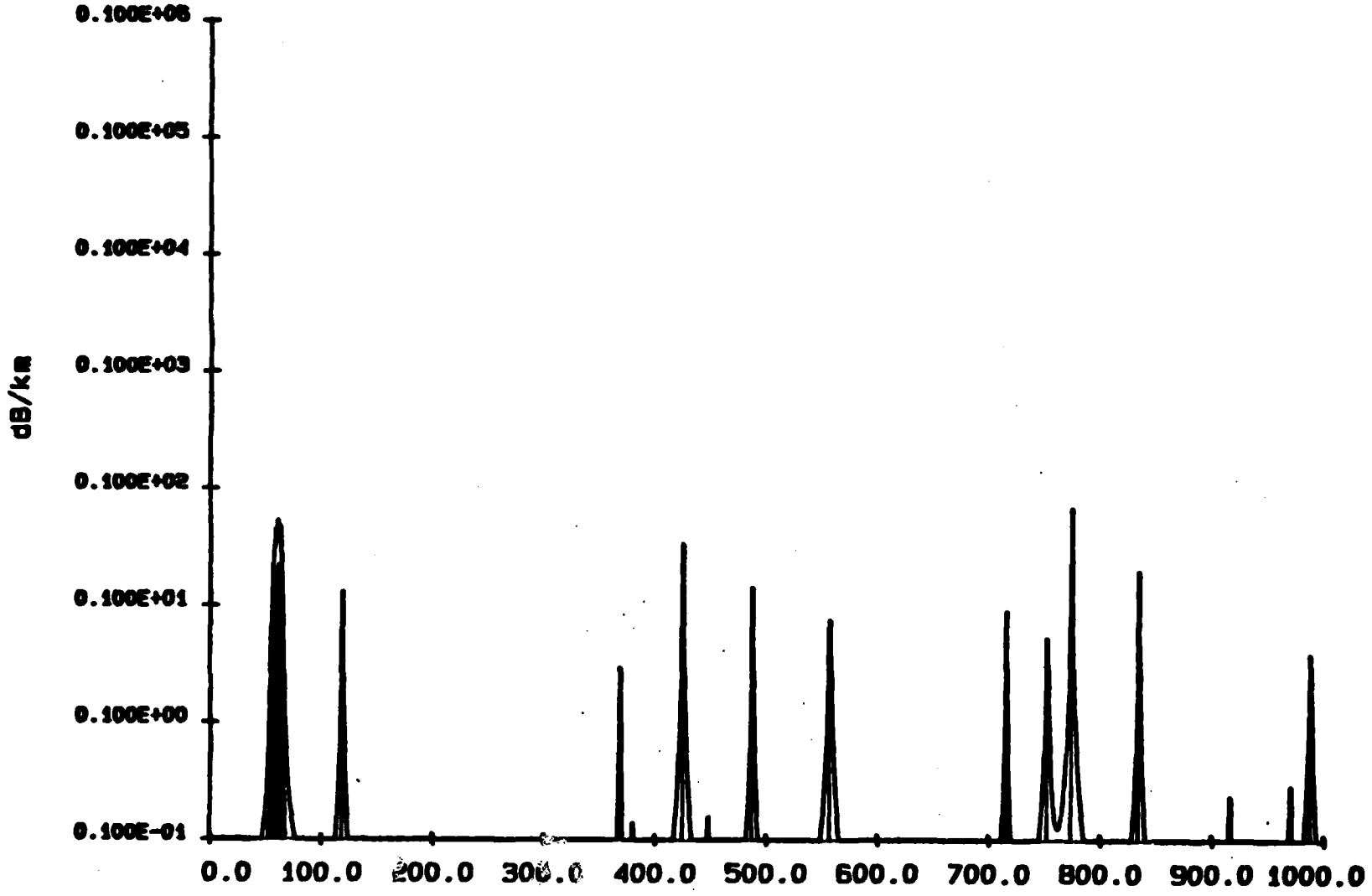

Figure 3. Atmospheric attenuation for ambient atmosphere at 25 km.

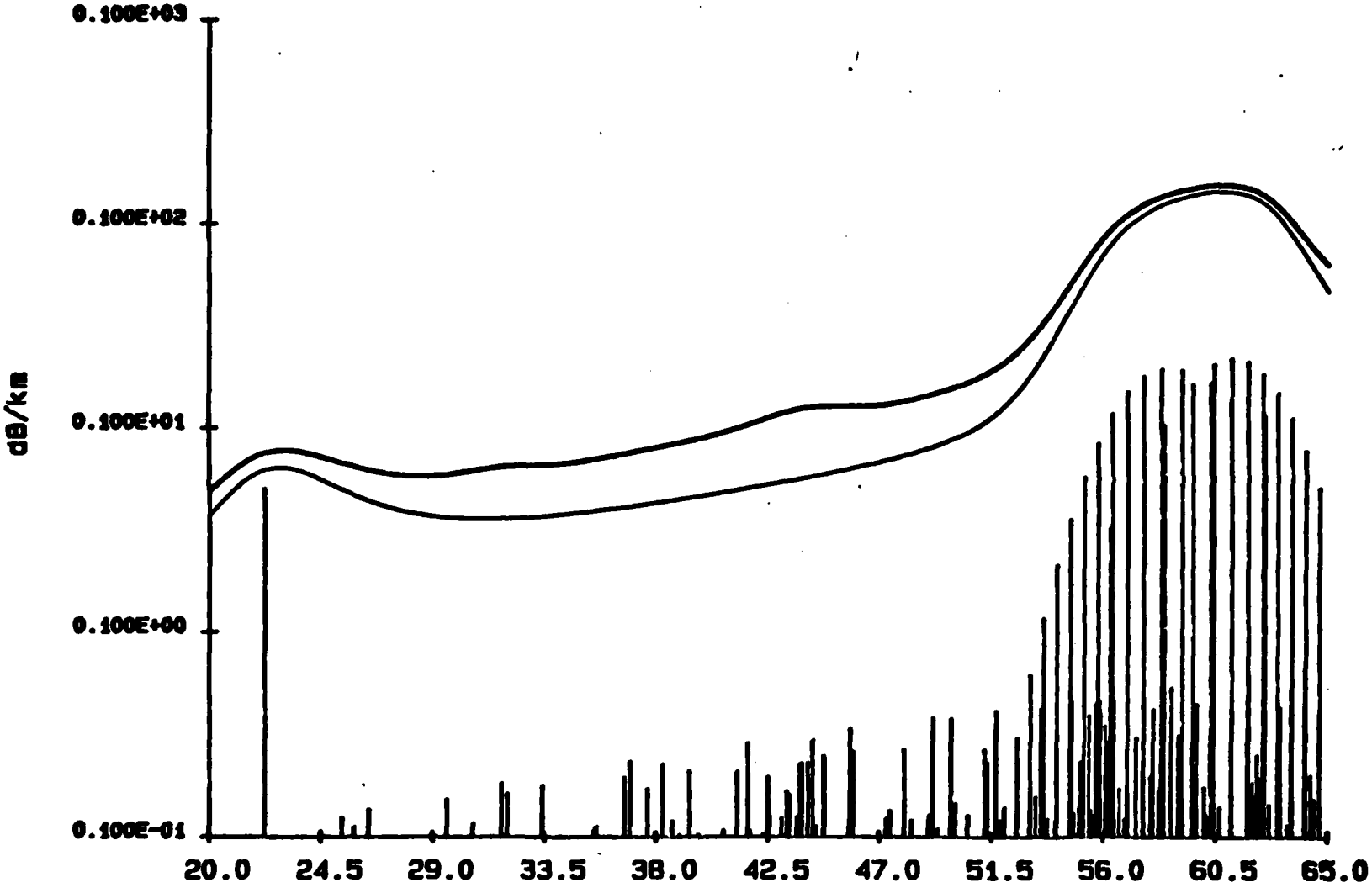

Figure 4. Atmospheric attenuation at sea level for ambient atmosphere with addition of $1 \times 10^{16}/cm^3$ of HNO_3. Upper line is sum; lower line ambient atmosphere only. Note that log scale minimized the difference.

where P_a is the pressure of the dry air (Torr) and T(Kelvin) is the temperature, for the linewidth contribution due to oxygen and nitrogen, and

$$\Delta\nu(\text{MHz}) = 18.04\, P_w\, [T/300]^{1.0},$$

where P_w is the partial pressure of water, as the linewidth contribution from water. In Figs. 5 and 6 we plot these function against our experimental measurement and find generally good agreement.

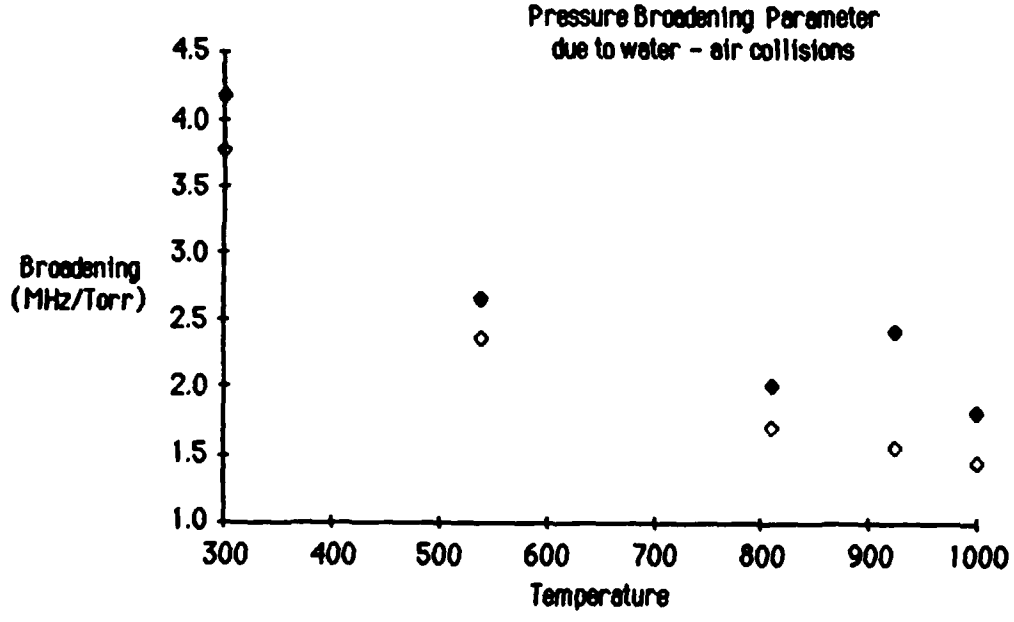

Figure 5. Comparison of experimental (solid) and theoretical (open) linewidth parameters. The experimental point at 925 K is believed to be spurious.

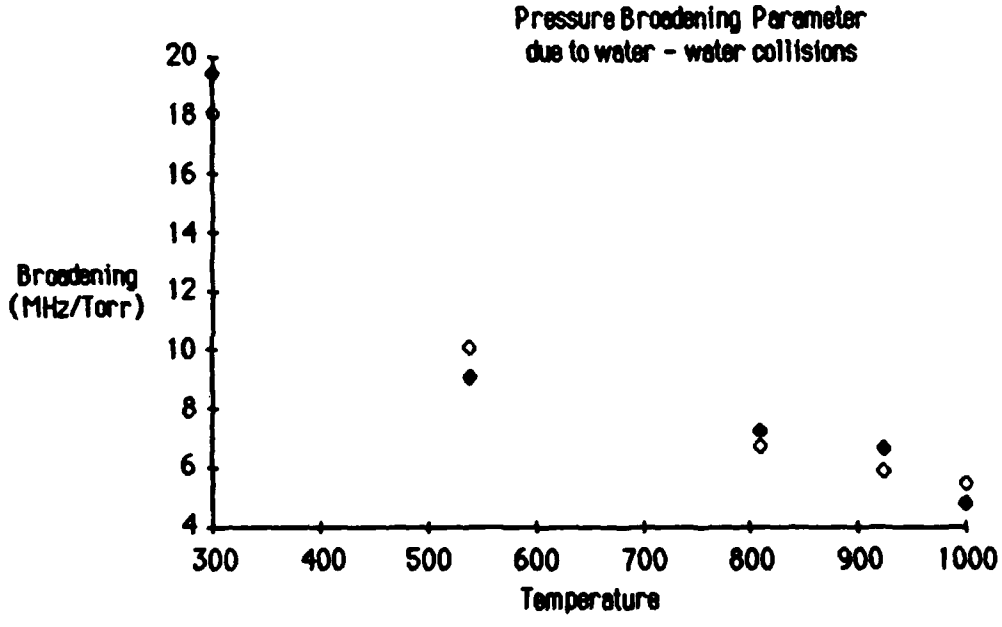

Figure 6. Comparison of experimental (solid) and theoretical (open) linewidth parameters.

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