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DNA-TR-87-239-V2A-10A

THE NORSE MANUAL

Volume 2A-10A—Local Thermal Equilibrium Molecular Band Shape
Parameters

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1 November 1988

Technical Report

CONTRACT No. DNA 001-88-C-0030

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Prepared for
Director
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SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

1a REPORT SECURITY CLASSIFICATION UNCLASSIFIED			1b RESTRICTIVE MARKINGS			
2a SECURITY CLASSIFICATION AUTHORITY N/A since Unclassified			3 DISTRIBUTION AVAILABILITY OF REPORT Approved for public release; distribution is unlimited.			
2b DECLASSIFICATION/DOWNGRADING SCHEDULE N/A since Unclassified						
4 PERFORMING ORGANIZATION REPORT NUMBER(S) PRI-NM-88-R002			5 MONITORING ORGANIZATION REPORT NUMBER(S) DNA-TR-87-239-V2A-10A			
6a NAME OF PERFORMING ORGANIZATION Physical Research, Inc.		6b OFFICE SYMBOL (If applicable)	7a NAME OF MONITORING ORGANIZATION Director Defense Nuclear Agency			
5c ADDRESS (City, State, and ZIP Code) 2201 Buena Vista SE Suite 301 Albuquerque, NM 87106			7b ADDRESS (City, State, and ZIP Code) Washington, DC 20305-1000			
8a NAME OF FUNDING SPONSORING ORGANIZATION		8b OFFICE SYMBOL (If applicable) RAAE/Schwartz	9 PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER DNA 001-88-C-0030			
9c ADDRESS (City, State, and ZIP Code)			10 SOURCE OF FUNDING NUMBERS			
			PROGRAM ELEMENT NO 63220C	PROJECT NO SA	TASK NO SA	WORK UNIT ACCESSION NO DH200780
11 TITLE (Include Security Classification) THE NURSE MANUAL Volume 2A-10A--Local Thermal Equilibrium Molecular Band Shape Parameters						
12 PERSONAL AUTHOR(S) Gorman, Thomas; Parker, Ronald; Generosa, John						
13a TYPE OF REPORT Technical		13b TIME COVERED FROM 870201 TO 870901		14 DATE OF REPORT (Year Month Day) 881101		15 PAGE COUNT 614
16 SUPPLEMENTARY NOTATION This work was sponsored by the Defense Nuclear Agency under RDT&E RMC Code B3200A7600D SA SA 00183 25904D.						
17 COSATI CODES			18 SUBJECT TERMS (Continue on reverse if necessary and identify by block number)			
FIELD	GROUP	SUB-GROUP	NORSE Optics, Molecular Effects, Nuclear Effects, <i>MOLECULAR SPECTRA</i> , Band Models <i>RADAR SYSTEMS, (TES)</i>			
12	8					
20	6					
19 ABSTRACT (Continue on reverse if necessary and identify by block number) The NORSE (Nuclear Optical and Radar System Effects) Code is being developed by DNA as a systems analysis tool. This report describes the local Thermal Equilibrium Emissions data base used by the NORSE code. Graphs of the Weakline and Strongline parameters in the spectral region of 10 cm^{-1} to $10,000\text{ cm}^{-1}$ are presented. A brief description of the band models used by NORSE is given.						
20 DISTRIBUTION AVAILABILITY OF ABSTRACT ☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT ☐ DTIC USERS			21 ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED			
22a NAME OF RESPONSIBLE INDIVIDUAL Bennie F. Maddox			22b TELEPHONE (Include Area Code) (202) 325-7042		22c OFFICE SYMBOL DNA/CSTI	

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PREFACE

This Manual is a graphical compendium of the NORSE LTE infrared data base. The complete NORSE data base is shown. Whenever possible the assumptions used to generate this information have been given. The theoretical background of the NORSE transmission model is briefly discussed.



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Justification	
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Distribution/	
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Conversion factors for U.S. Customary to metric (SI)
Units of Measure

MULTIPLY -----> TO GET <-----	BY -----> BY <-----	TO GET DIVIDE
angstrom (A)	1.000 000 X E -10	meters (m)
atmosphere (normal)	1.013 25 X E +2	kilo pascal (kPa)
bar	1.000 000 X E +2	kilo pascal (kPa)
barn	1.000 000 X E -28	meter ² (m ²)
British thermal unit (thermochemical)	1.054 350 X E +3	joule (J)
caloric (thermochemical)	4.184 000	joule (J)
cal (thermochemical)/cm ²	4.184 000 X E -2	mega joule/m ² (MJ/m ²)
degree (angle)	1.745 329 X E -2	radian (rad)
degree Fahrenheit	$t_K = (t_F + 459.67)/1.8$	degree kelvin (K)
electron volt	1.692 19 X E -19	joule (J)
erg	1.000 000 X E -7	joule (J)
erg/second	1.000 000 X E -7	watt (W)
foot	3.048 000 X E -1	meter (m)
foot-pound-force	1.355 818	joule (J)
gallon (U.S. liquid)	3.785 412 X E -3	meter ³ (m ³)
inch	2.540 000 X E -2	meter (m)
joule/kilogram (J/kg) (radiation dose absorbed)	1.000 000	Gray (Gy)
kilotons	4.183	terajoules
kip (1000 lbf)	4.448 222 X E +3	newton (N)
kip/inch ² (ksi)	6.894 757 X E +3	kilo pascal (kPa)
klap	1.000 000 X E +2	newton-second/m ² (N·s/m ²)
micron	1.000 000 X E -6	meter (m)
mil	2.540 000 X E -5	meter (m)
mile (international)	1.609 344 X E +3	meter (m)
ounce	2.834 952 X E -2	kilogram (kg)
pound-force (lbs avoirdupois)	4.448 222	newton (N)
pound-force inch	1.129 848 X E -1	newton-meter (N·m)
pound-force/inch	1.751 268 X E +2	newton/meter (N/m)
pound-force/foot ²	4.788 026 X E -2	kilo pascal (kPa)
pound-force/inch ² (psi)	6.894 757	kilo pascal (kPa)
pound-mass (lbm avoirdupois)	4.535 924 X E -1	kilogram (kg)
pound-mass-foot ² (moment of inertia)	4.214 011 X E -2	kilogram-meter ² (kg·m ²)
pound-mass/foot ³	1.601 846 X E +1	kilogram/meter ³ (kg/m ³)
rad (radiation dose absorbed)	1.000 000 X E -2	**Gray (Gy)
roentgen	2.579 760 X E -4	coulomb/kilogram (C/kg)
shake	1.000 000 X E -8	second (s)
torr (mm Hg, 0°C)	1.333 22 X E -1	kilo pascal (kPa)

*The becquerel (Bq) is the SI unit of radioactivity; 1 Bq = 1 event/s.

**The Gray (Gy) is the SI unit of absorbed radiation.

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SECTION 1

INTRODUCTION

1.1 DESCRIPTION OF THE DATA.

This manual describes the NORSE LTE (Local Thermodynamic Equilibrium) database including, when possible, the input assumptions used to generate the data. The NORSE LTE data base consists of values for the weak-line parameter (S/d - SOD) and the inverse line spacing ($1/d$ - DEI) arranged by wavenumber, temperature and molecule. This information is used by NORSE for thermal emission calculations.

The NORSE database contains emission information for twenty-six molecules and thirteen temperatures. The spectral range of this data is from 10 cm^{-1} (far infrared) to $100,000\text{ cm}^{-1}$ (visible).

The spectral data presented later in this report represents the NORSE LTE data base 87244.

1.2 DATA SOURCES.

The data sources for this database include: Band model programs, Air Force Geophysical Laboratory Line Atlas, Air Force Weapons Laboratory opacity database and other sources. Some of the information within this database originated over twenty years ago. During that time period the source of the data and the assumptions used to generate the information have been lost. When possible the source of the LTE data and the input assumption, will be presented in sections describing individual molecules.

1.3 LTE DATA BASE.

The LTE data base is stored as an ASCII file at the Los Alamos National Laboratory Central Computing Facility. The data base consists of over 260,000 eighty character lines of information. Further information about the structure and contents of the data base is contained in the NC RSE Manual 4-10 Model Data Files¹.

1.4 FUTURE EFFORTS.

Enhancement and verification of the LTE data base is a continuing effort. The Local Thermal Equilibrium (LTE) data base is updated and reviewed on a regular basis. Work is underway to bring this data in line with current spectroscopic data.

SECTION 2

BACKGROUND²

2.1 TRANSMISSION BAND MODELS.

The presentation in this section has been adapted from a discussion given in reference 2. Given a spectral line atlas it is possible to calculate photon transport along an optical path with varying temperature and pressure. In practice, a line-by-line calculation is impractical because of the large number of lines which need to be considered. To simplify the numerics, various band models have been developed.

Band models differ in their method of treating rotation lines; in fact, a rotational line-by-line reconstruction (or prediction) is often called the "line-by-line model" recognizing that even in the most painstaking predictions, there are assumptions, improper methods of including coupling, etc., which prevent the accurate representation of the actual situation.

A brief review of the different types of band models follows. As an introduction, it can be shown from radiative transfer considerations that the energy, E_a , absorbed through a path length s , in a solid angle Ω and reaching an area A is given by

$$\frac{d^2 E_a}{dA d\Omega} = \int_0^\infty I_\nu^o [1 - \exp(-a_\nu s)] d\nu \quad (1)$$

whereas the energy emitted, E_e , to A by a gas is given by

$$\frac{d^2 E_e}{dA d\Omega} = \int_0^\infty I_\nu^b [1 - \exp(-a_\nu s)] d\nu \quad (2)$$

where I_ν^o is the incident intensity at wavenumber ν , I_ν^b is the Blackbody emission intensity, and a_ν is the line absorption coefficient. It will be assumed that a_ν is zero, except in the small wavenumber interval near to ν_{ij} . For small path lengths, the integrals in Eqns. (1) and (2) will be large only within this narrow interval, so that the integration need only be performed over this interval. Within this interval, I_ν^o and I_ν^b are assumed to be constant, at their value of ν . Then the two equations become

$$\frac{d^2 E_a}{dA d\Omega} = I_{\nu_{ij}}^o \int_0^s [1 - \exp(-a_{\nu_{ij}} s)] d\nu \quad (3)$$

and

$$\frac{d^2 E_e}{dA d\Omega} = I_{\nu_{ij}}^b \int_0^s [1 - \exp(-a_{\nu_{ij}} s)] d\nu \quad (4)$$

where ij indicates the two levels involved in the line transition. The absorbed energy as well as the emitted energy for the line in question are seen to be dependent on the same integral; this integral is called "effective line width" $\bar{A}_{ij}$, i.e.,

$$\bar{A}_{ij} = \int_0^s [1 - \exp(-a_{\nu_{ij}} s)] d\nu \quad (5)$$

and has the units of ν (cm^{-1}). $\bar{A}_{ij}$ can be interpreted as follows. If $a_{\nu_{ij}}$ is considered infinitely large, and there is no absorption outside this line, $\bar{A}_{ij}$ can be considered as the width of a black line centered at ν_{ij} that produces the identical emission as the actual line.

$\bar{A}_{ij}$ can be evaluated for two limiting cases. If the product $(a_{\nu_{ij}} s)$ is small (i.e., $\ll 1$) an expansion of the exponent in Eqn. (5) gives:

$$1 - \exp(-a_{\nu_{ij}} s) = a_{\nu_{ij}} s - \frac{(a_{\nu_{ij}} s)^2}{2!} + \dots \quad (6)$$

Keeping only the first term, Eqn. (5) becomes

$$\bar{A}_{ij} = s \int_0^{\infty} a_{\nu_{ij}} d\nu \quad (7)$$

where the integral represents the "integrated absorption coefficient." The effective line width is therefore linear with path length, s , regardless of the line profile; a line with this linear behavior is called a "weak-line." [*"Line profiles" arise because the upper and lower energy levels, which determine the energy of a spectral "line", are in reality a distribution of levels; transitions from one distribution (say, the upper) to another distribution (lower) gives rise to a spectral line "profile". Depending on the statistical nature of these distributions, profiles are called Lorentzian, Gaussian, or Voigt (a convolution of Lorentzian and Gaussian). For our purposes, the major cause of Gaussian profiles is Doppler broadening, the term we will use in this work. The importance of line profiles cannot be overemphasized*].

The other limit concerns a large optical path (optically thick). In this limit, $a_{\nu_{ij}} s \gg 1$, the absorption coefficient is written

$$a_{\nu_{ij}} = b_{ij} \int_0^{\infty} a_{\nu_{ij}} d\nu \quad (8)$$

where b_{ij} is the line profile. Using the Lorentz profile for b_{ij} , substituting Eqn. (8) into Eqn. (7) and performing integration and rearrangements, it is found that

$$\bar{A}_{ij} = (2s\gamma_L \int a_{\nu_{ij}} d\nu)^{1/2}, \quad (9)$$

where γ_L is the Lorentzian width at half-maximum. Thus, the "strong-line" approximation leads to an absorption varying with the square root of the path length (s) in contrast to the "weak-line" approximation where it varies linearly with s .

In a similar manner, an "effective band width", $\bar{A}_e$ can be defined as

$$\bar{A}_e = \int_{band} [1 - \exp(-a_{\nu_y} s)] d\nu \quad (10)$$

The boundaries of the band can be defined as the wavenumber interval outside of which there is only a predetermined fractional contribution to $\bar{A}_e$. As the path length increases, the width of the wavenumber interval increases slowly due to absorption taking place in the wings of the line profiles (the profiles are bell shaped). Note that $\bar{A}_e$ for the band is the sum of the $\bar{A}_y$ for all the lines that constitute the band, only if all the $\bar{A}_y$ do not overlap. Since the lines overlap, each line absorbs less energy than if there were no overlap.

In the derivation of appropriate band models, simplified forms of the absorption coefficient a_{ν} must be devised. The two more common types of band models are the Regular and Random Band Models.

The most familiar of the Regular techniques is due to Elsasser. In this model, the individual lines all have the same profile, the same height and the same spacing. Elsasser's approach uses the Lorentz line profile (the Doppler and Voigt profiles may also be used). The absorption coefficient at a specified wavenumber is calculated by adding all the contributions from neighboring lines. If the specified position is ν_o , the distance of the centers of the other lines from the specified wavenumber ν_o is $|\nu_o - 0|$, $|\nu_o - d|$, $|\nu_o - 2d|$, ... Summing the contributions results in:

$$a(\nu_o) = \frac{\int a_L d\nu}{2\pi} \sum_{-\infty}^{\infty} \frac{\gamma_L}{\frac{\gamma_L^2}{4} + (\nu_o - nd)^2} \quad (11)$$

where $a(\nu_o)$ is the absorption coefficient at the specified wavenumber (ν_o), $\int a_L d\nu$ is the integrated absorption coefficient for each line, n is the number of lines contributing, d is the spacing between adjacent peaks and γ_L is the Lorentzian width.

This function is substituted in Eqn. (7). By using the "weak-line" and "strong-line" limits, analytic solutions are practical, otherwise numerical methods are necessary.

The Random (or Statistical) band model uses a statistical array of individual lines. In this case, there can be a random spacing of identical or dissimilar lines. In order to apply this model, probability distributions of line strengths and positions must be assumed. Once the nature of a line, and its position, are chosen, the effective band width $\bar{A}_\ell$ is calculated from Eqn. (10). Note that $\bar{A}_\ell$ depends on the line spacing, the width of the line profile, and the integrated absorption. Since these parameters rely on temperature and density, it is necessary to know how they change with temperature and pressure.

2.2 BAND MODEL PARAMETERS.

An important source of radiation from low-altitude fireballs is thermal emission due to equilibrium processes in the hot gas. The magnitude of the radiation is determined by the temperature and the optical absorption properties of the fireball. For infrared wavelengths, the vibrational-rotational bands of

molecular species are major contributors to thermal emission. Particularly important emitters in a fireball are CO_2 , CO , NO and NO^+ . Other potential infrared emitters include O_3 , NO_2 , N_2O , H_2O , OH and metal oxides (MeO).

A procedure has been developed for the NORSE³ code that uses band absorption models to calculate fireball thermal emission. These models require the fireball sight-path length, the average pressure over the path, an isothermal temperature of the emitting gas, and the population of species in the fireball. The spectral radiance of the path length is then calculated as a function of wavenumber. The models described in Section 2.1 include:

- o Elsasser model. This model is appropriate for a band of lines with uniform intensity, width and spacing.
- o Random Elsasser model. This model assumes n randomly superimposed Elsasser bands. The limit n corresponds to the statistical model, while $n = 1$ corresponds to the Elsasser model.
- o Statistical model. This model assumes lines with arbitrary strength and width distributions, and random spectral frequency.

For molecules of the asymmetrical top (three moments of inertia, all unequal) form, such as H_2O , the rotational structure is quite irregular, and the statistical model is clearly preferred. Symmetric top (rotor) molecules, such as diatomic or linear polyatomic species, have more regular rotational structures. Such a structure is best described by the Elsasser or random Elsasser models for lower temperatures. At elevated temperatures, many such regular bands will overlap. If the number of bands is $n > 10$, there is little difference between the predictions of the random Elsasser and statistical models. Since the statistical model offers the advantage of rapid calculation, and requires a minimum number of parameters to be determined from often scanty data, it is used in the fireball thermal emission model.

In many situations, lines show both Doppler and Lorentz profiles characterized by broadening widths denoted by γ_D and γ_L , respectively. If $\gamma_L \gg \gamma_D$, the absorption predicted by a pure Lorentz line shape is an excellent approximation. The corresponding approximation does not hold for $\gamma_D \gg \gamma_L$, however. In this case, the center of the line will reflect the Doppler profile, while the wings will reflect the Lorentz shape. For small path length, the absorption is well approximated by a pure Doppler line shape. For larger path lengths absorption by the line wings will dominate, so the Lorentz profile is needed.

Stephens⁴ discusses the details of the transmission model. Of interest herein is the fact that in either limit of Doppler or Lorentz shapes, the value of transmission over an optical path of varying temperature, composition, and pressure (affecting the Lorentz profile) can be reduced to functions of γ_L, γ_D , pressure, and so-called weak-line parameters, average line strength, SOD, and effective inverse line spacing, DEI, for individual species. For temperature T and wavenumber ν

$$\text{SOD}(T, \nu) = \sum_i S_i / \Delta \nu \quad (12)$$

$$\text{DEI}(T, \nu) = \left[\sum_i (S_i)^{1/2} / \Delta \nu \right]^2 / \text{SOD}(T, \nu) \quad (13)$$

where $\Delta \nu$ refers to a small wavenumber interval within which there are a limited number of individual quantum mechanical lines of strength S_i .

Thus, calculations of radiation transport are reduced to calculations involving the weak-line parameters SOD and DEI which approximate molecular absorption processes as a function of energy and temperature.

SECTION 3 SAMPLE CALCULATIONS

A sample transmissivity calculation for CO₂ gas in LTE is presented. The data used for this calculation are a subset of the CO₂ data presented in section 5.2 of this report. For simplicity, only data for the 626 (the 626 label denotes the ¹⁶O-¹²C-¹⁶O molecule) isotopic species of carbon dioxide will be used. The temperature, path length, and mole fraction for the absorbing CO₂ gas are chosen to match the experimental conditions as reported.⁵ This exercise will show how the data contained in this volume may be used to predict transmissivity and emissivities using the statistical band model approach.

The transmissivity predicted by various forms of the statistical band model is given by:

$$\tau = \exp[-F(x)(2\pi\gamma_L/d_\nu)] \quad (14)$$

where the curve of growth for the particular model is defined as, $-\ln(\tau)$. The variable x is defined here as:

$$x = (S/d)_\nu u(2\pi\gamma_L/d_\nu)^{-1} \quad (15)$$

where

$$\begin{aligned} \gamma_L & \text{ is the full width at half maximum for a single line with} \\ & \text{Lorentzian shape} \\ \gamma_L & = \gamma_L^o (T_o/T)^\eta \end{aligned} \quad (16)$$

d_ν is the mean line spacing

$(S/d)_w$ is the weak-line parameter

u is related to the number of absorber/emitters

$$u = L\chi P(T_o/T) \quad (17)$$

where χ is the mole fraction of the absorbing/emitting species, P is the pressure, T is the temperature, L is the path length and η is an empirical parameter which is usually about 0.5.

Here it is assumed that all lines have the Lorentz shape and equal widths. The function $F(x)$ is determined by the distribution of line strengths. For example, the probability distribution

$$P(S) \propto (1/S) \exp (-S/S_o) \quad (18)$$

results in

$$F(x) = (1/\pi)[(1+2\pi x)^{1/2} - 1] \quad (19)$$

As $x \rightarrow 0$ the function $F(x)$ becomes proportional to x and the curve of growth is said to be in the linear (weak-line) region. The square root (strong-line) region of the curve of growth obtains when $x \rightarrow \infty$. The curve of growth or $F(x)$ is then proportional to $(x)^{1/2}$. Different choices of the distribution function $P(S)$, will result in the same form for the curve of growth (or $F(x)$) for the asymptotic regions. However, for intermediate values of u (where $x \approx 1$) the various curve of growth functions will be different, with the exponential S^{-1} probability distribution having the largest change between the two asymptotic forms⁶.

The statistical curve of growth which results from the distribution function given in Eqn. 18 is assumed and predictions are made of the transmissivity for a

given optical depth and temperature. In Figure 1 the weak-line parameter as a function of wavenumber is plotted for the 626 isotopic species of the CO_2 molecule for a temperature of $T = 292^\circ\text{K}$. The weak-line parameter is the absorption coefficient for the linear region of the curve of growth. Note the strong P and R branch lobes from the ν_3 fundamental transition located about the band center near 2350 cm^{-1} .

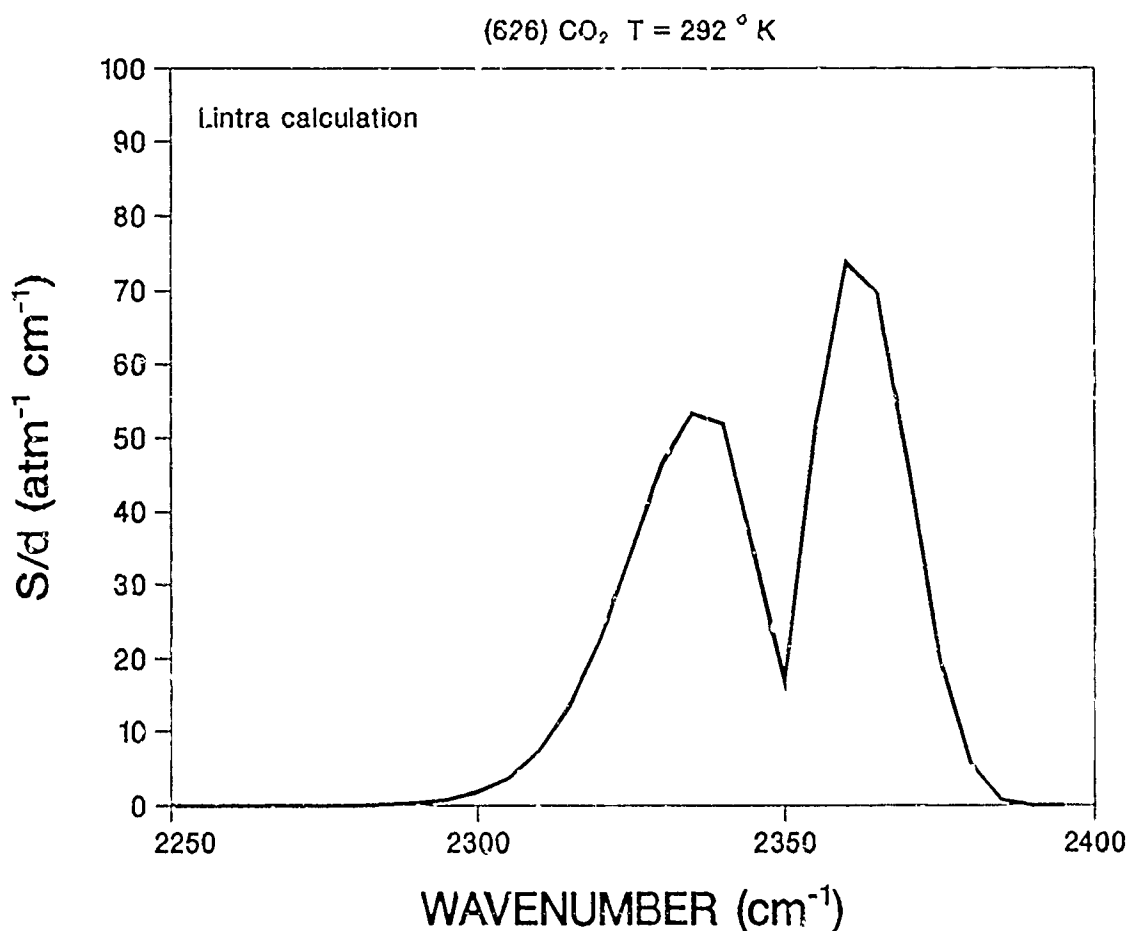


Figure 1. Weak-line parameter for 626 CO_2 .

In Figure 2 the inverse line spacing parameter is displayed as a function of wavenumber for a temperature $T = 292^\circ \text{K}$. The two band model parameters listed in this report are the weak-line parameter $(S/d)_v$ and the strong-line parameter used by Malkmus⁷. The strong line parameter is related to the inverse line spacing parameter by

$$A = (S/d)_v (2\pi\gamma_L/d_v)^{-1} = x/u \quad (20)$$

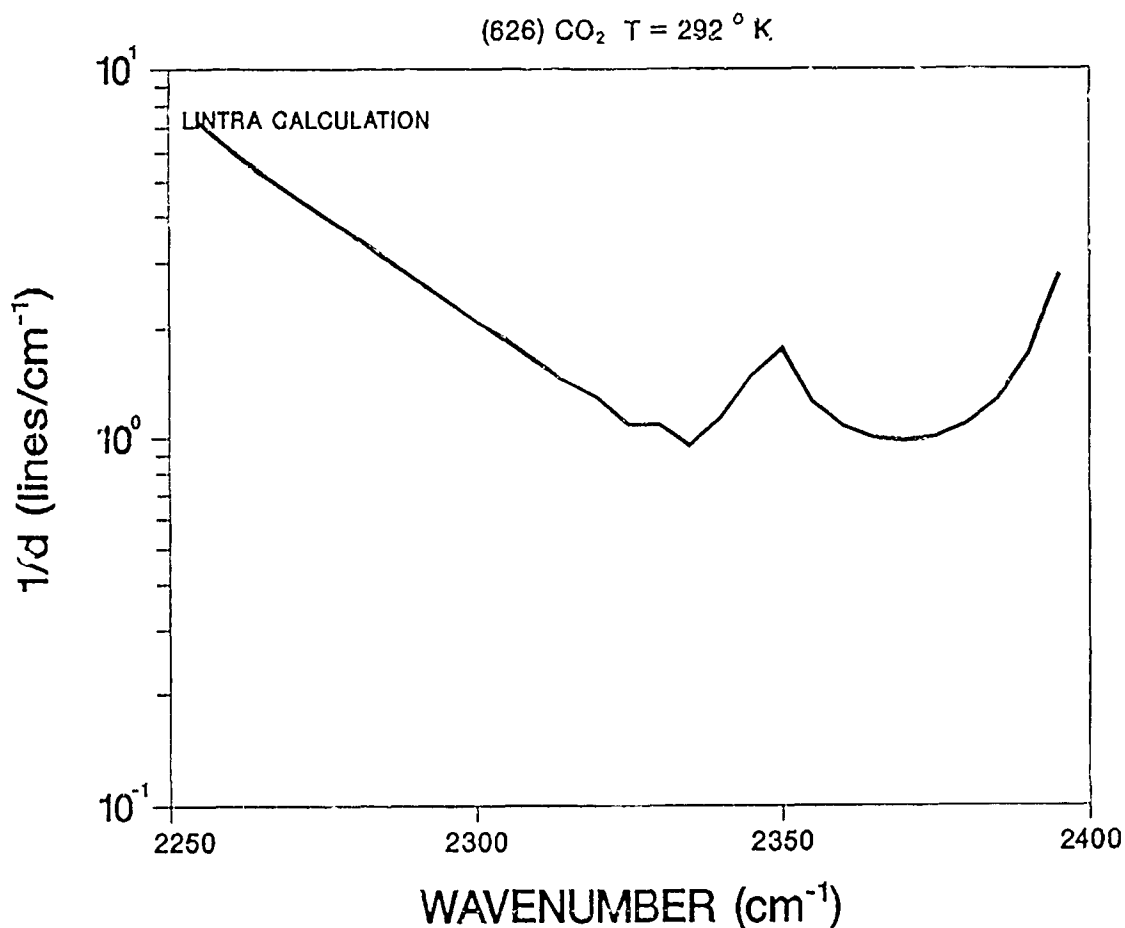


Figure 2. Inverse line spacing for 626 CO₂.

The weak-line and inverse line spacing parameters are input to the statistical model (Eqn. 14) with the optical conditions of a homogenous sample of gas at a temperature of $T = 292$ °K. The path length is 9.84 cm and the total pressure of the gas is 0.6128 atm, with the mole fraction for CO_2 , $\chi = 0.0230$. The statistical band model gives the transmissivity shown in Figure 3. This predicted transmissivity curve agrees with recent experimental data taken under the same conditions⁵.

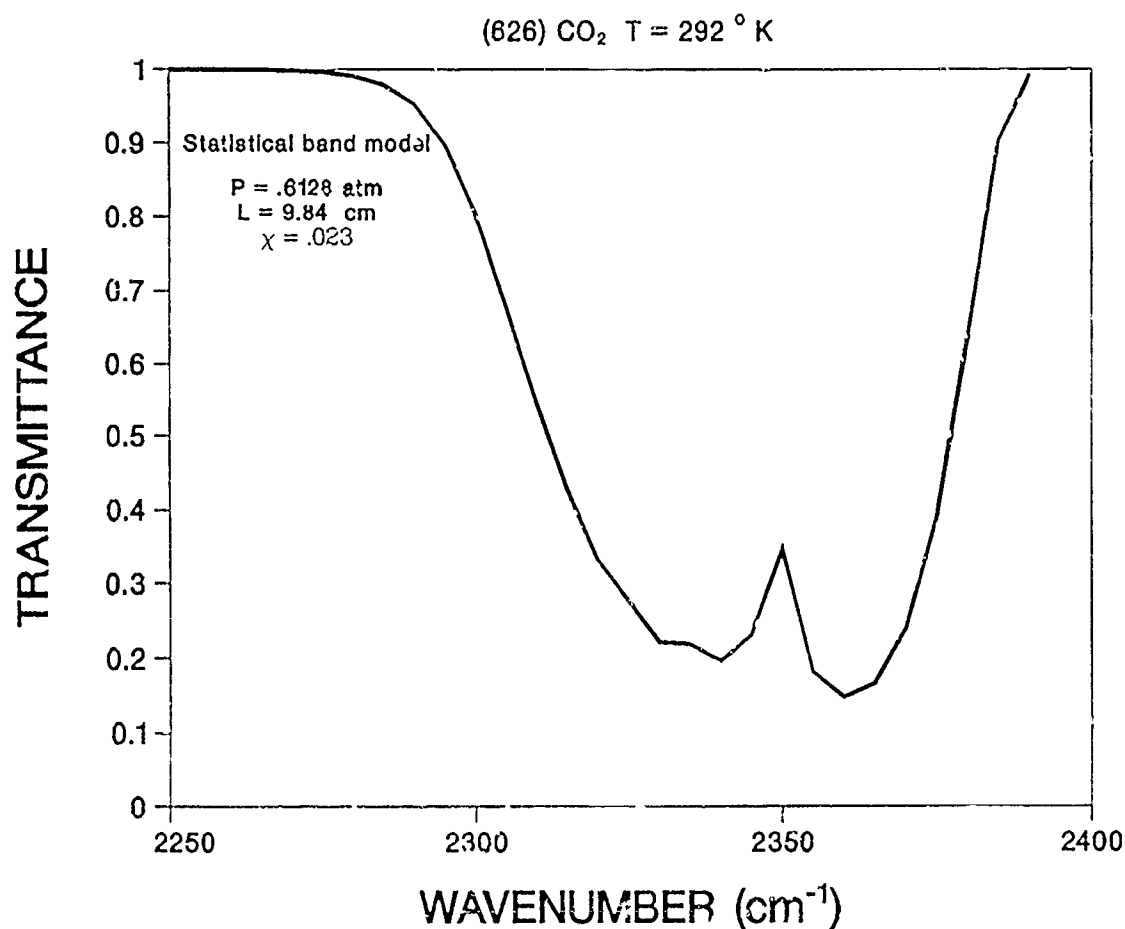


Figure 3. Transmittance for 626 CO_2 .

SECTION 4

DIATOMIC MOLECULES

Local thermal equilibrium emission spectra for all diatomic molecules within the spectral range $10 - 10,000 \text{ cm}^{-1}$ have been computed using the DiAtomic Thermal Emissions (DATE) code⁸. In the case of certain molecules, NO, N_2 , N_2^+ and O_2 , data available in the spectral range $5,000 - 100,000 \text{ cm}^{-1}$ was obtained from the VisiDyne Corporation using a database developed by the Air Force Weapons Laboratory (AFWL) in the late sixties and used by the RADiation FLOW (RADFLO) code.

The band strengths given in this section are listed in $\text{cm}^{-2} \text{ atm}^{-1}$ at STP.

4.1 CARBON MONOXIDE (CO).

Data for the CO molecule in the spectral range 10 - 12,000 cm^{-1} has been computed using the DATE code.

Table 1. Spectroscopic data for CO.

$X \ ^1\Sigma^+$		
$\omega_e = 2169.8233^*$	$\omega_e x_e = 13.2939^*$	$\omega_e y_e = 0.01158^*$
$\omega_e z_e = -1.119 \times 10^{-5}^b$	$\omega_e a_e = 2.85 \times 10^{-6}^*$	$\omega_e b_e = -4.94 \times 10^{-6}^*$
$\alpha_e = 0.017513^*$	$B_e = 1.931271^*$	$\gamma_e = 2.96 \times 10^{-6}^*$
$S_{10} = 260.0^\dagger$	$S_{20} = 2.06^\dagger$	$S_{30} = 0.0132^\dagger$
$\gamma_t(300^\circ\text{K}) = 0.06^\dagger$		

Data Source:

*J.T. Yardley, J. Mol. Spectrosc. 35, 314 (1970).

†R.A. Toth, R.H. Hunt, and E.K. Plyler, J. Mol. Spectrosc. 32, 85 (1969).

‡Fit to the data of D.A. Draegert, and D. Williams, J. Opt. Soc. Am. 58 1399 (1968).

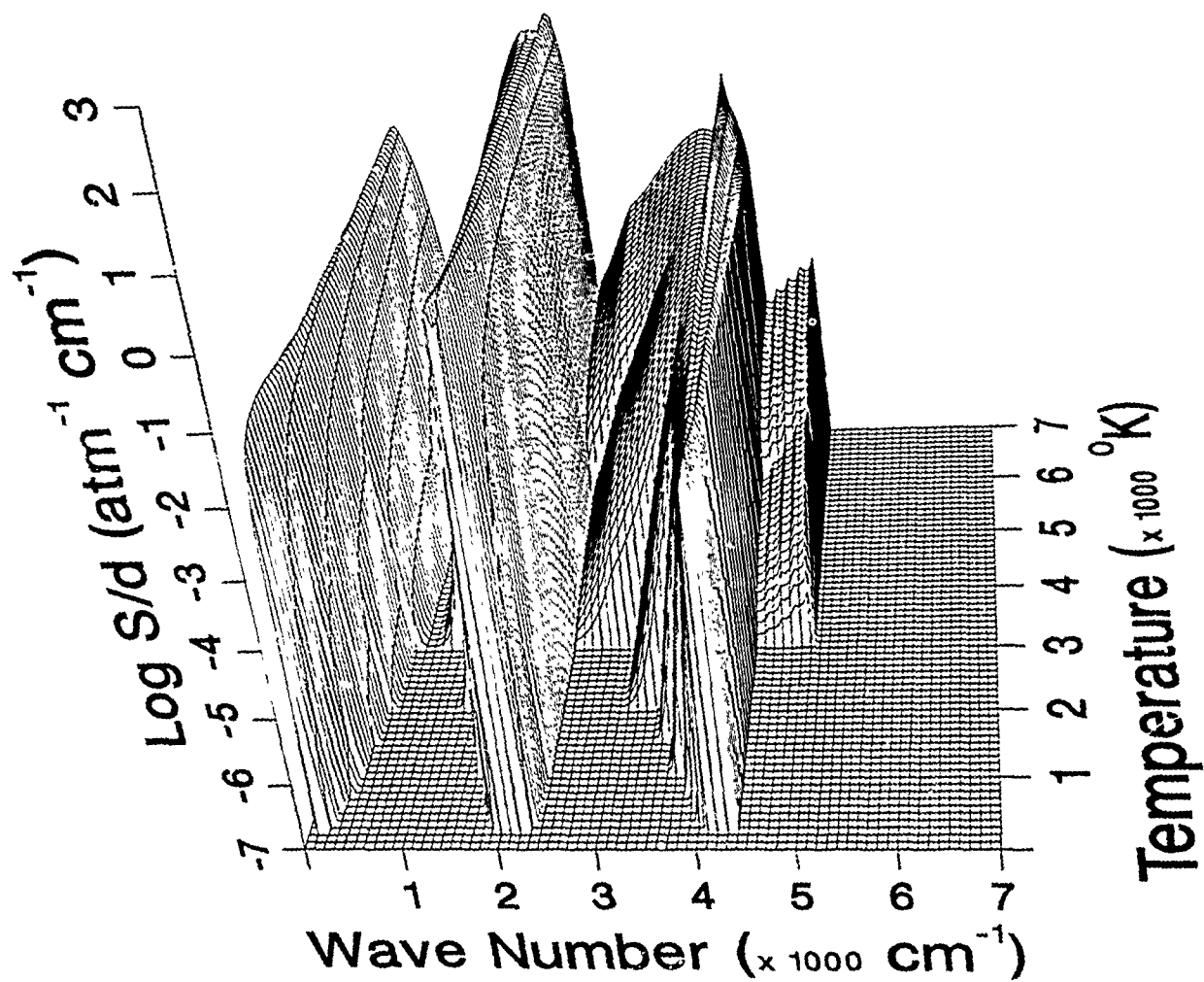


Figure 4. Weak-line parameter for CO.

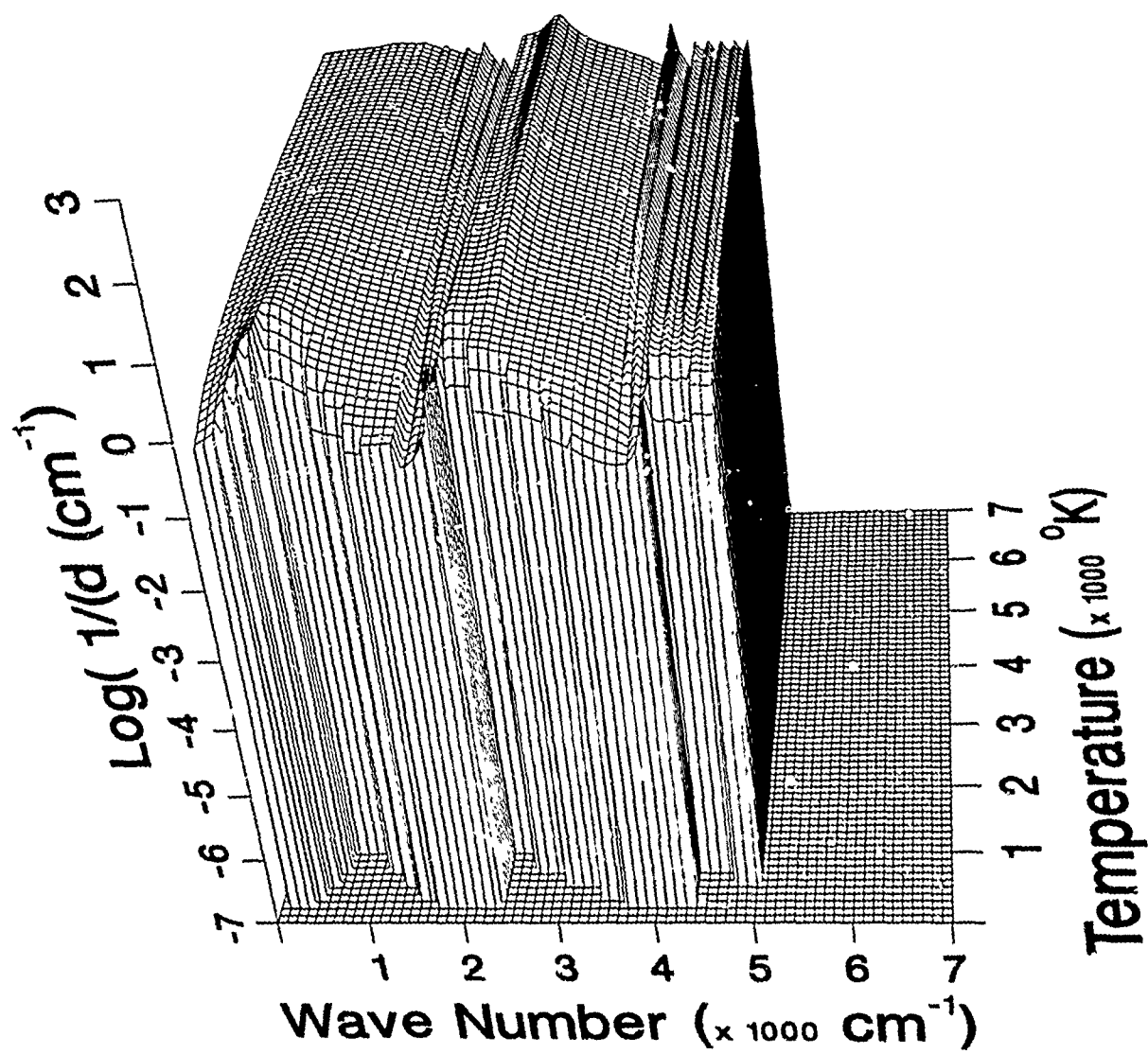


Figure 5. Inverse line spacing for CO.

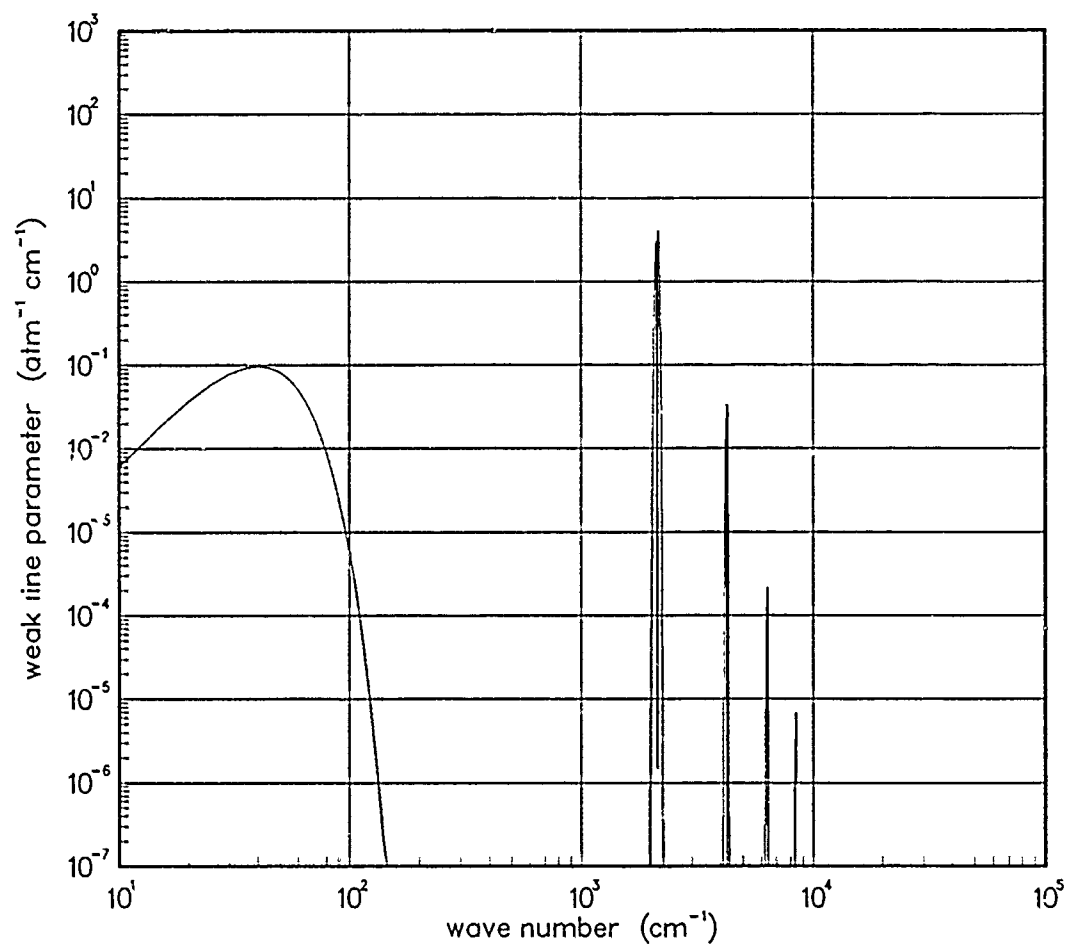


Figure 6. Weak-line parameter for CO at 200°K.

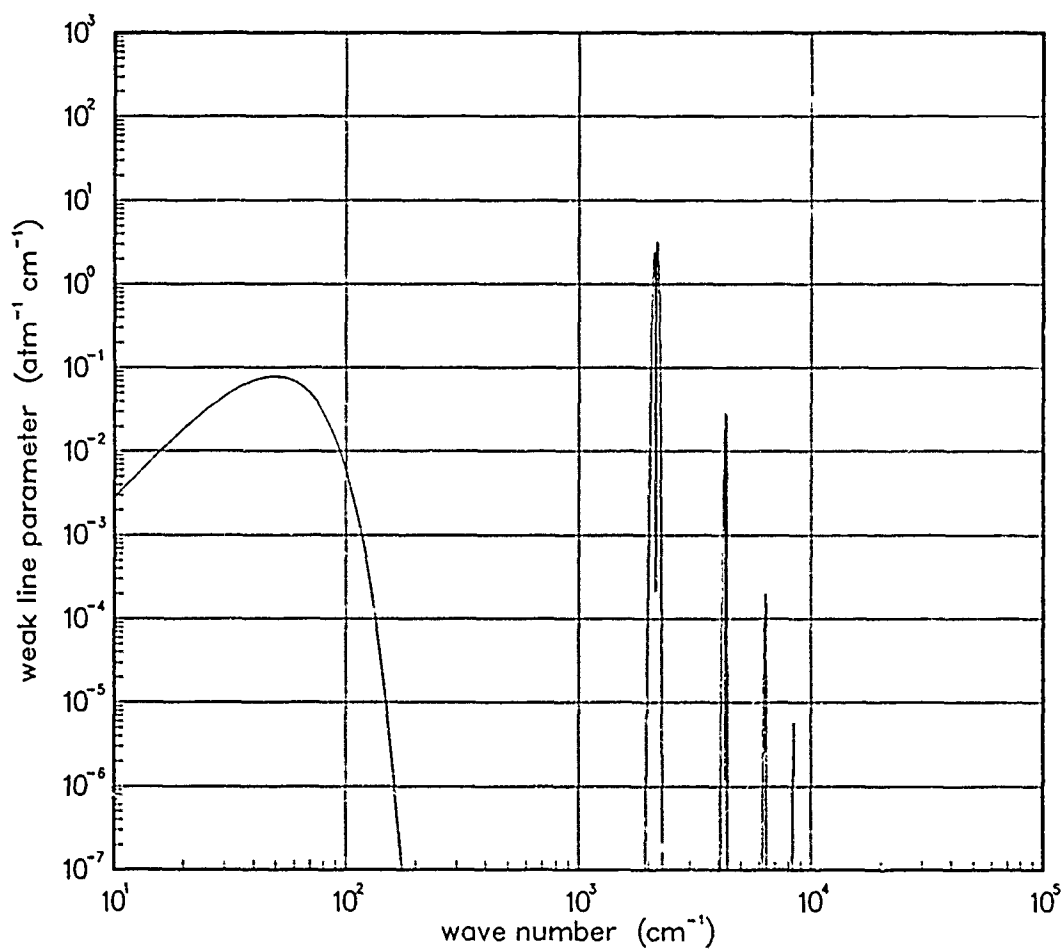


Figure 7. Weak-line parameter for CO at 300°K.

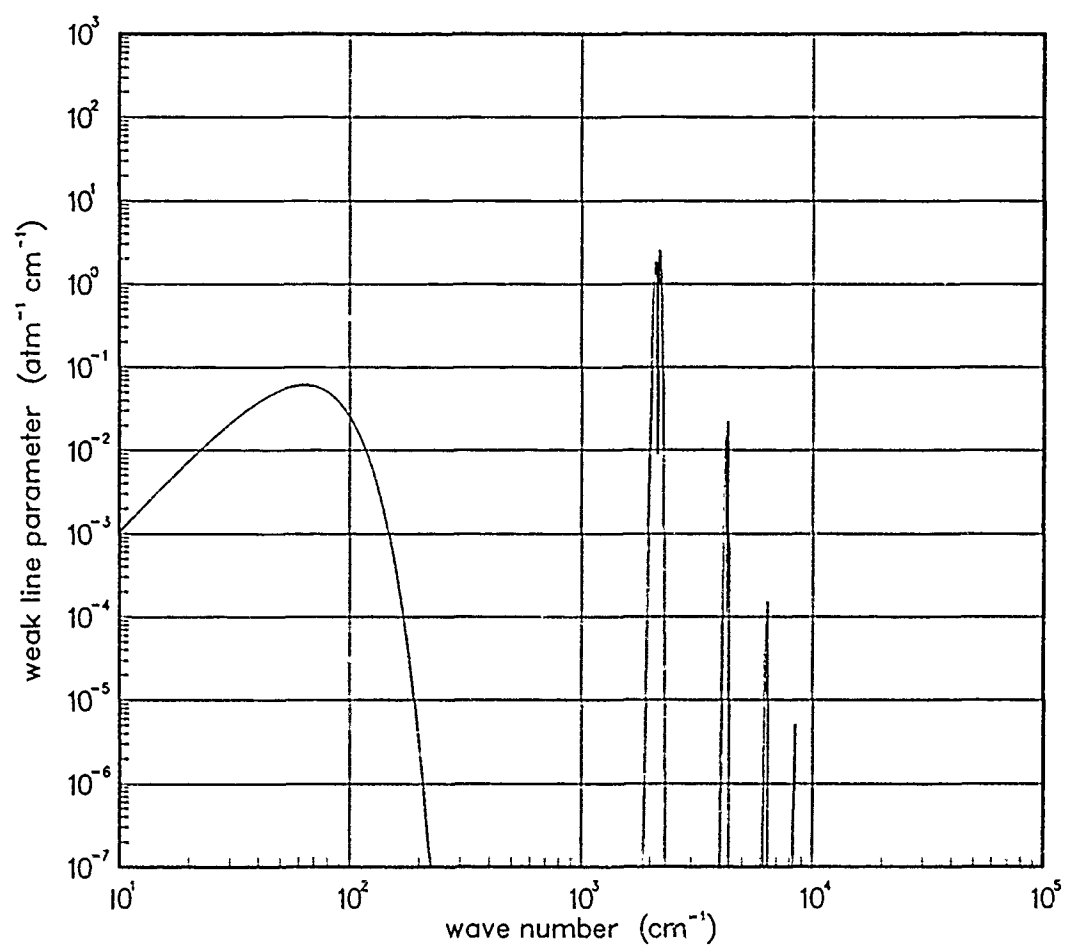


Figure 8. Weak-line parameter for CO at 500°K.

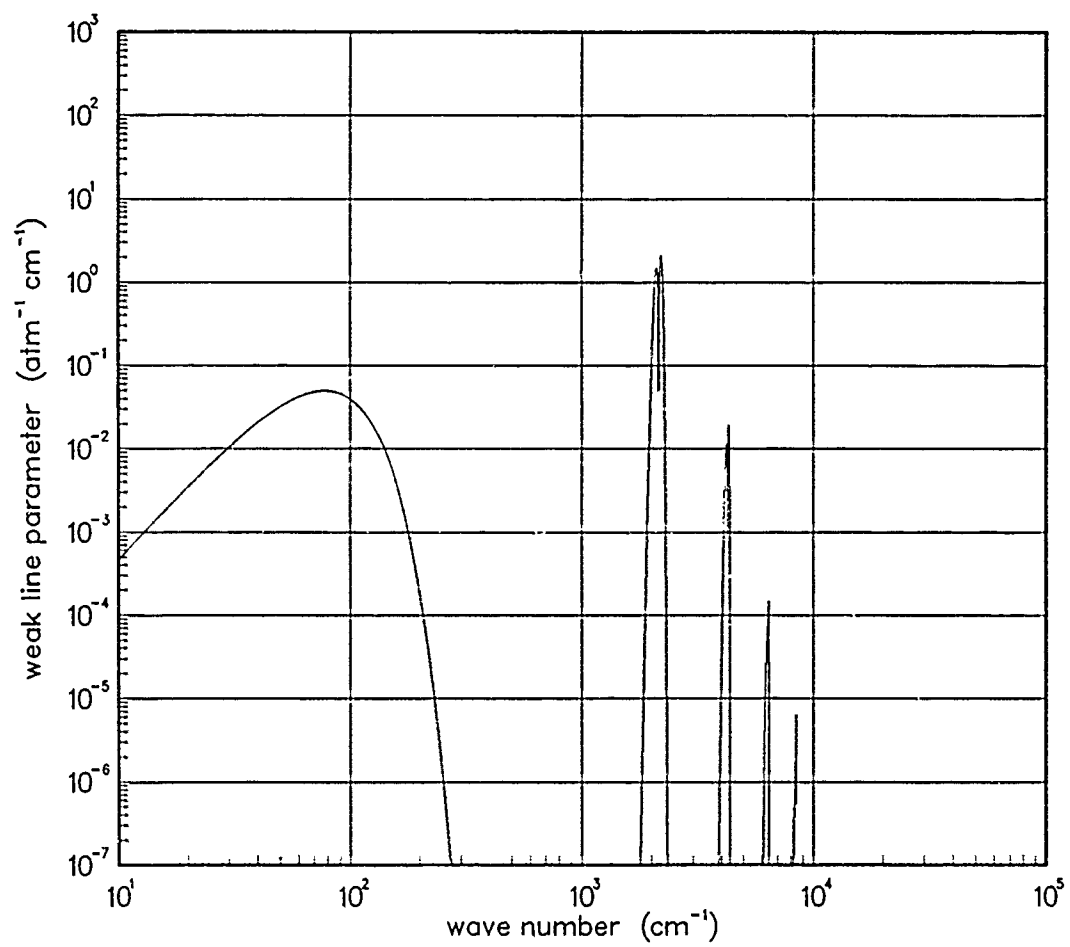


Figure 9. Weak-line parameter for CO at 750°K.

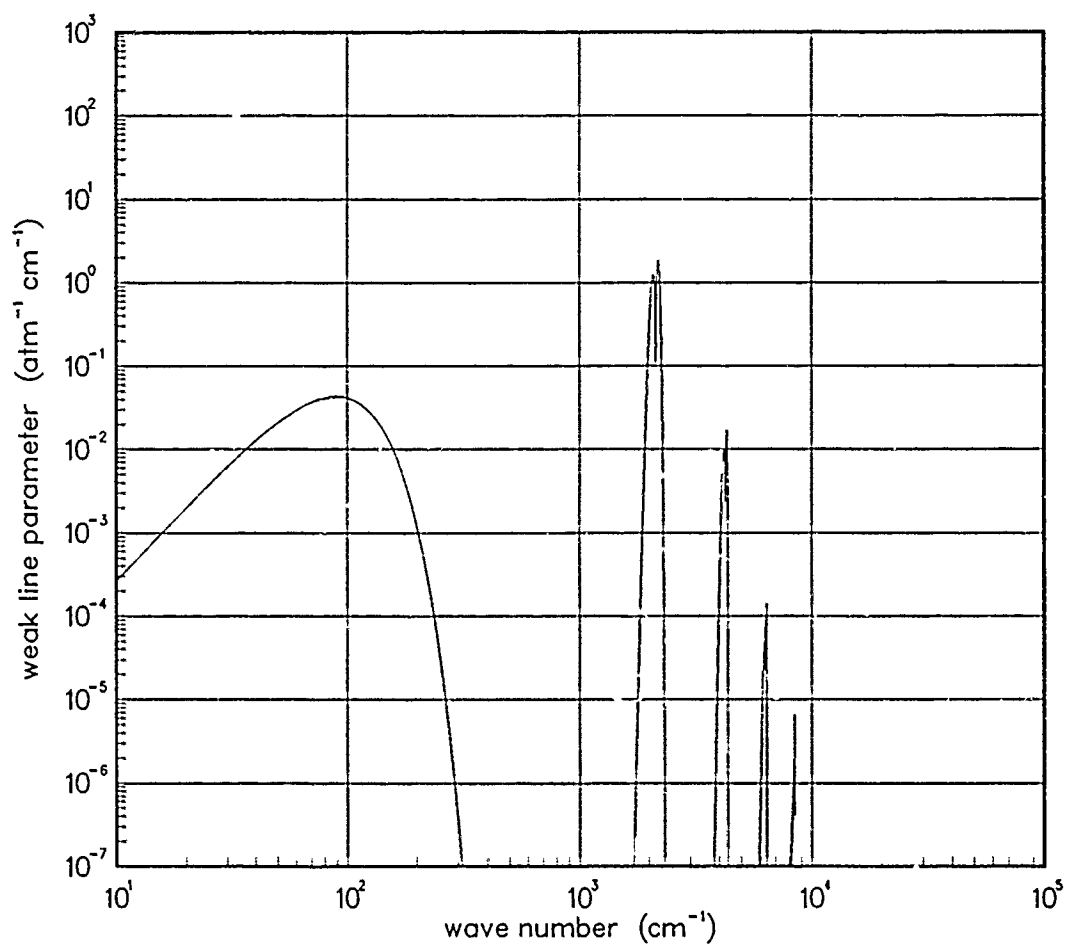


Figure 10. Weak-line parameter for CO at 1000°K.

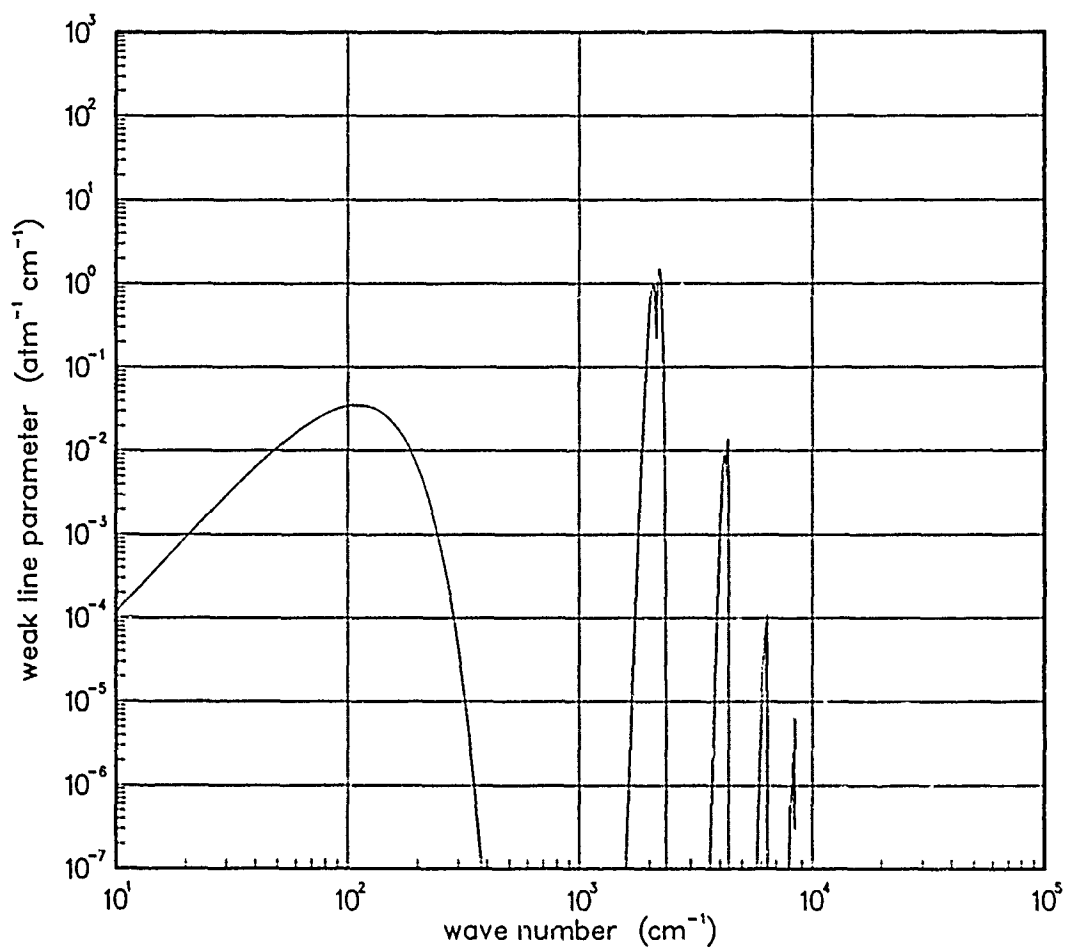


Figure 11. Weak-line parameter for CO at 1500°K.

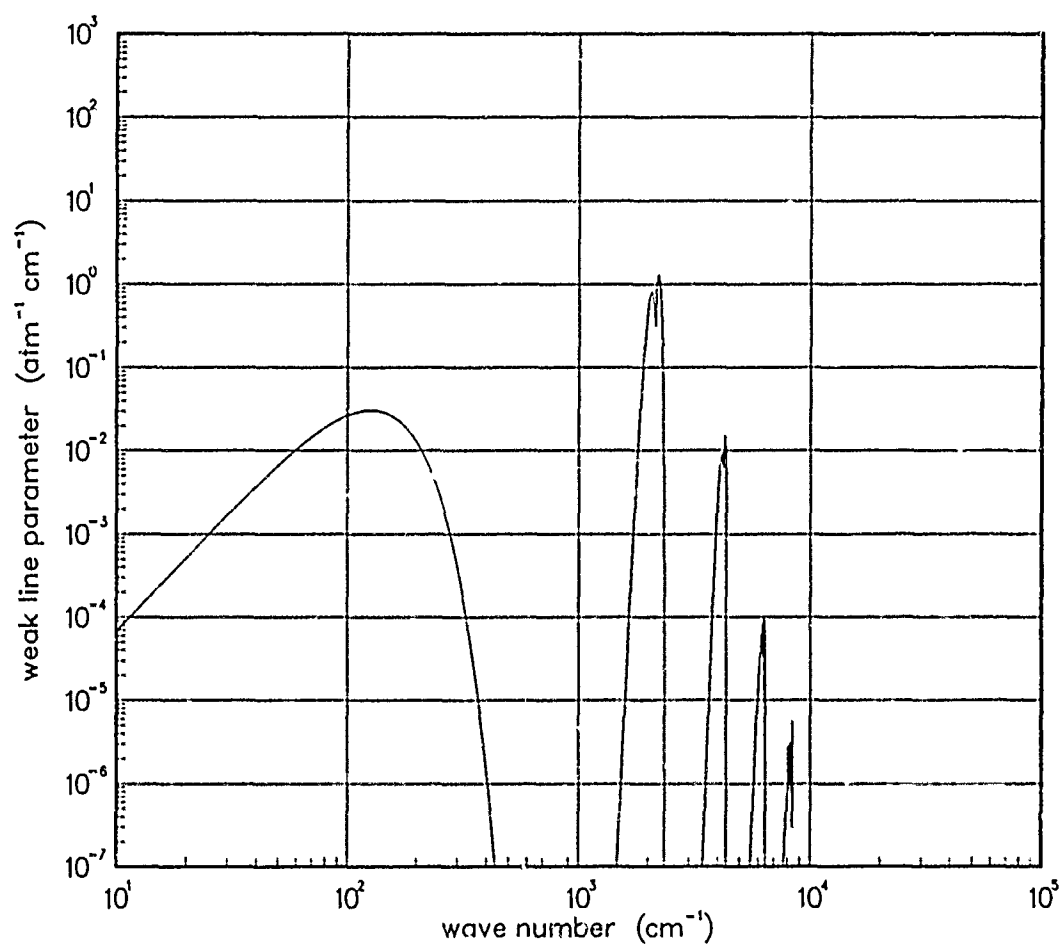


Figure 12. Weak-line parameter for CO at 2000°K.

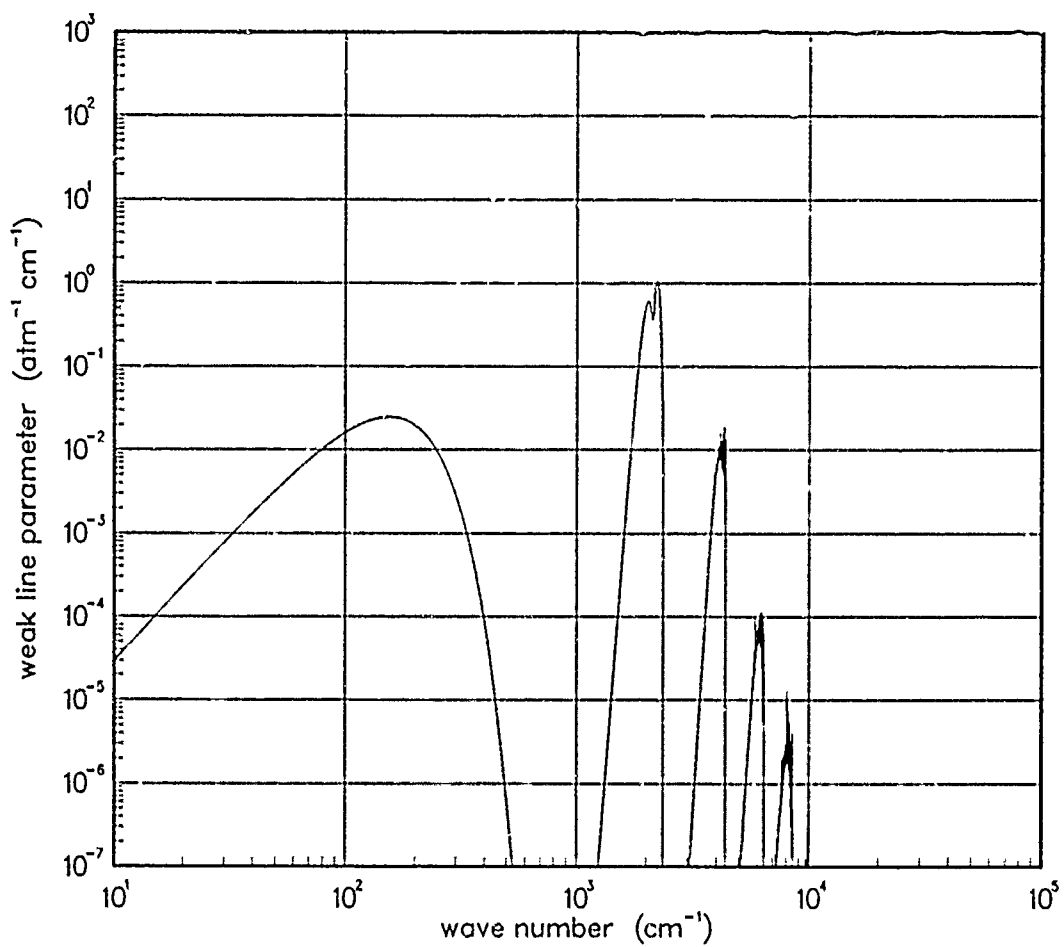


Figure 13. Weak-line parameter for CO at 3000°K.

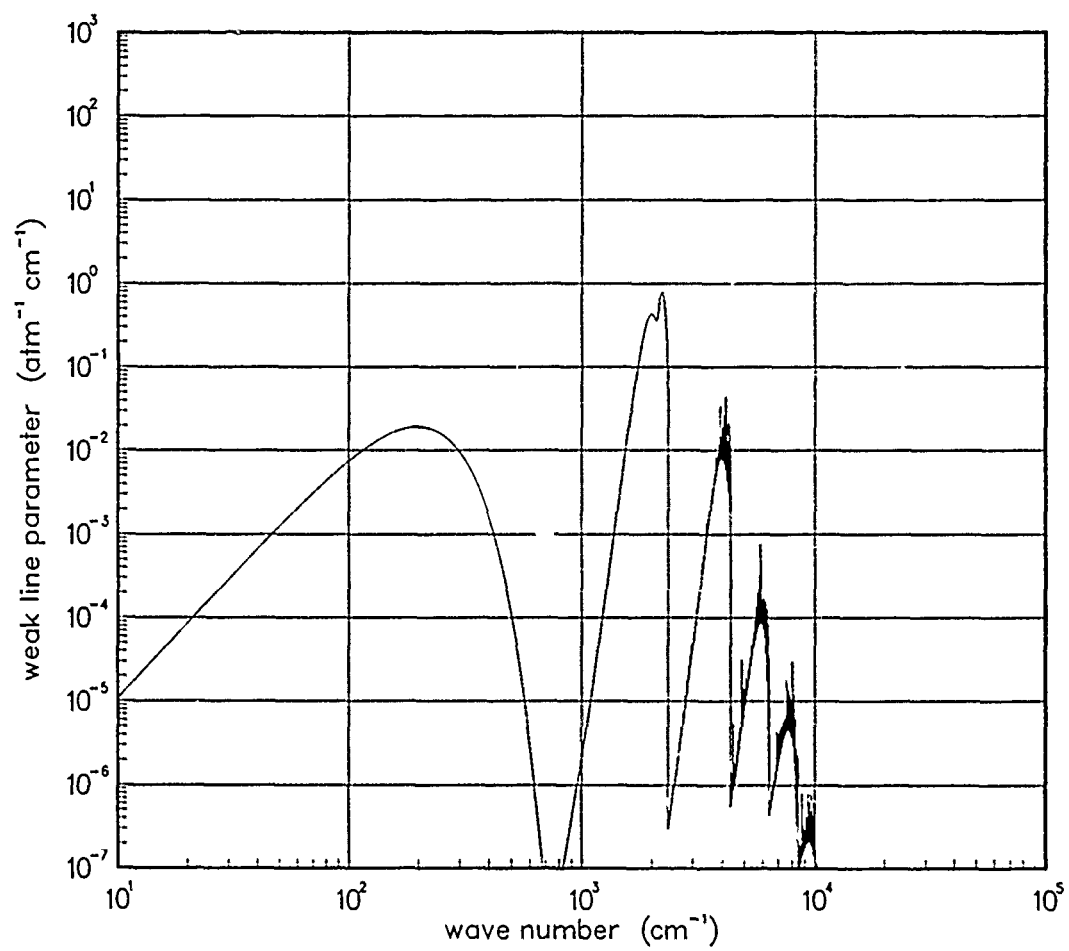


Figure 14. Weak-line parameter for CO at 5000°K.

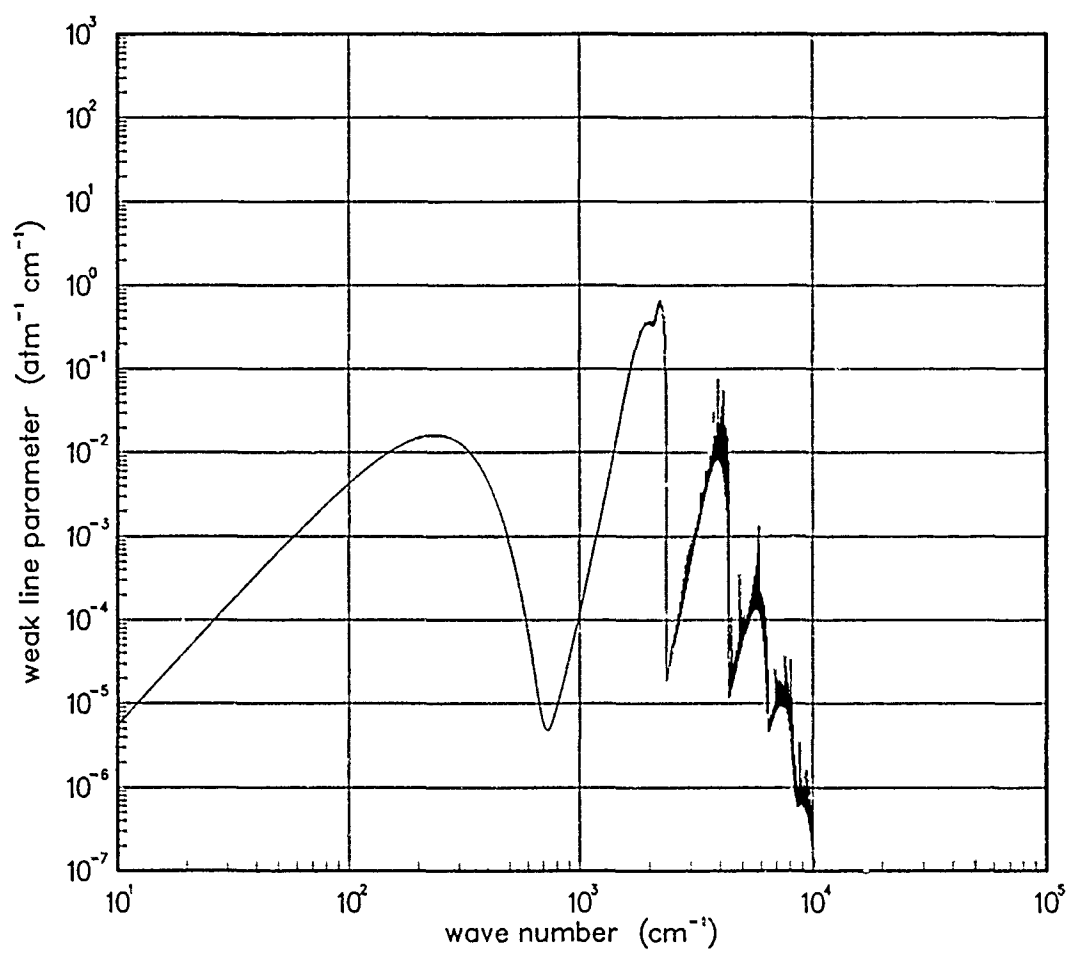


Figure 15. Weak-line parameter for CO at 7000°K.

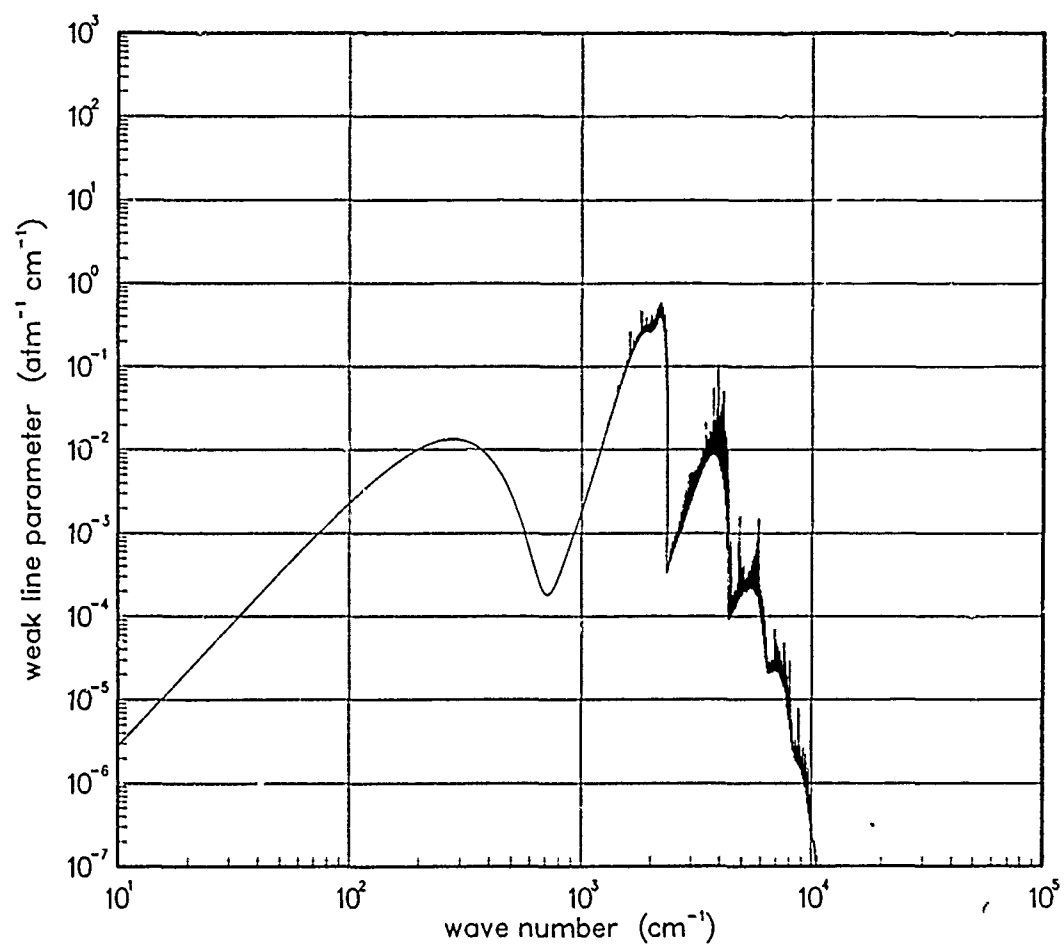


Figure 16. Weak-line parameter for CO at 10000°K.

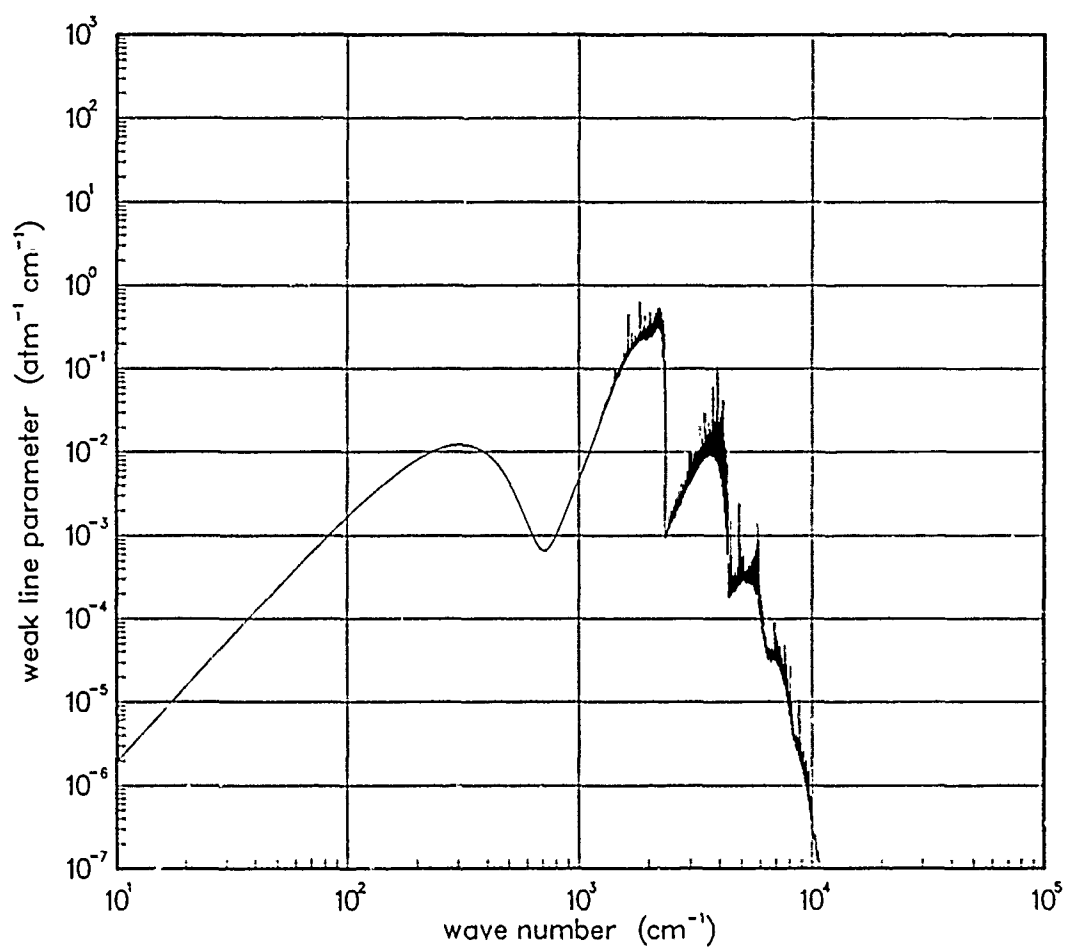


Figure 17. Weak-line parameter for CO at 12000°K.

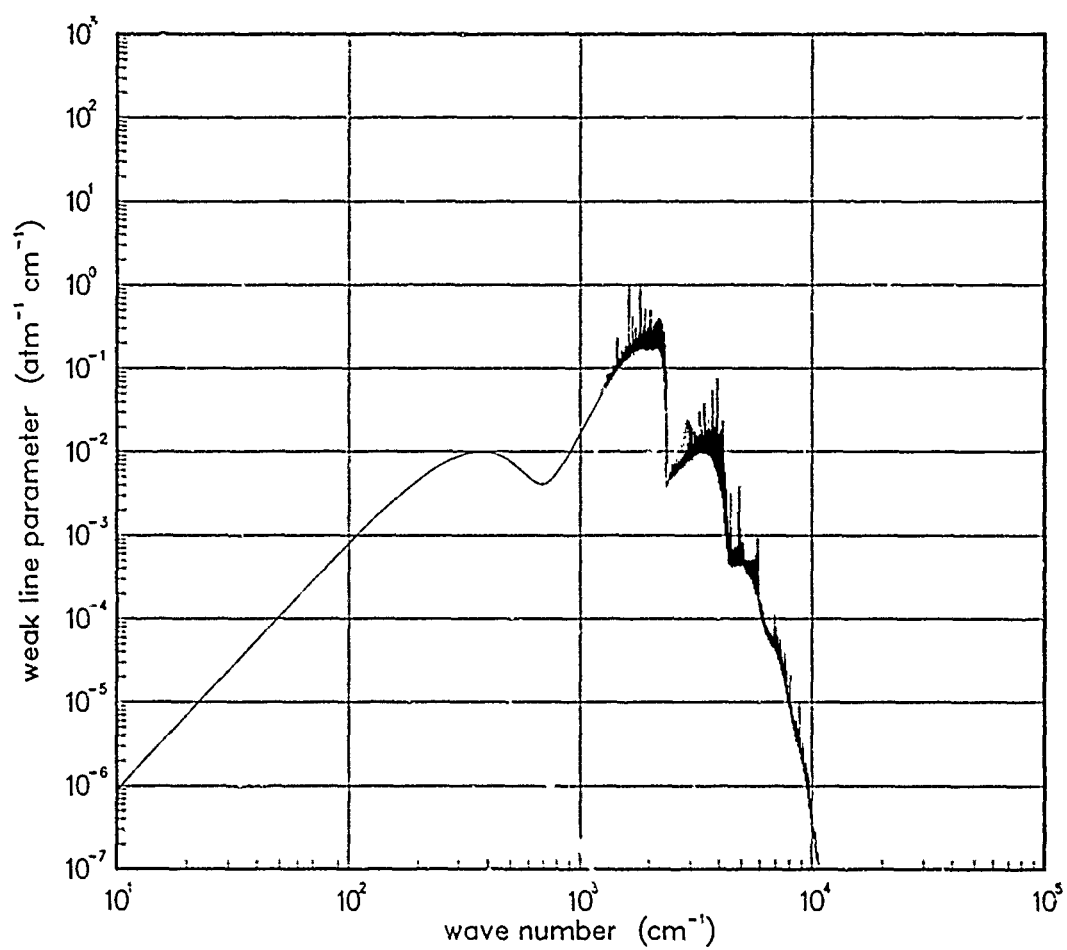


Figure 18. Weak-line parameter for CO at 18000°K.

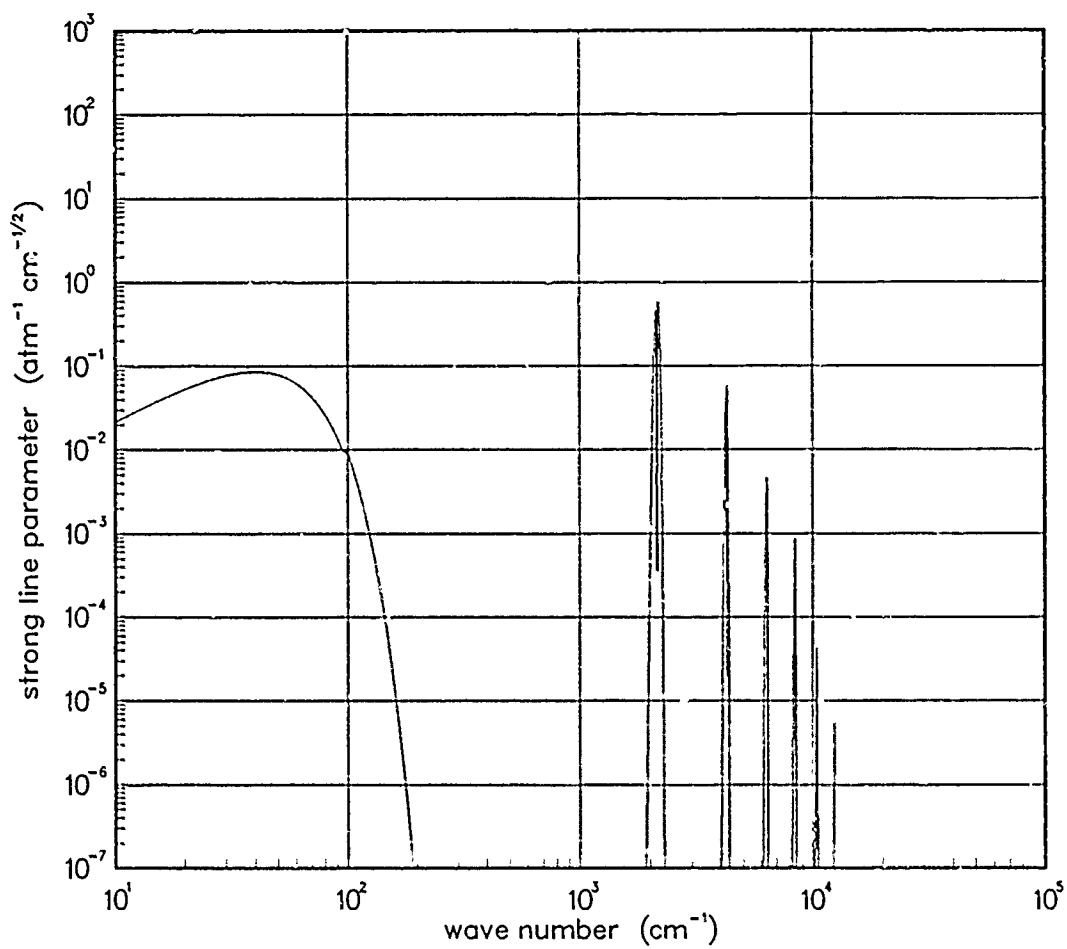


Figure 19. Strong-line parameter for CO at 200°K.

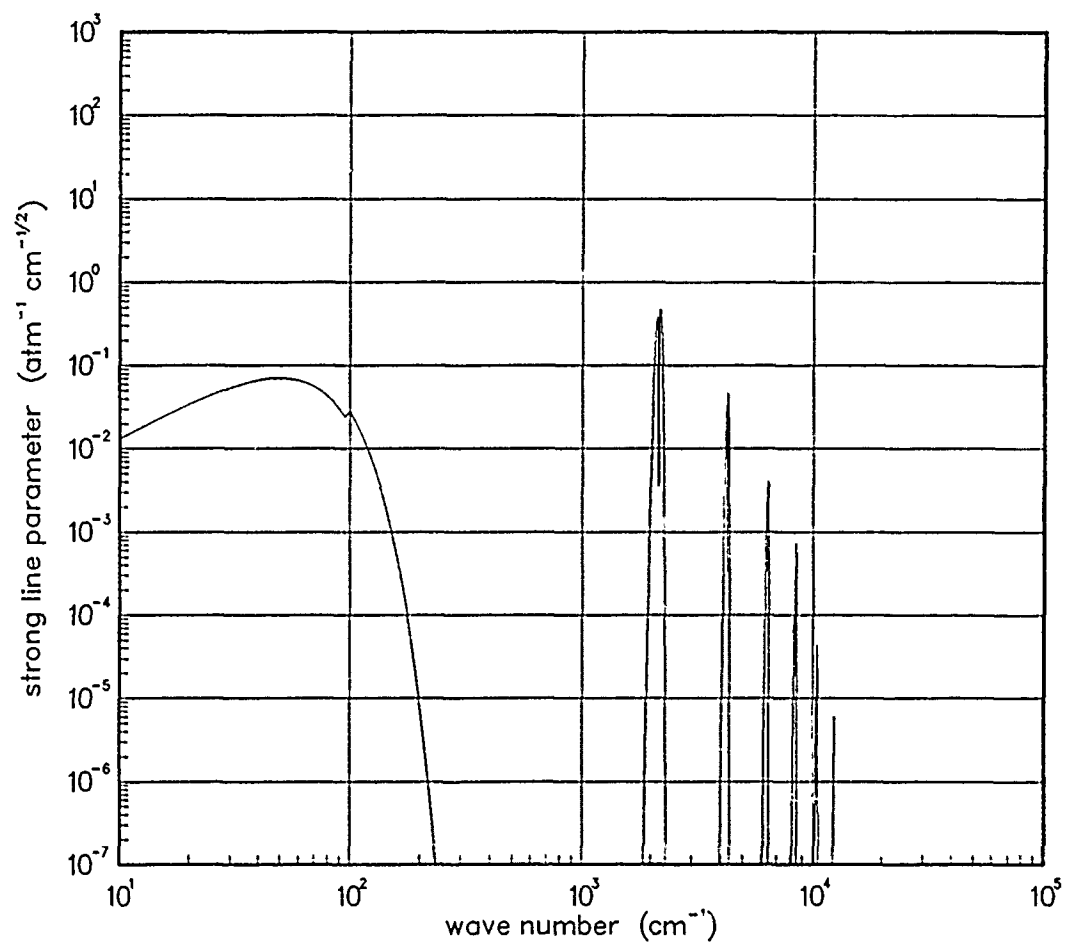


Figure 20. Strong-line parameter for CO at 300°K.

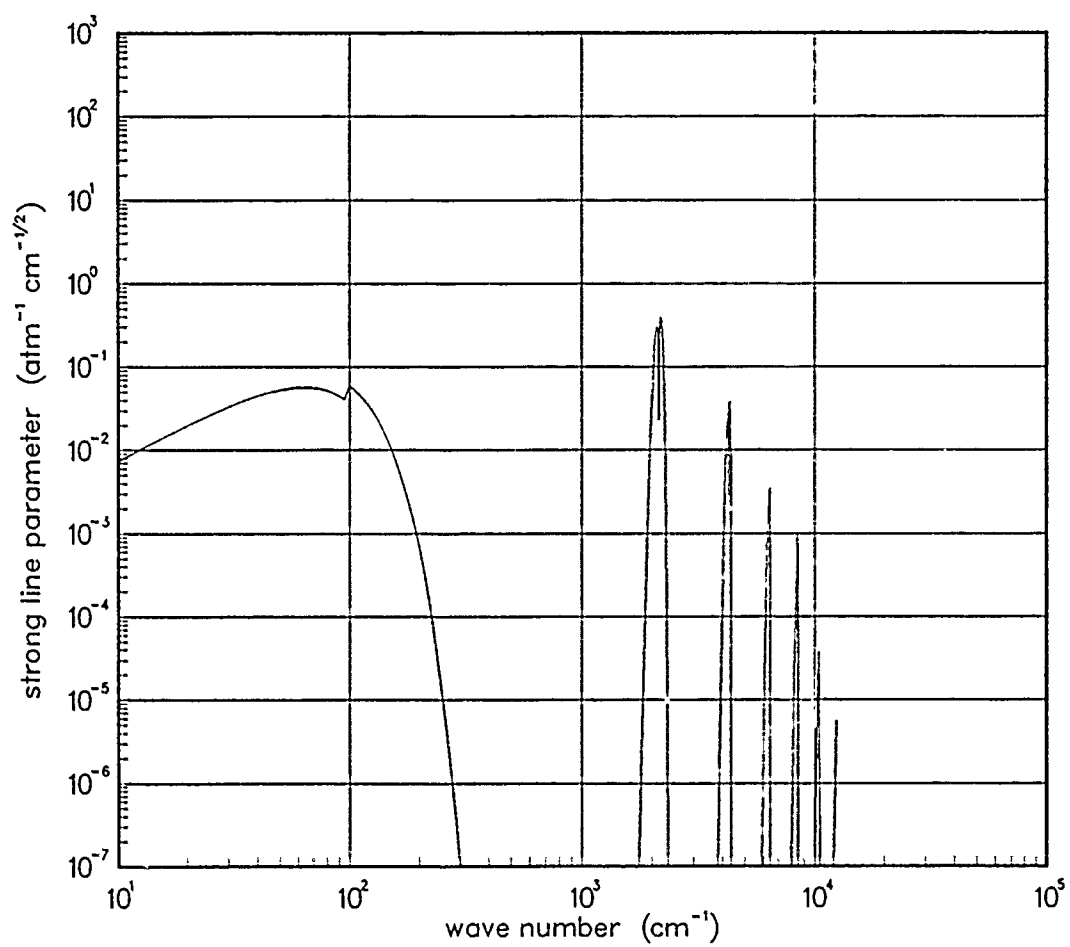


Figure 21. Strong-line parameter for CO at 500°K.

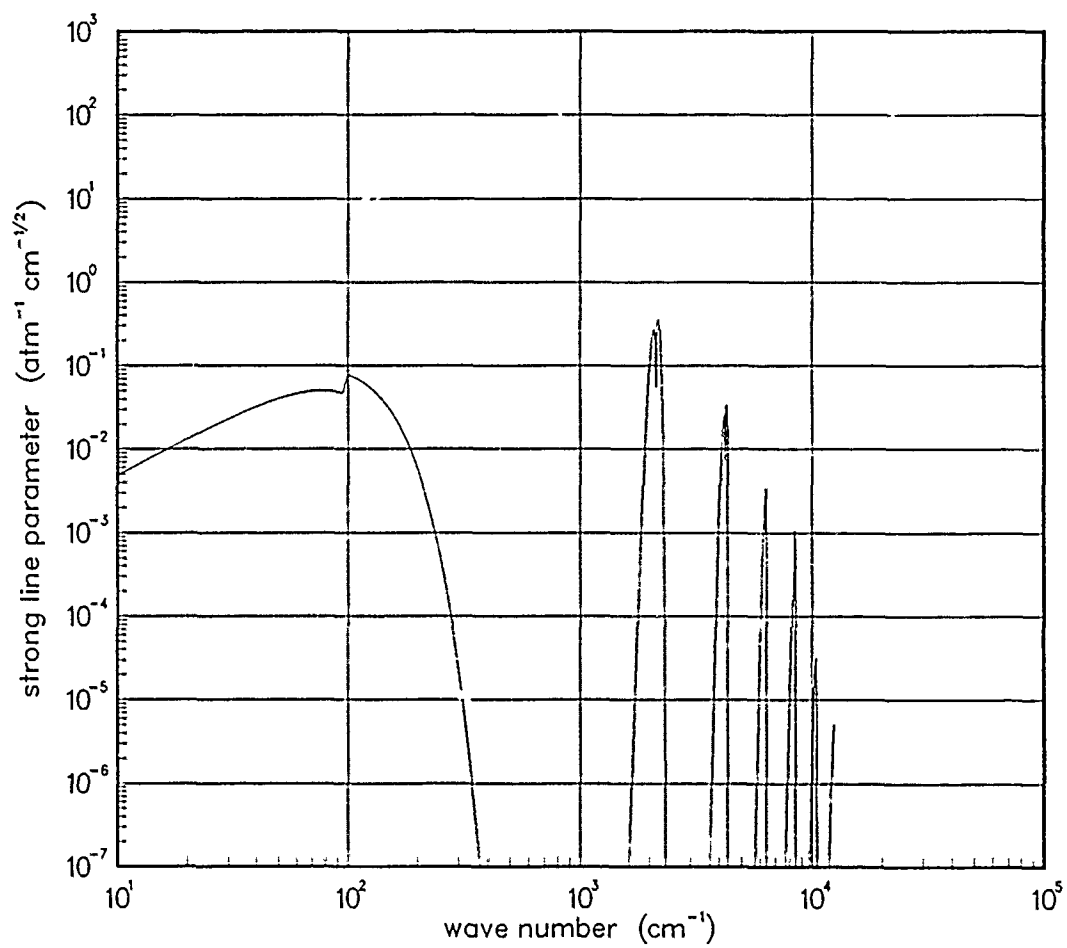


Figure 22. Strong-line parameter for CO at 750°K.

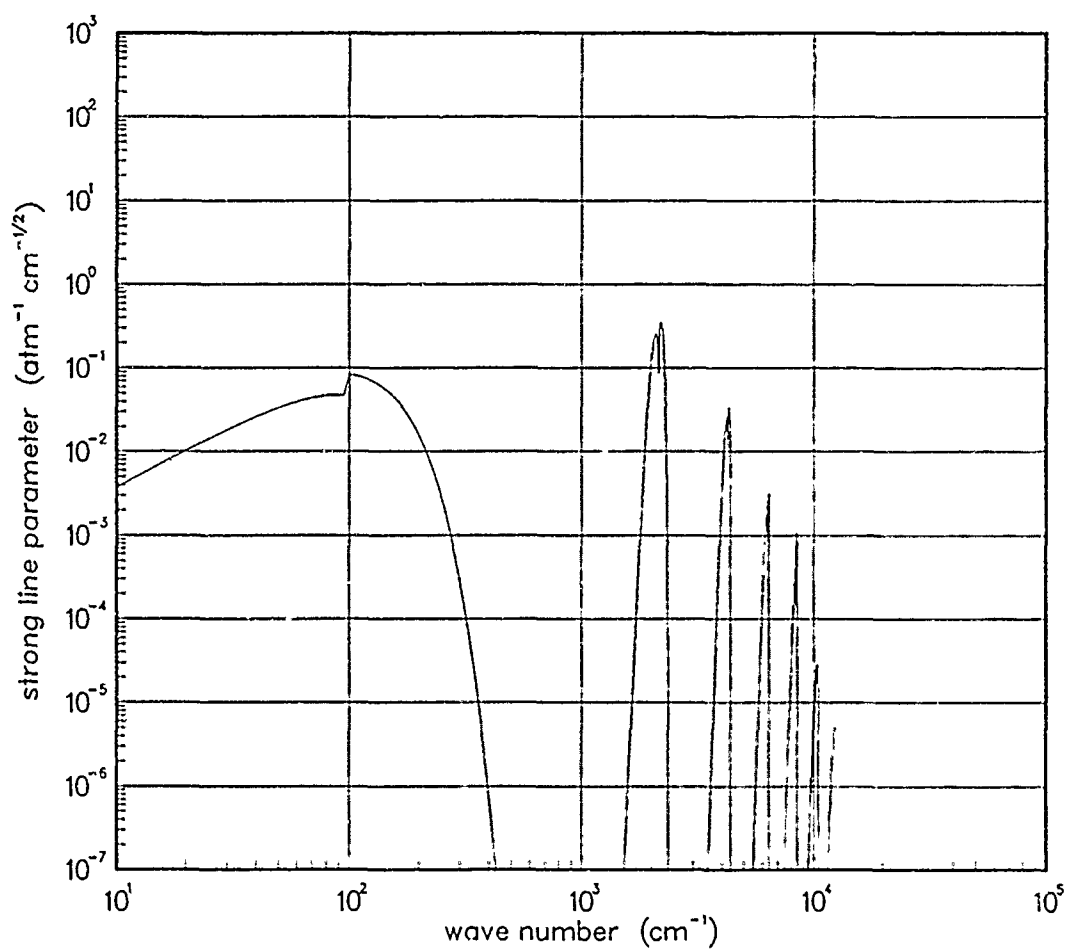


Figure 23. Strong-line parameter for CO at 1000°K.

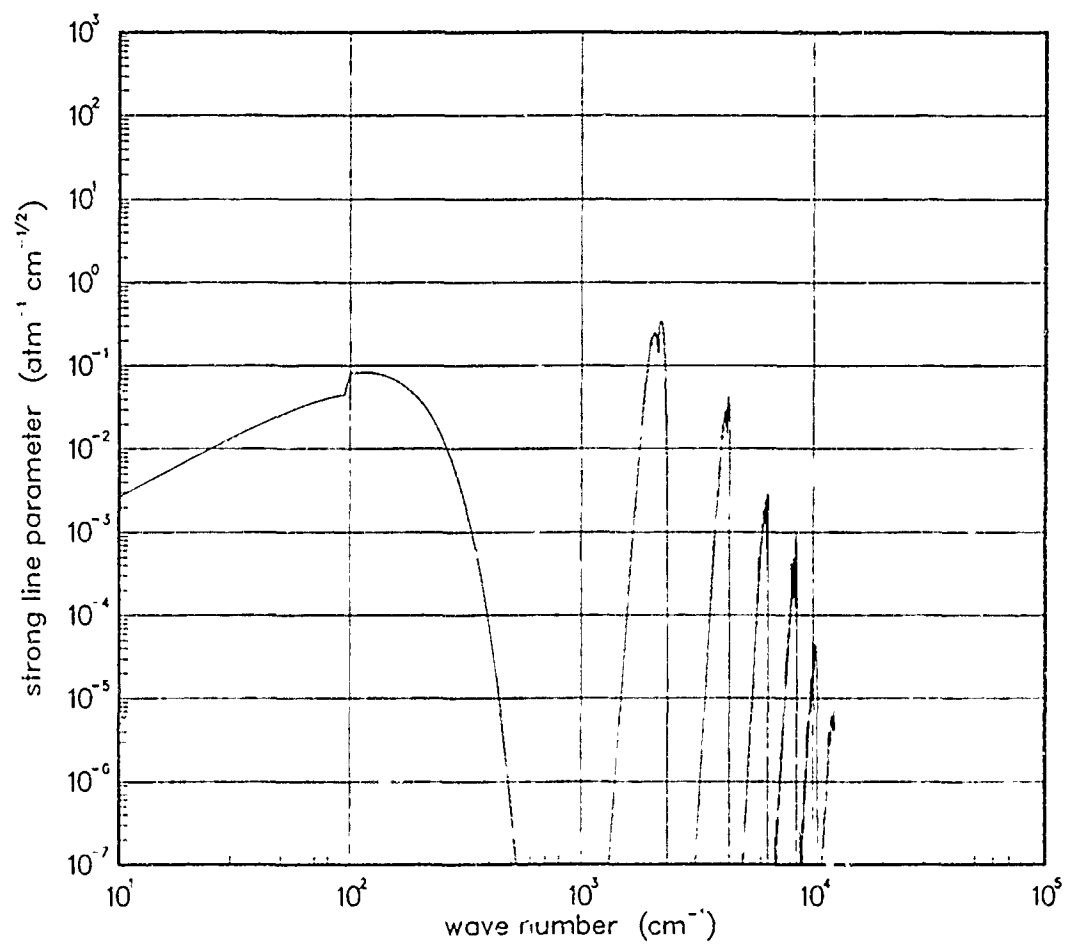


Figure 24. Strong-line parameter for CO at 1500°K.

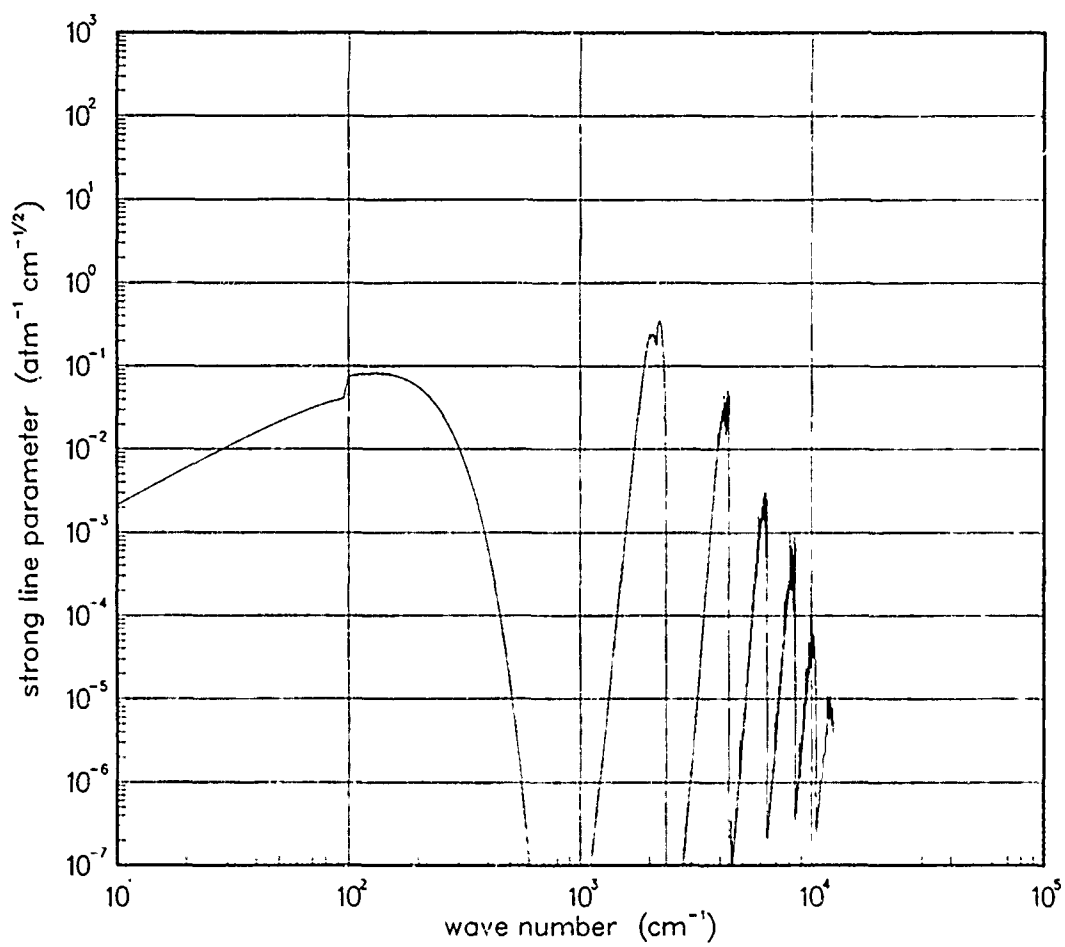


Figure 25. Strong-line parameter for CO at 2000°K.

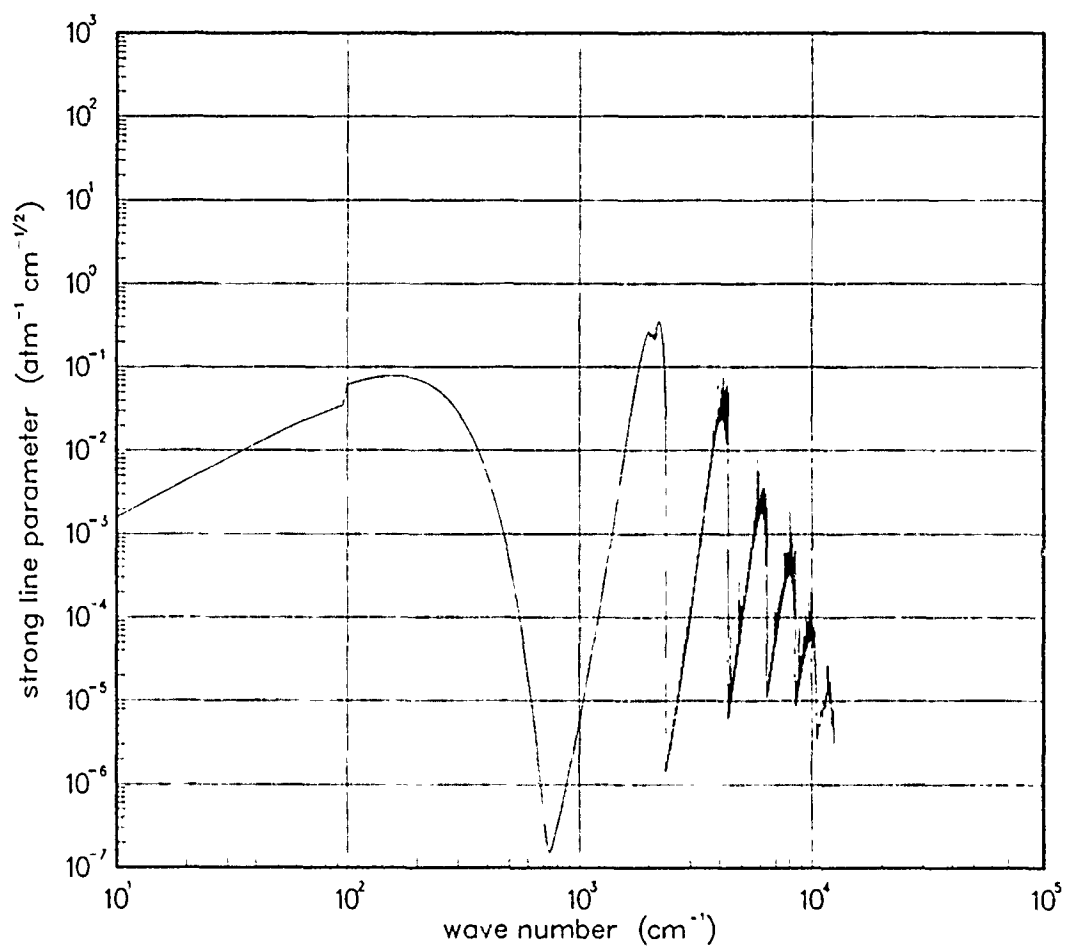


Figure 26. Strong-line parameter for CO at 3000°K.

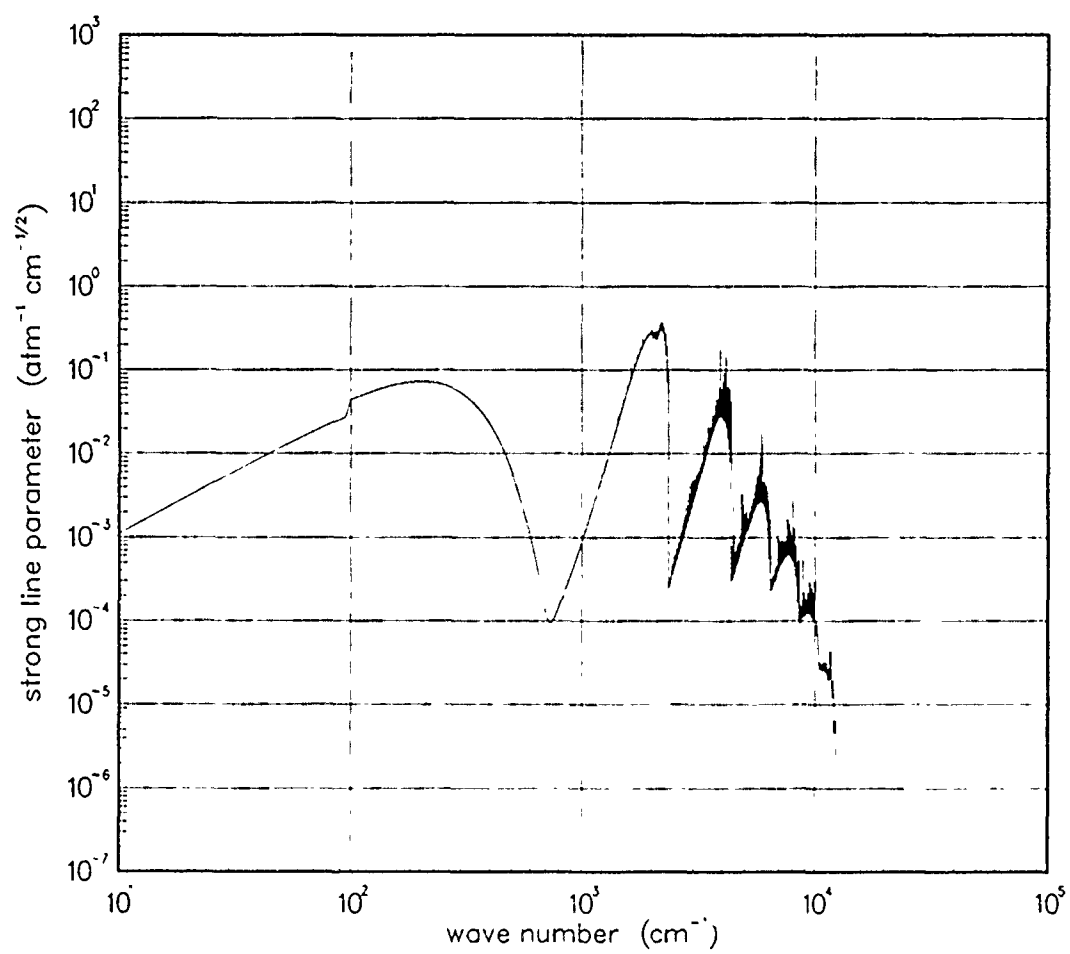


Figure 27. Strong-line parameter for CO at 5000°K.

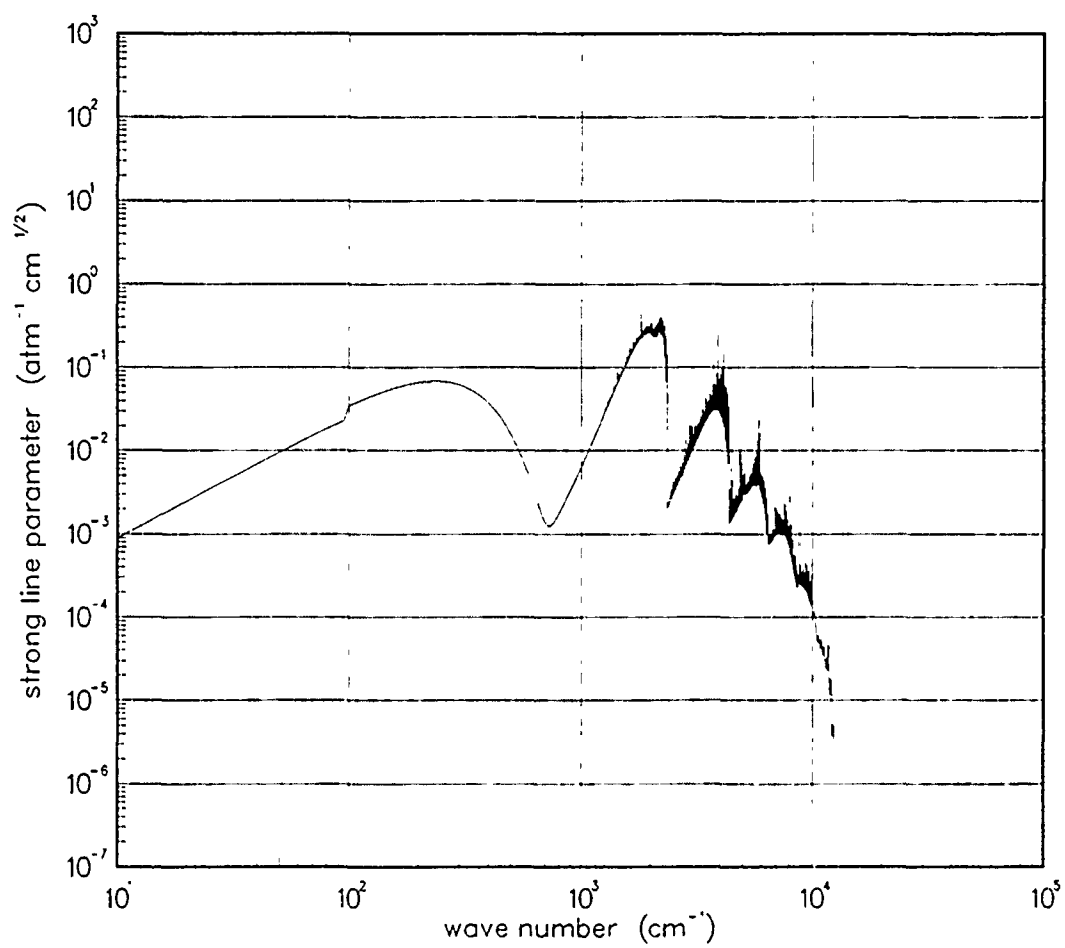


Figure 28. Strong-line parameter for CO at 7000°K.

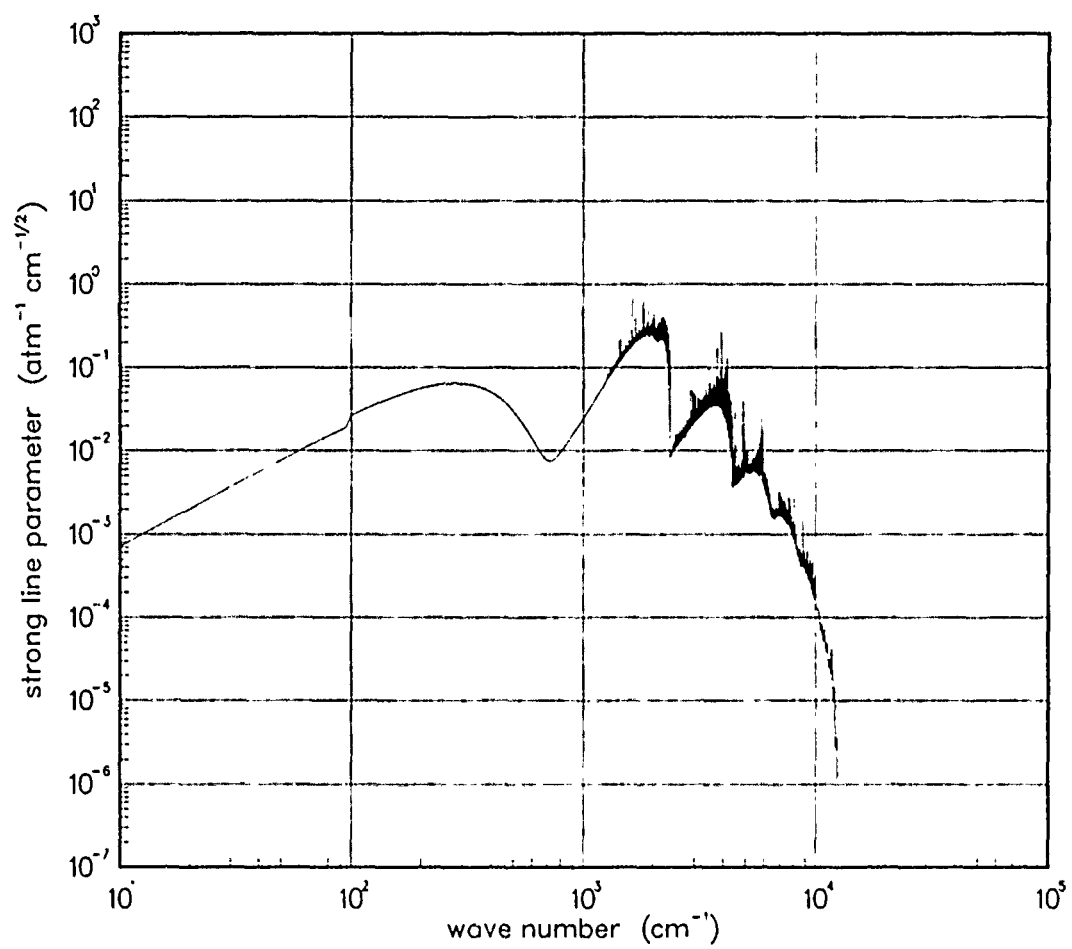


Figure 29. Strong-line parameter for CO at 10000°K.

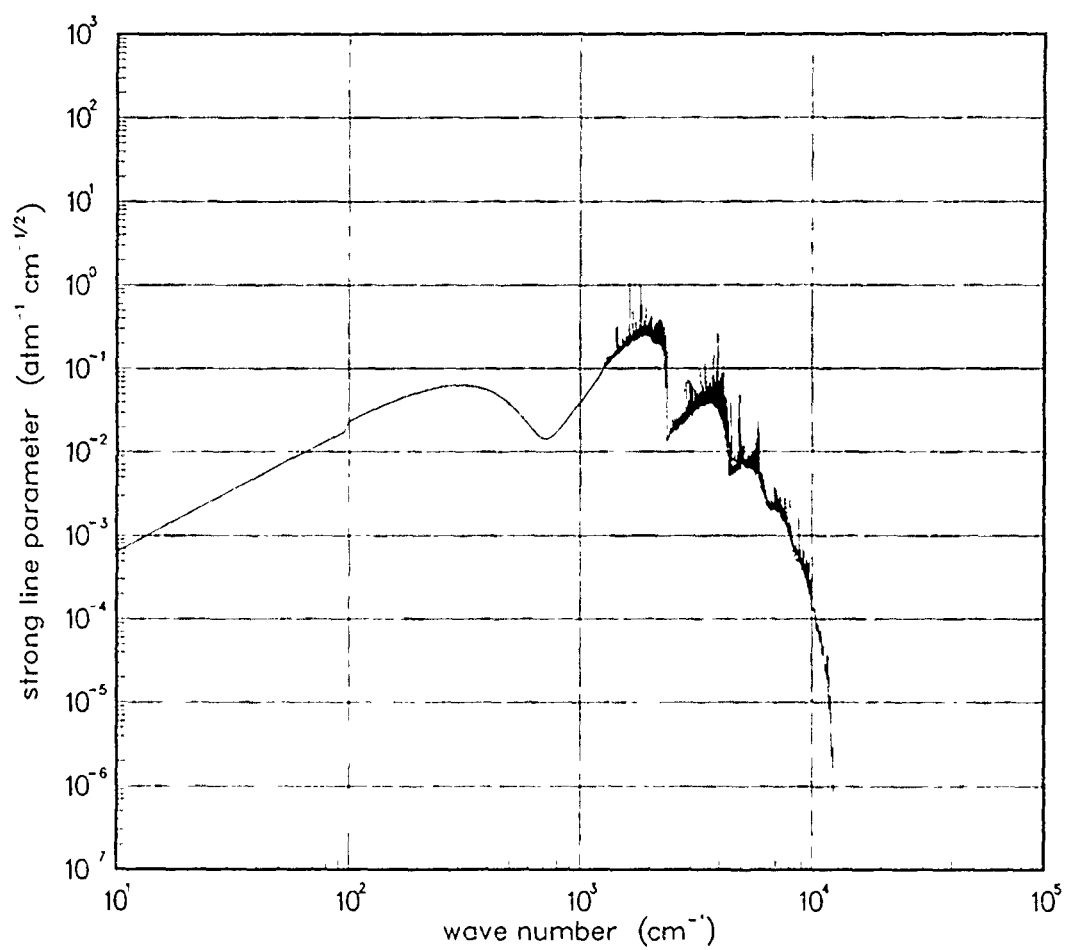


Figure 30. Strong-line parameter for CO at 12000°K.

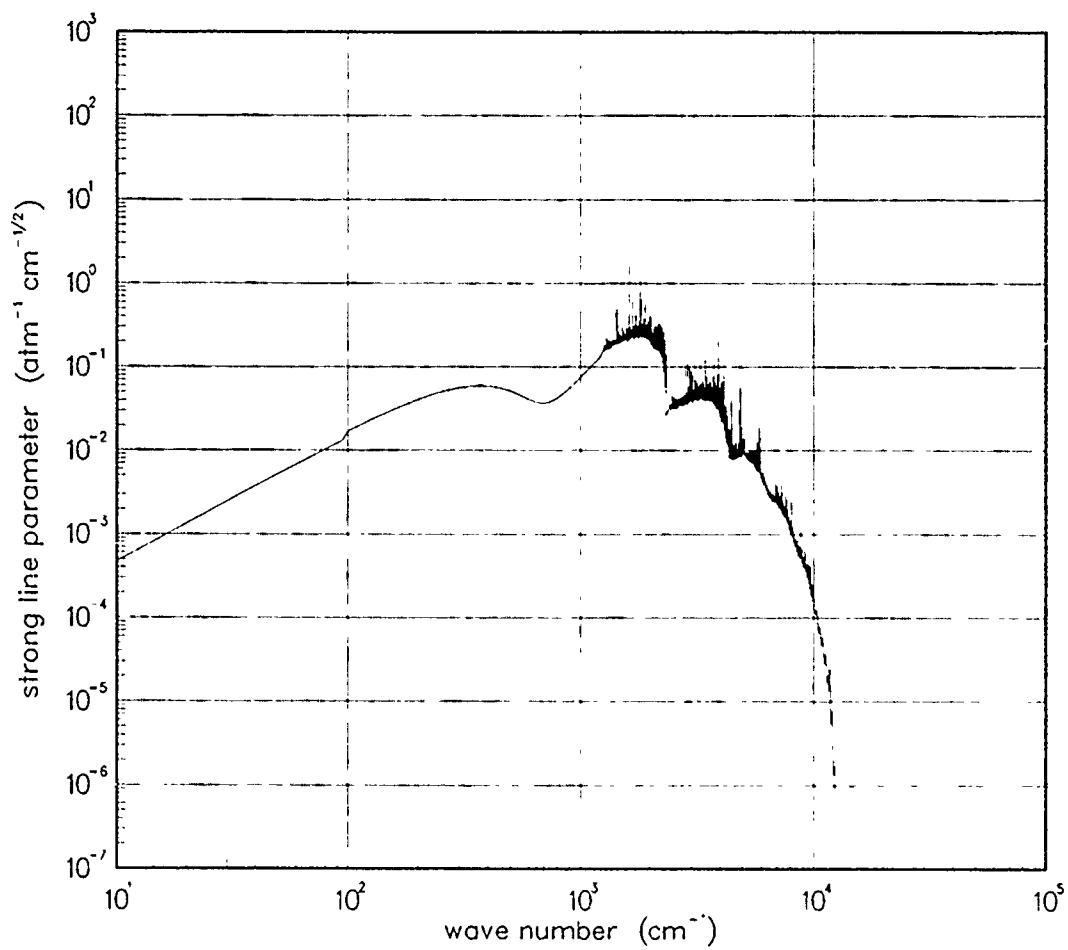


Figure 31. Strong-line parameter for CO at 18000°K.

4.2 HYDROXYL (OH).

Table 2. Spectroscopic data for OH.

Ground Electronic State

$$\begin{array}{ll} \omega_e = 3735.21 \text{ cm}^{-1*} & \omega_e x_e = 82.82 \text{ cm}^{-1*} \\ \alpha_e = 0.714 \text{ cm}^{-1*} & B_e = 18.871 \text{ cm}^{-1*} \end{array}$$

$$S_{10} = 120 \text{ atm}^{-1} \text{ cm}^{-2*}$$

$$\gamma_t(300 \text{ }^\circ\text{K}) = 0.06^\dagger$$

Data Source:

*W.S. Benedict, and E.K. Plyler, High-Resolution Spectra of Hydrocarbon Flames in the Infrared, Energy Transfer in Hot Gases, National Bureau of Standards Circular 523, p. 57 (1954).

†D. Bastard, et al, Spectroscopic Hertzienne -- Etude experimental dela saturation de l'absorption hertzienne du radical OH, C.R. Acad. Sc. Paris, vol 284, Series B, p. 445 (1977).

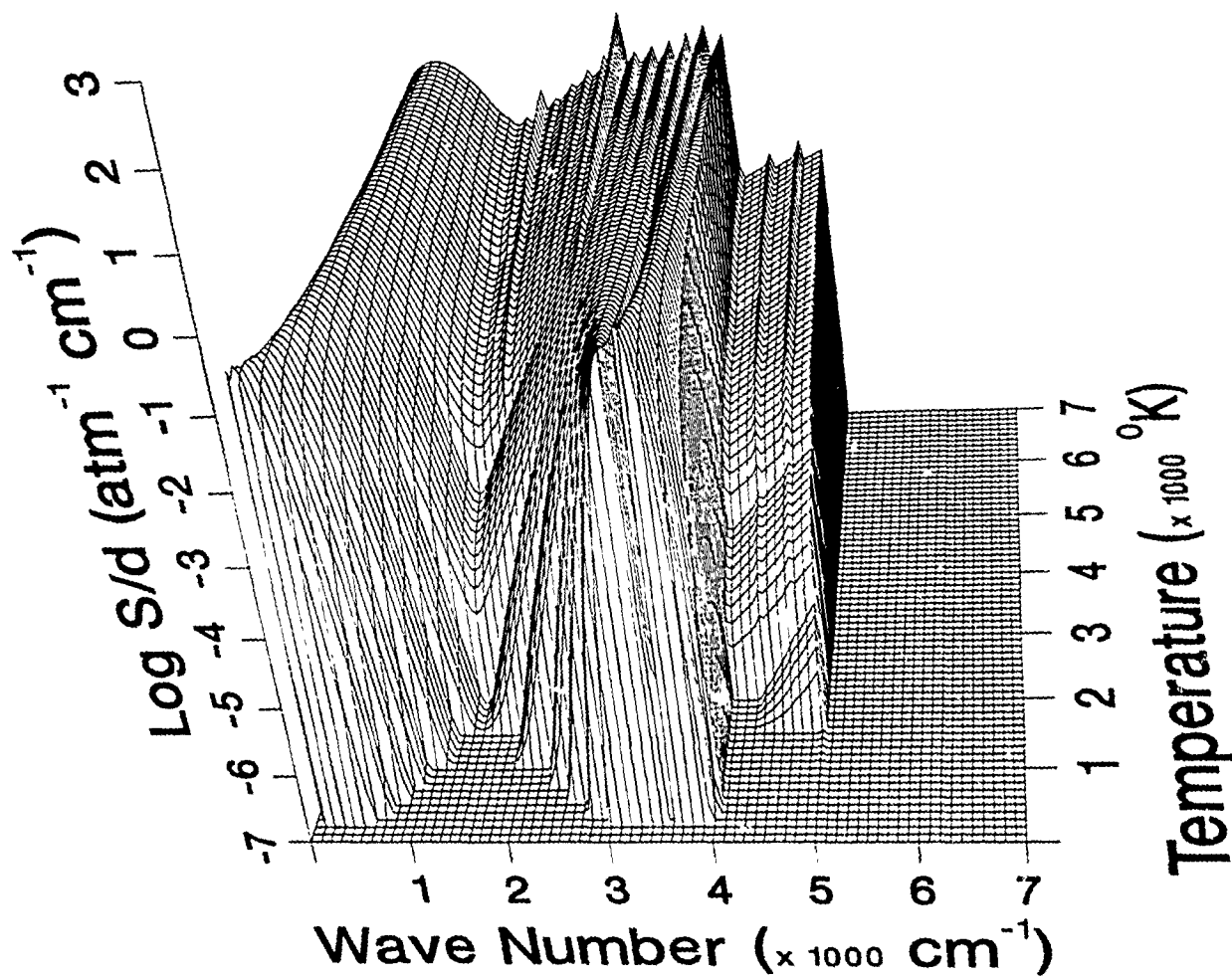


Figure 32. Weak-line parameter for OH.

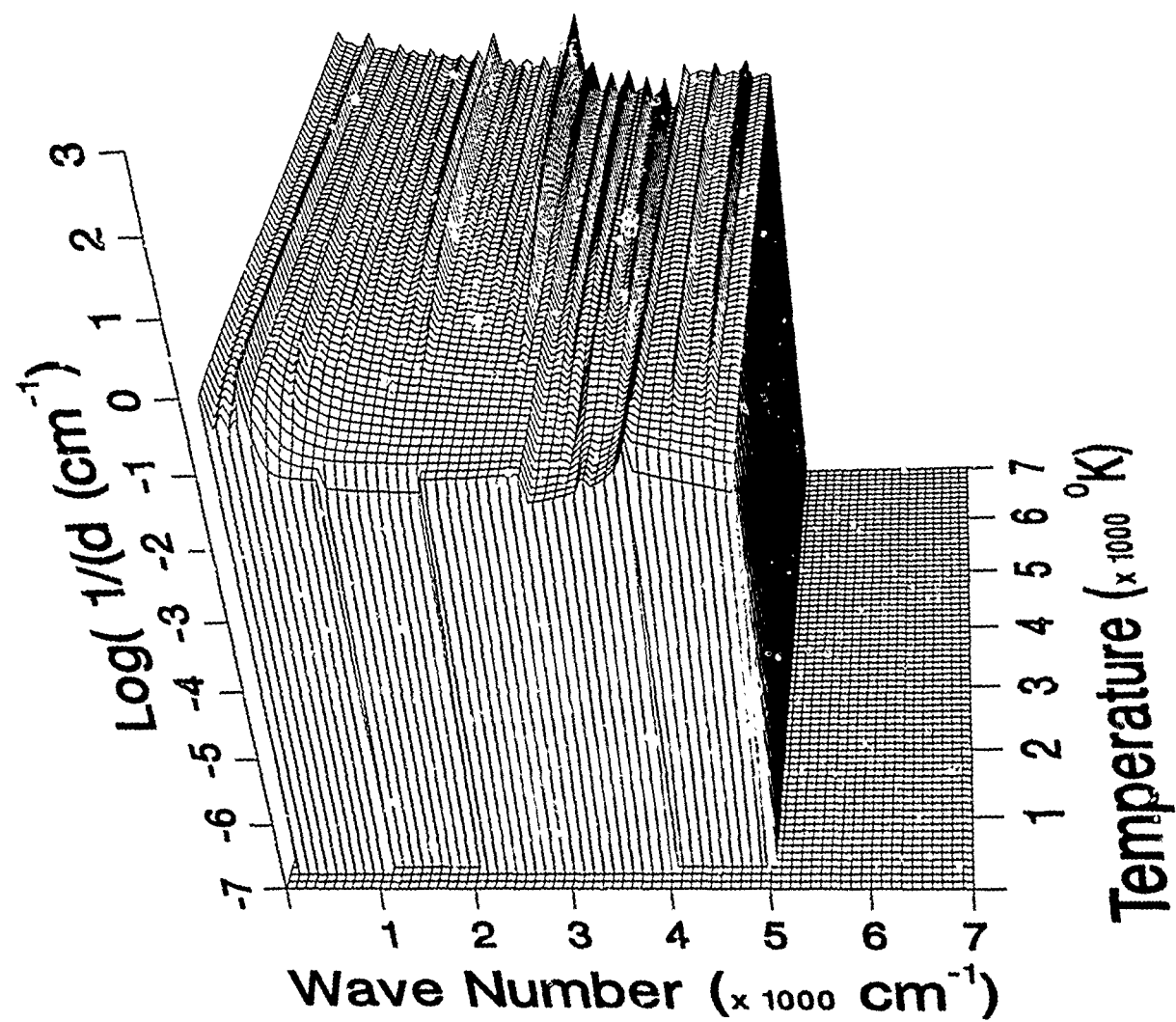


Figure 33. Inverse line spacing for OH.

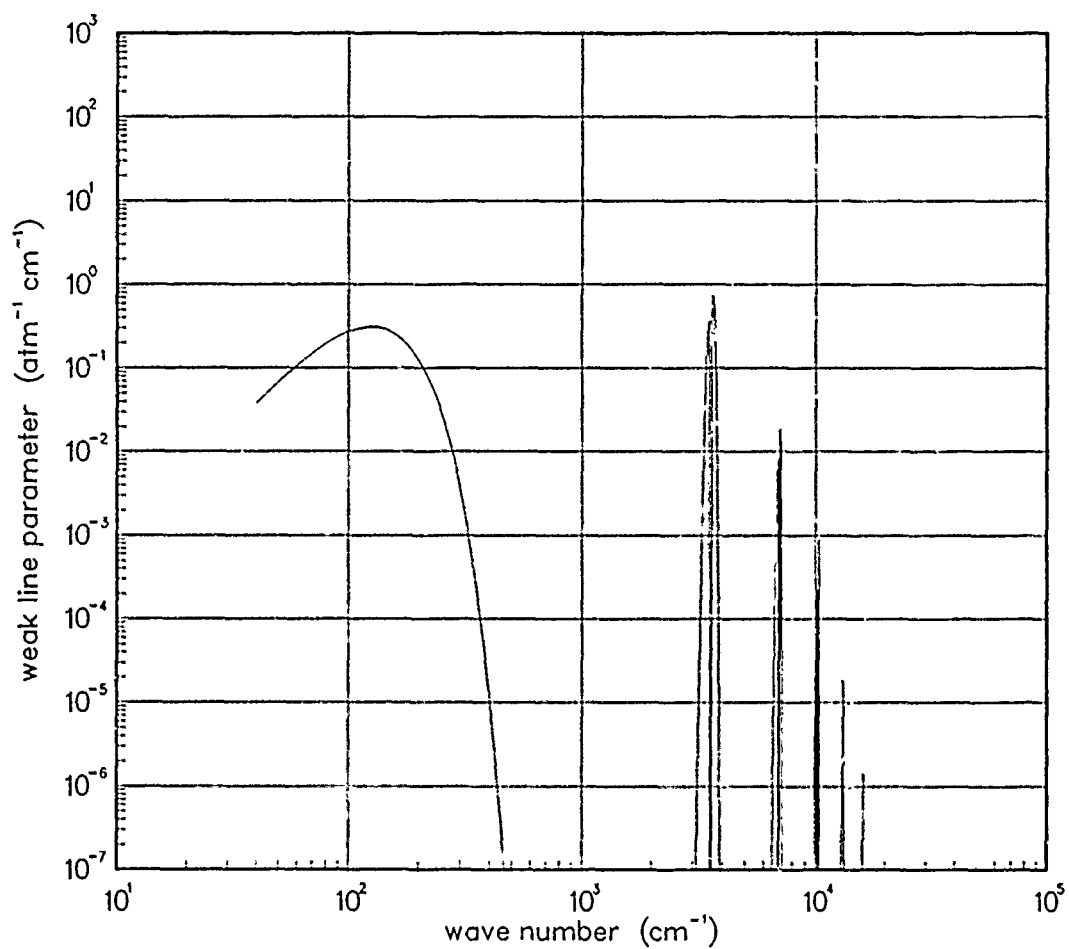


Figure 34. Weak-line parameter for OH at 200°K.

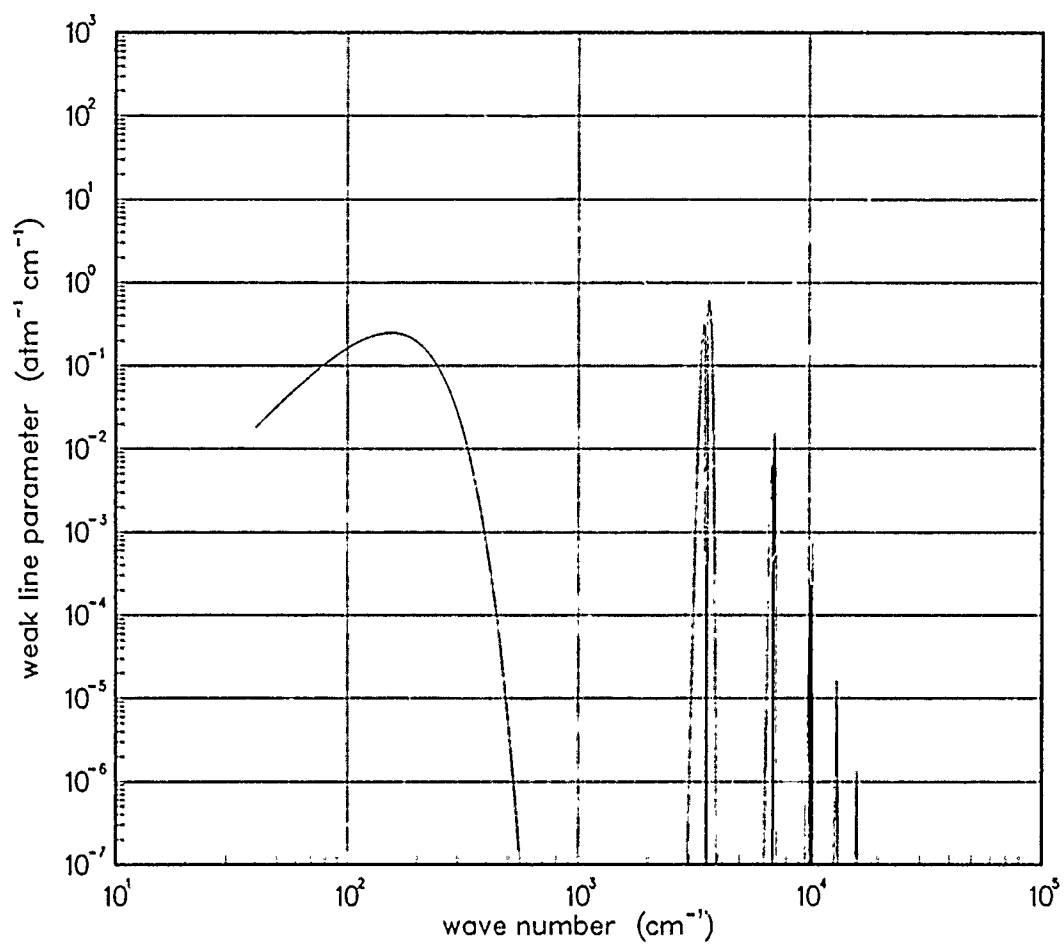


Figure 35. Weak-line parameter for OH at 300°K.

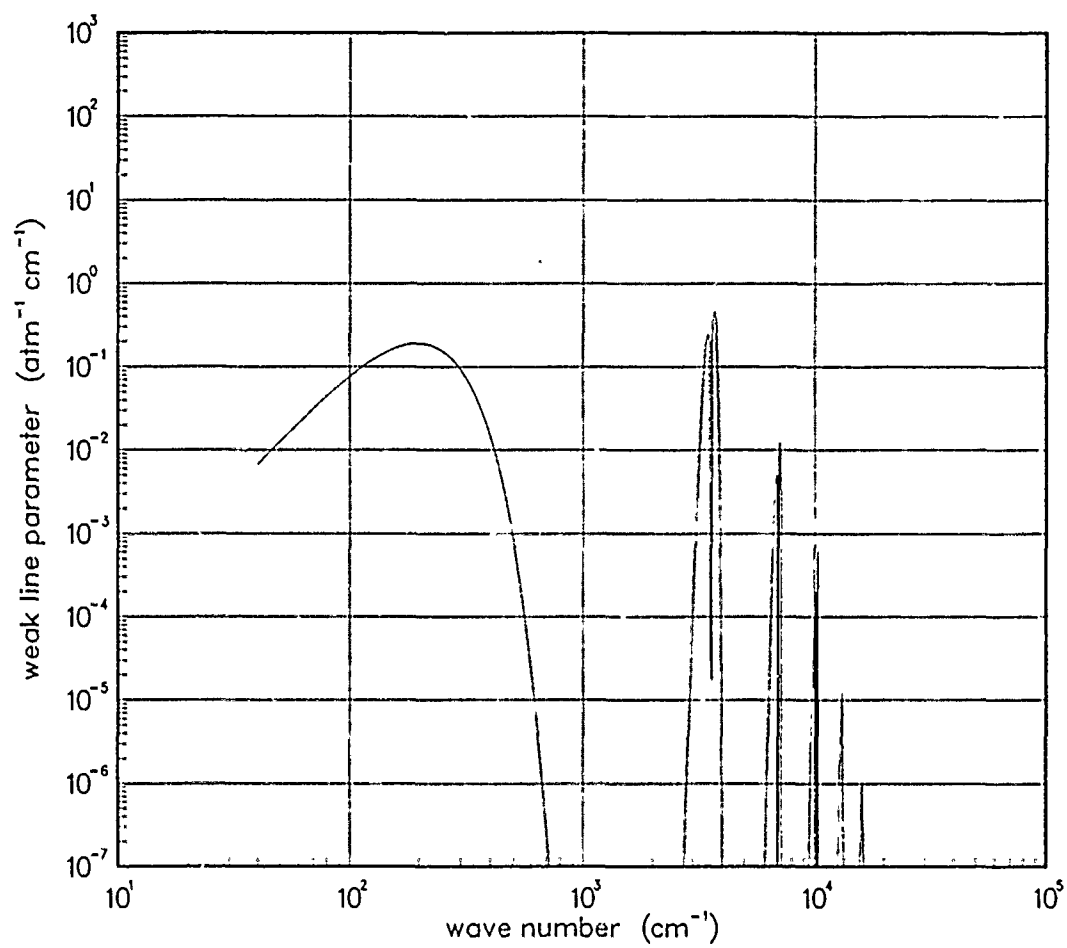


Figure 36. Weak-line parameter for OH at 500°K.

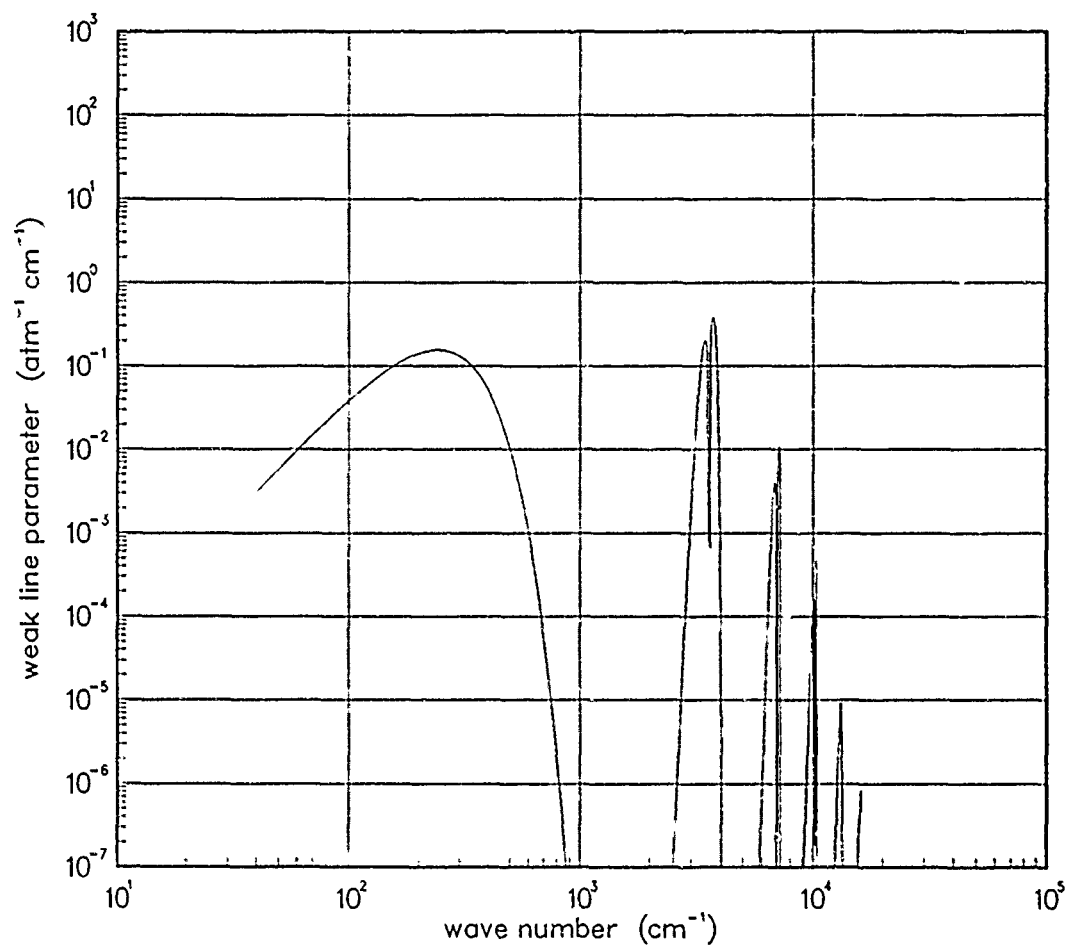


Figure 37. Weak-line parameter for OH at 750°K.

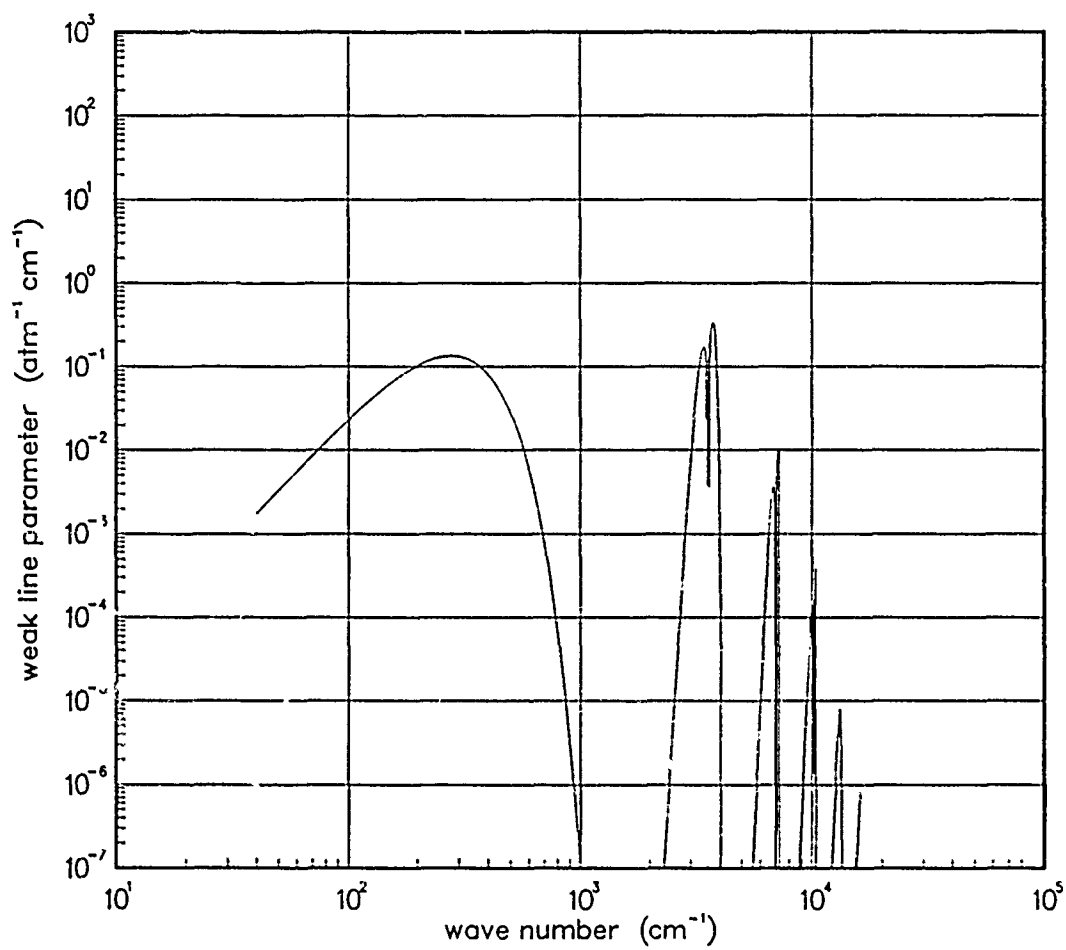


Figure 38. Weak-line parameter for OH at 1000°K.

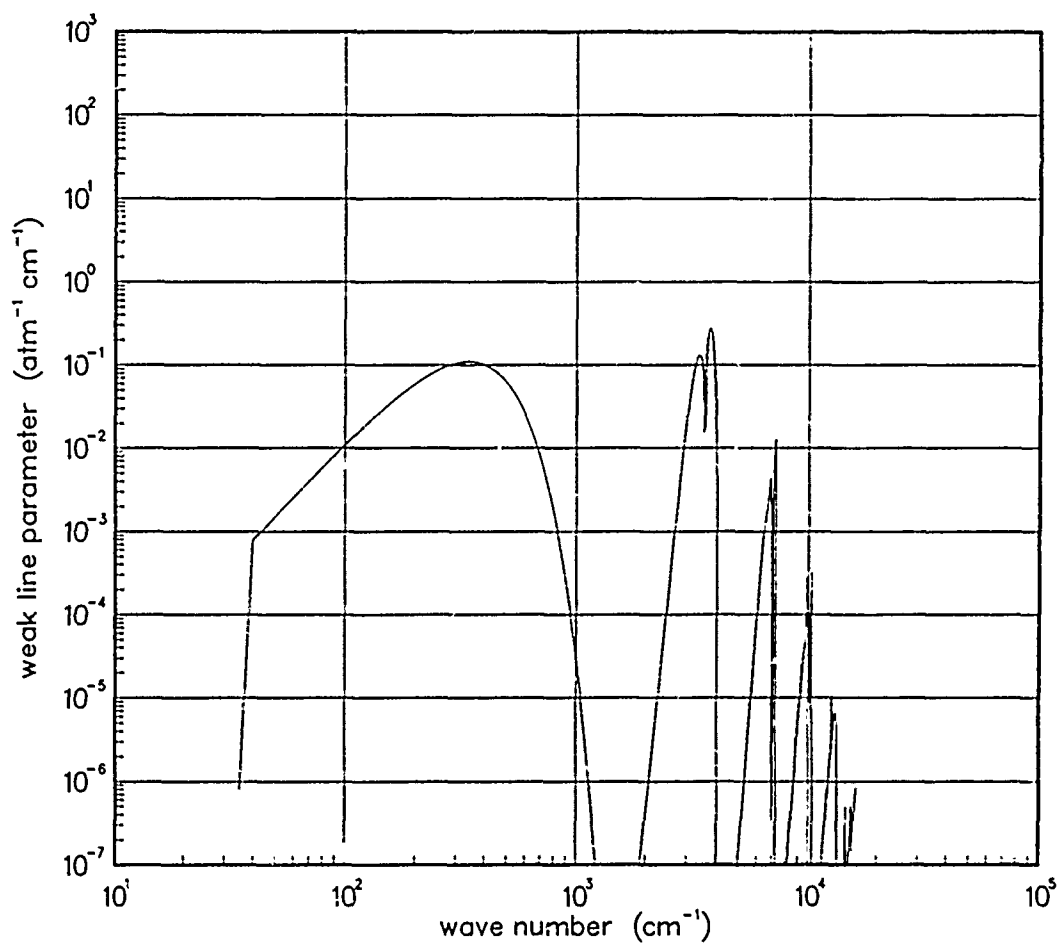


Figure 39. Weak-line parameter for OH at 1500°K.

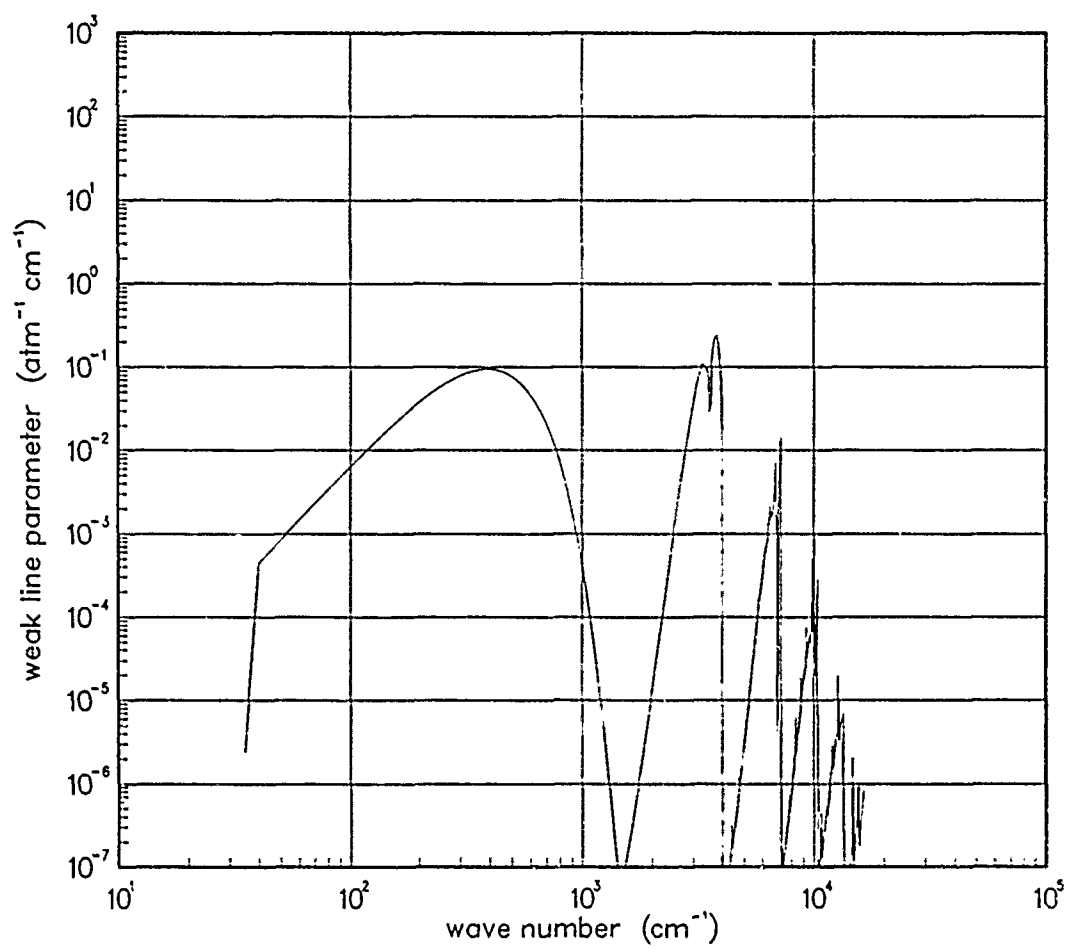


Figure 40. Weak-line parameter for OH at 2000°K.

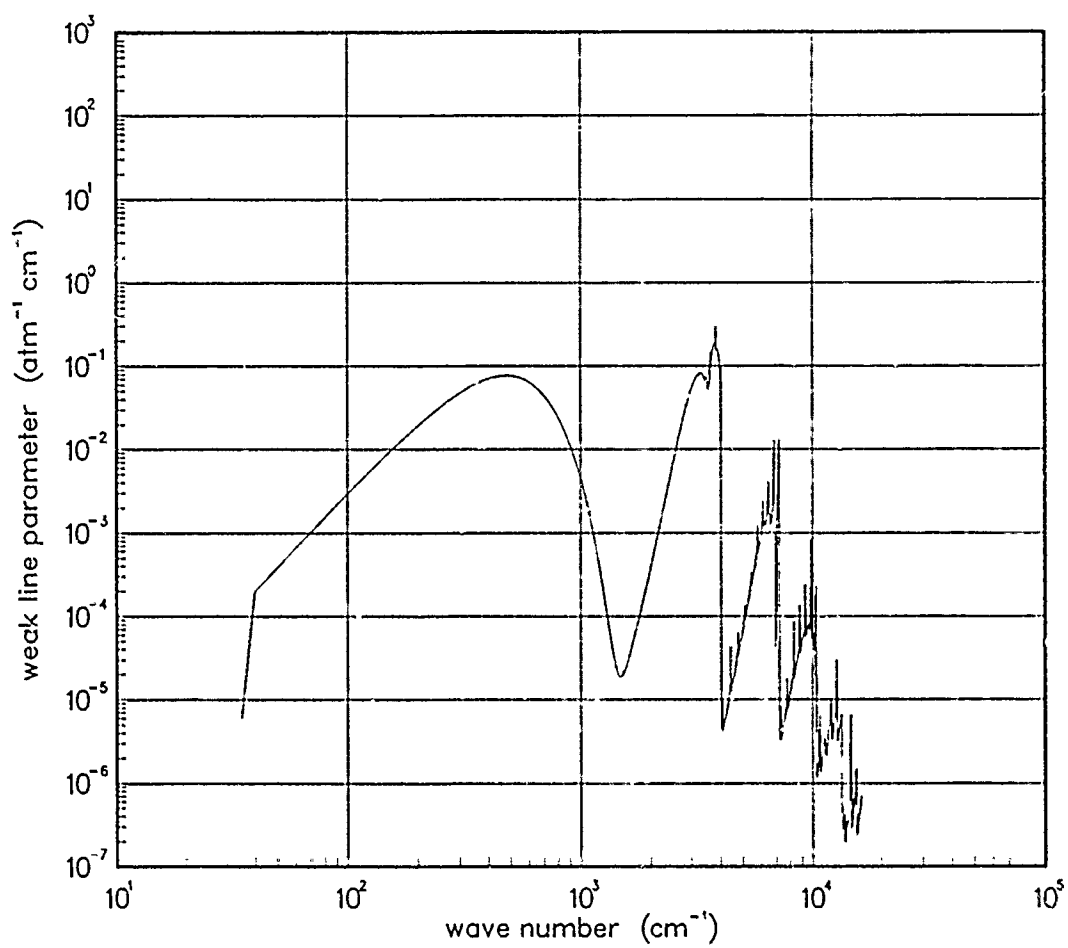


Figure 41. Weak-line parameter for OH at 3000°K.

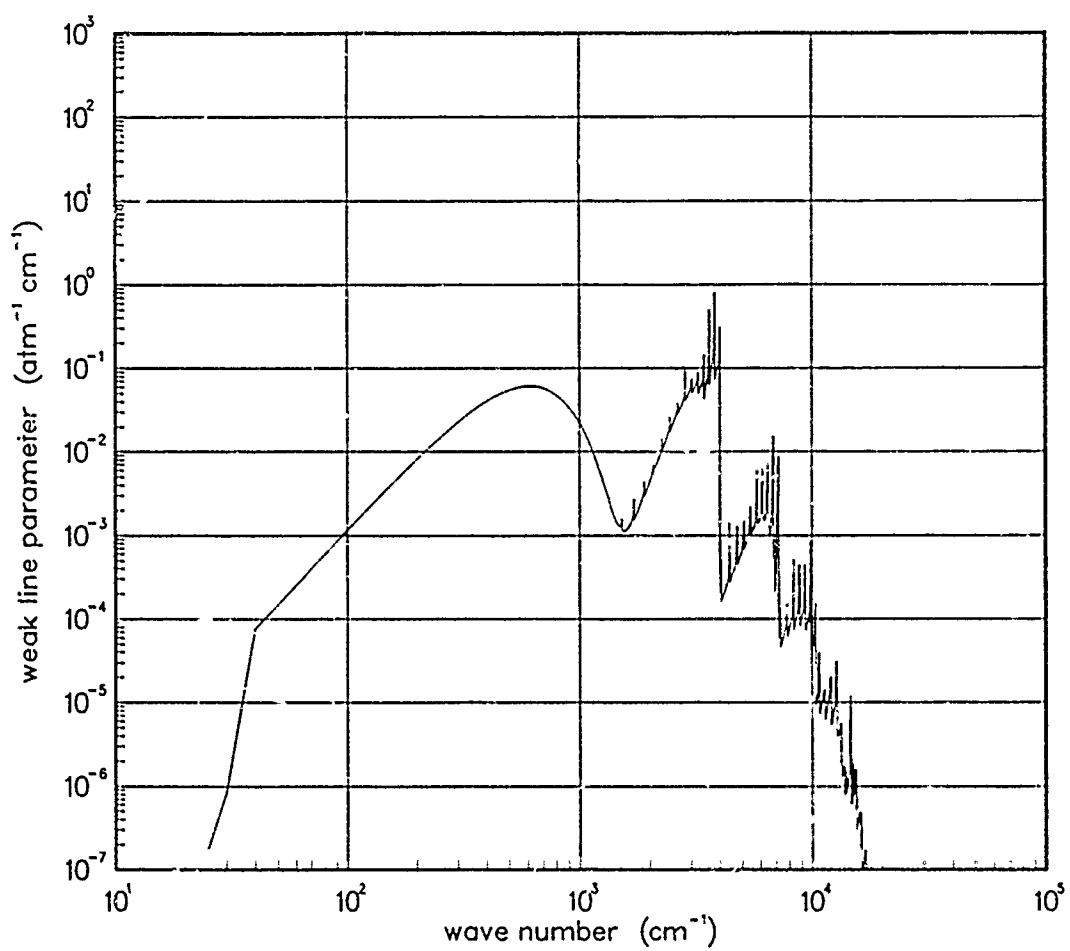


Figure 42. Weak-line parameter for OH at 5000°K.

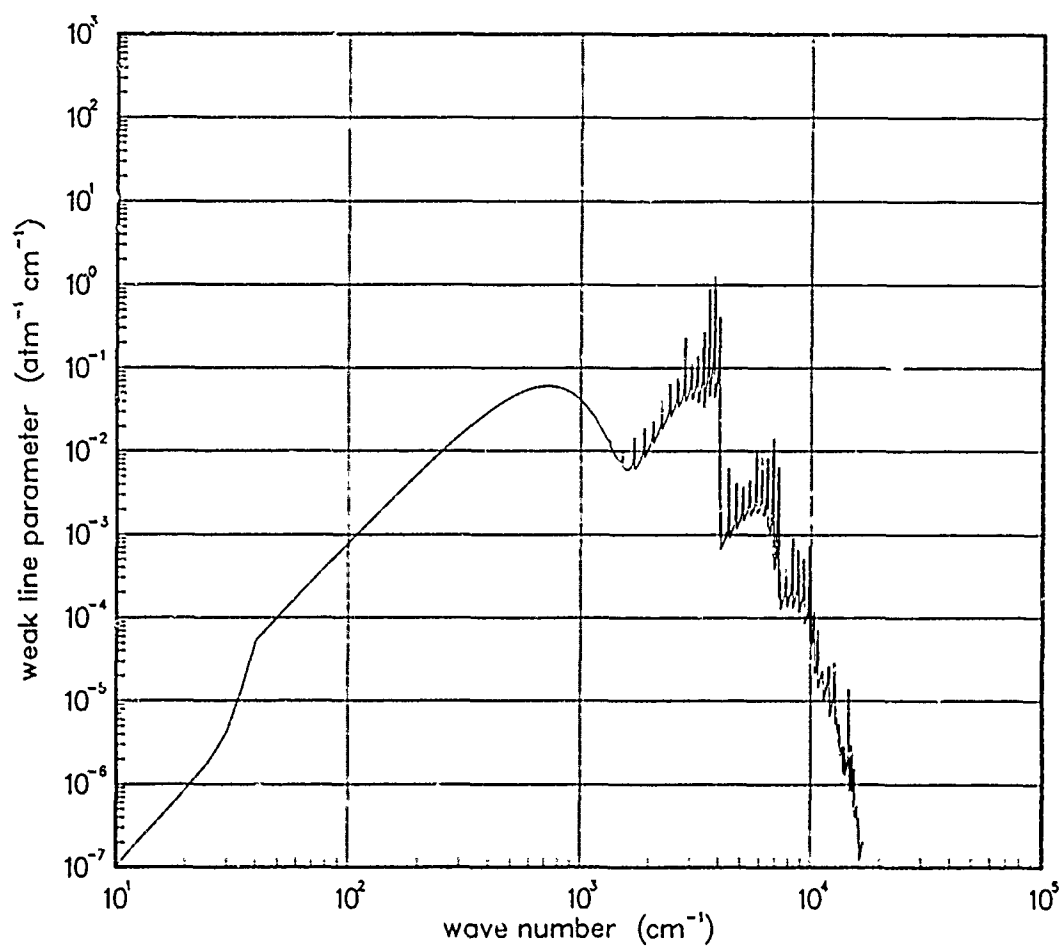


Figure 43. Weak-line parameter for OH at 7000°K.

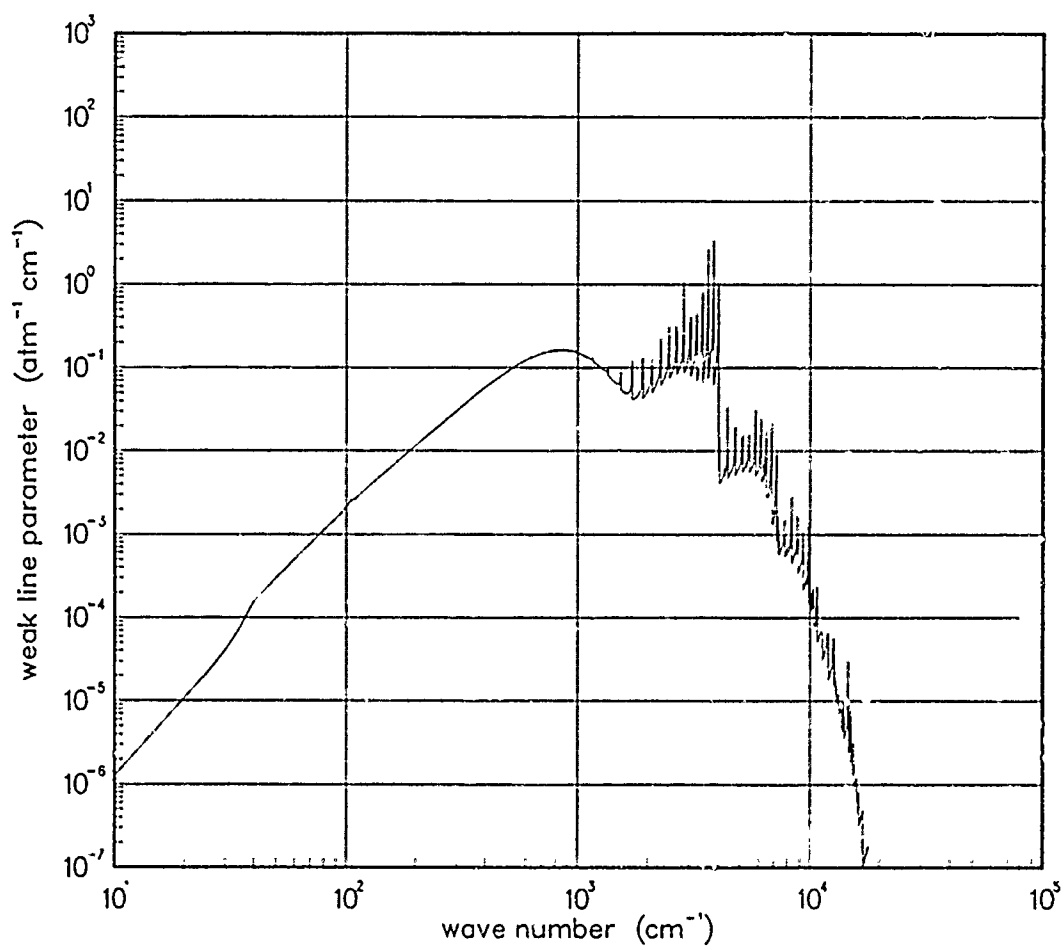


Figure 44. Weak-line parameter for OH at 10000°K.

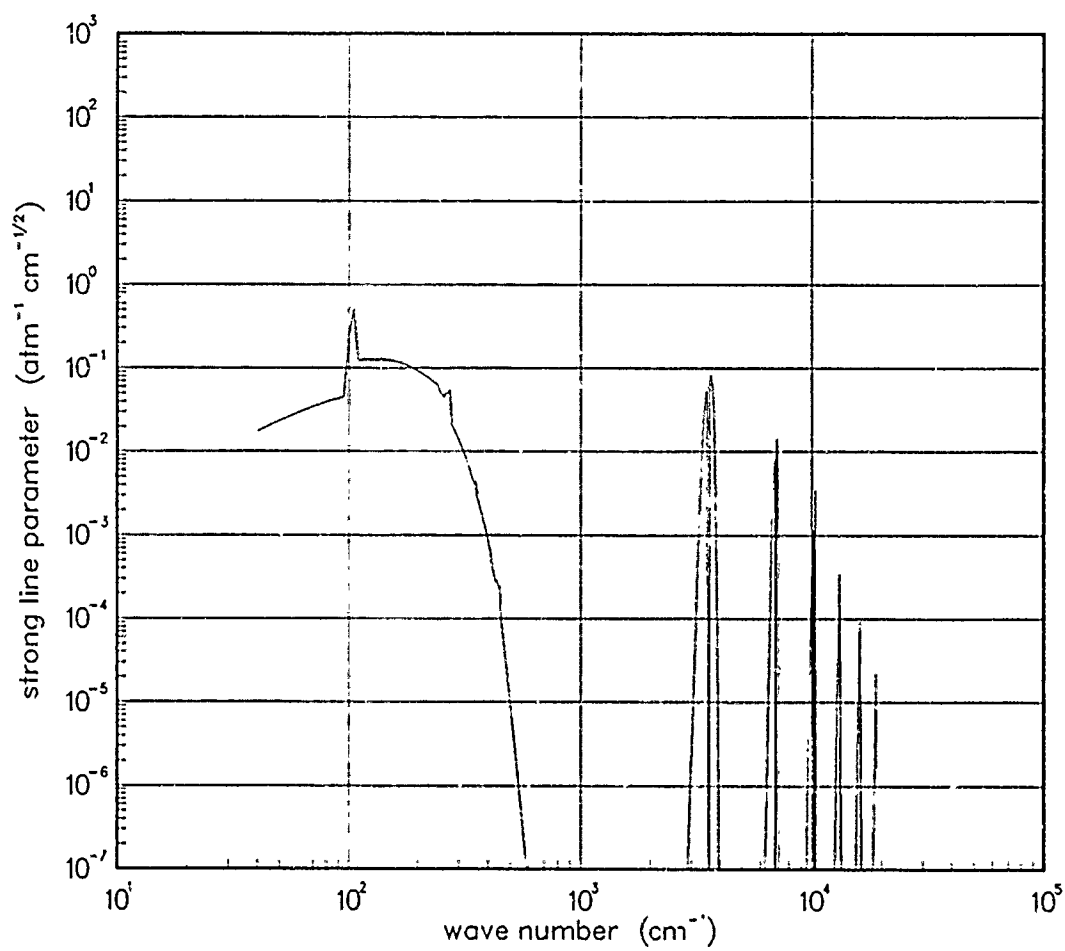


Figure 45. Strong-line parameter for OH at 200°K.

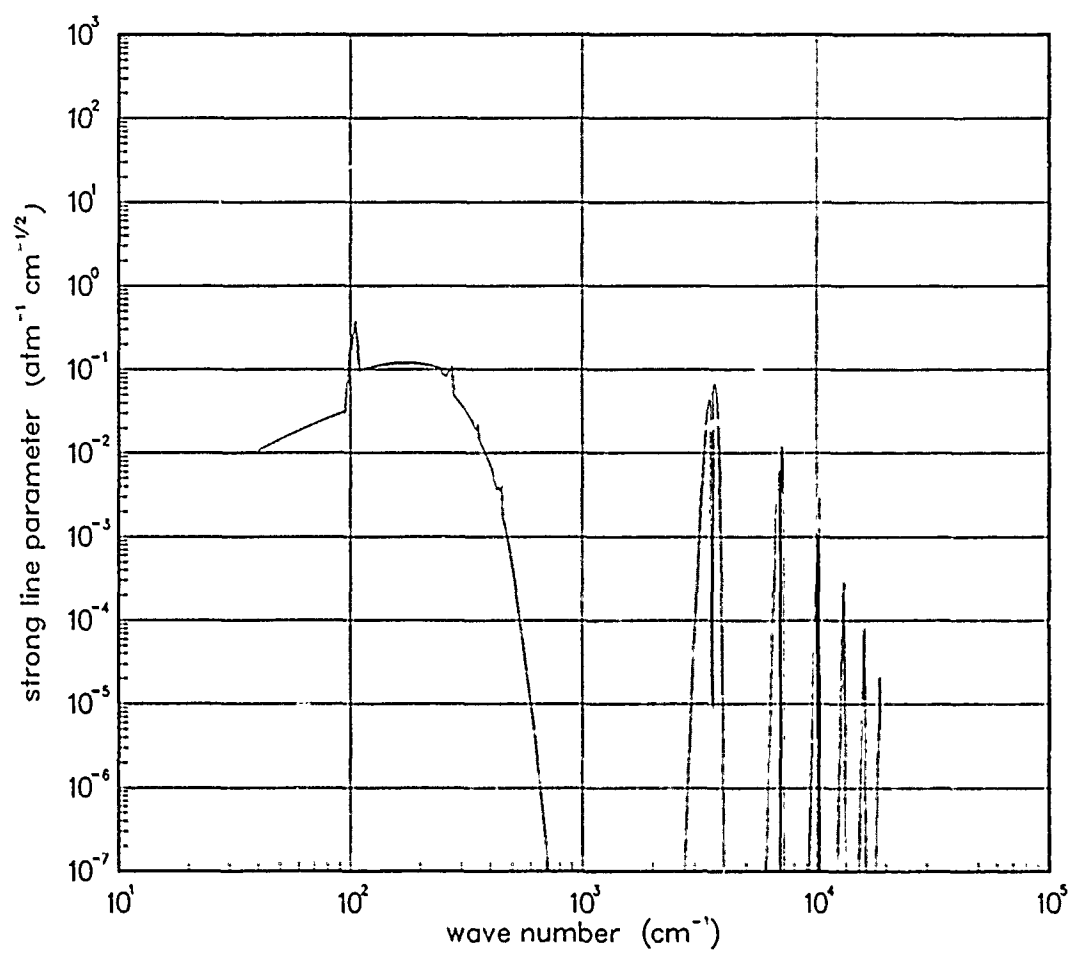


Figure 46. Strong-line parameter for OH at 300°K.

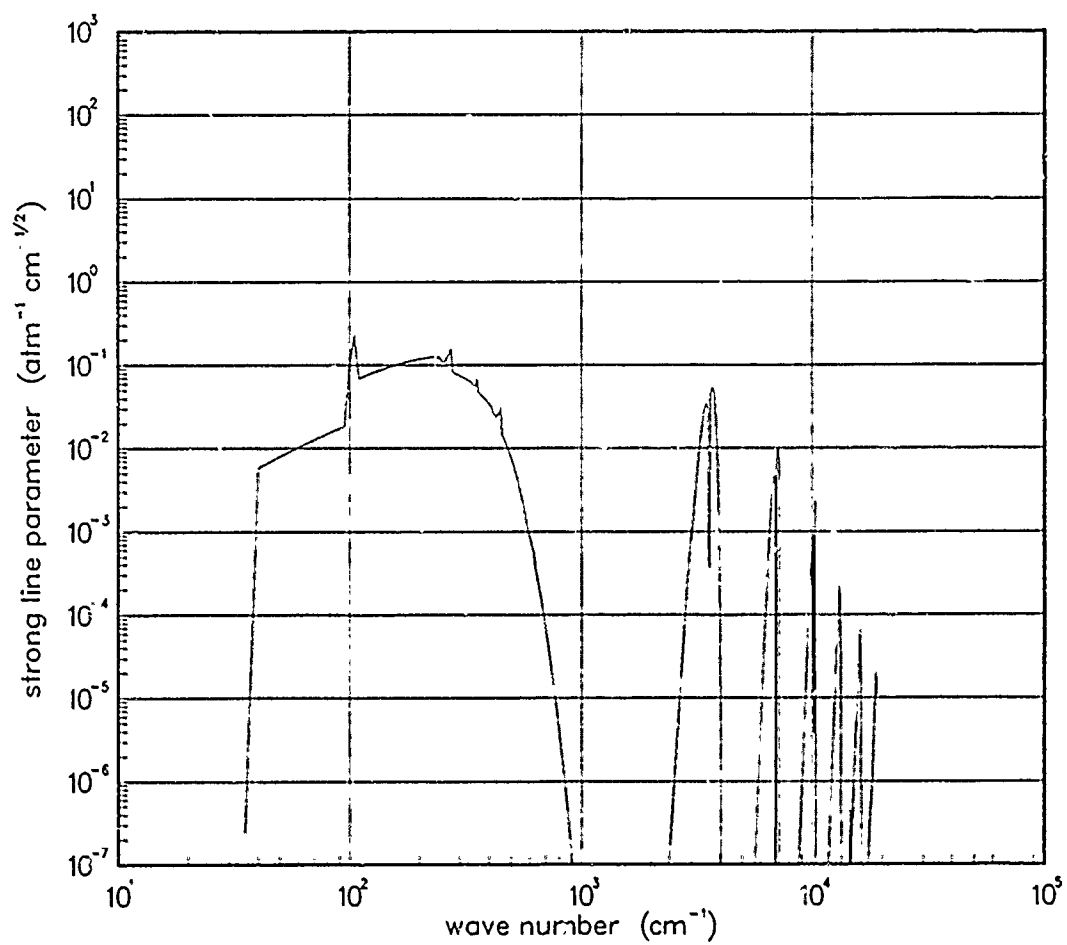


Figure 47. Strong-line parameter for OH at 500°K.

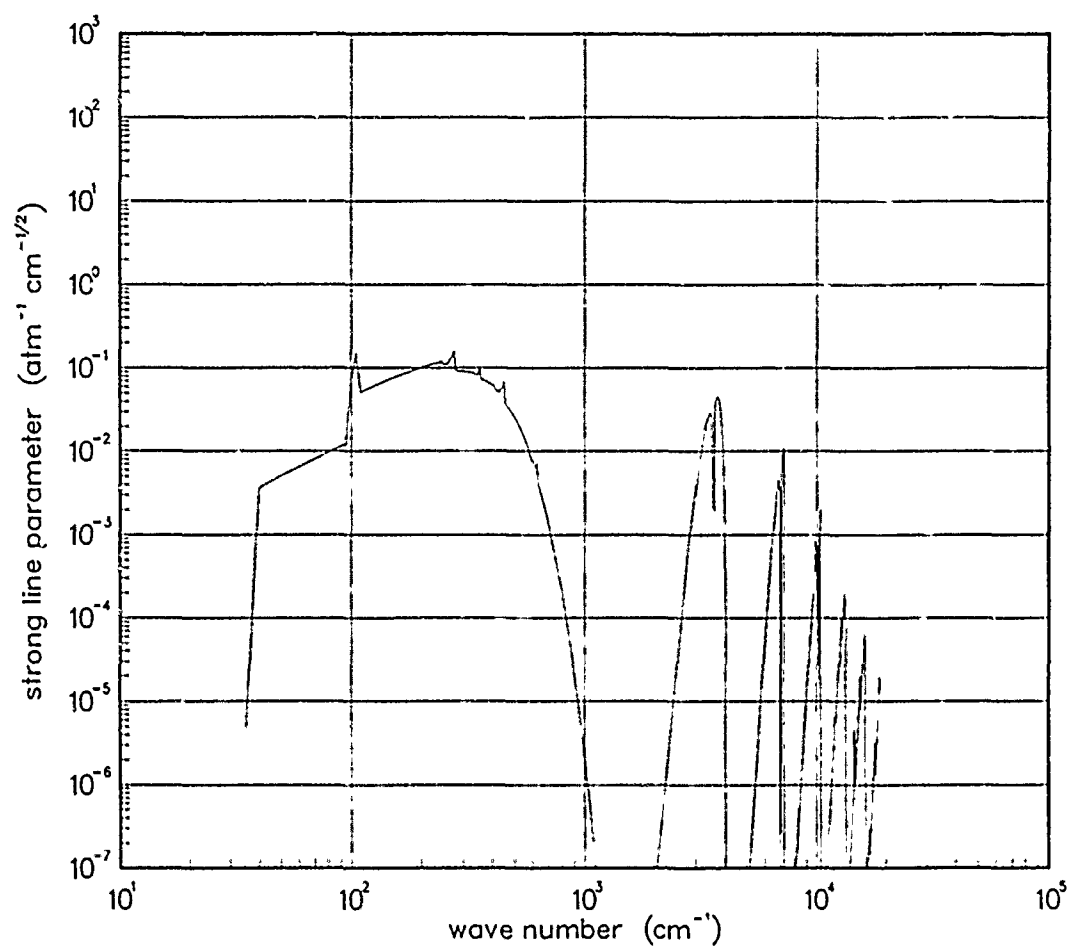


Figure 48. Strong-line parameter for OH at 750°K.

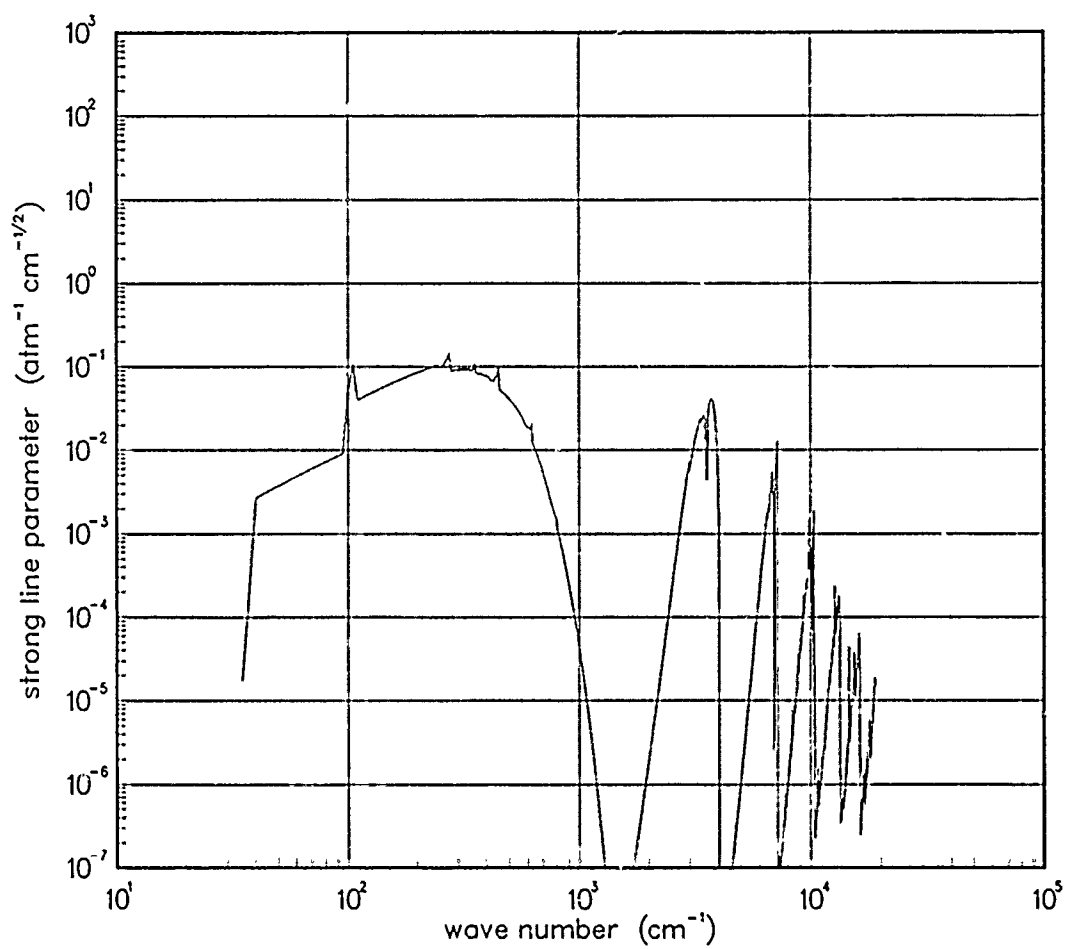


Figure 49. Strong-line parameter for OH at 1000°K.

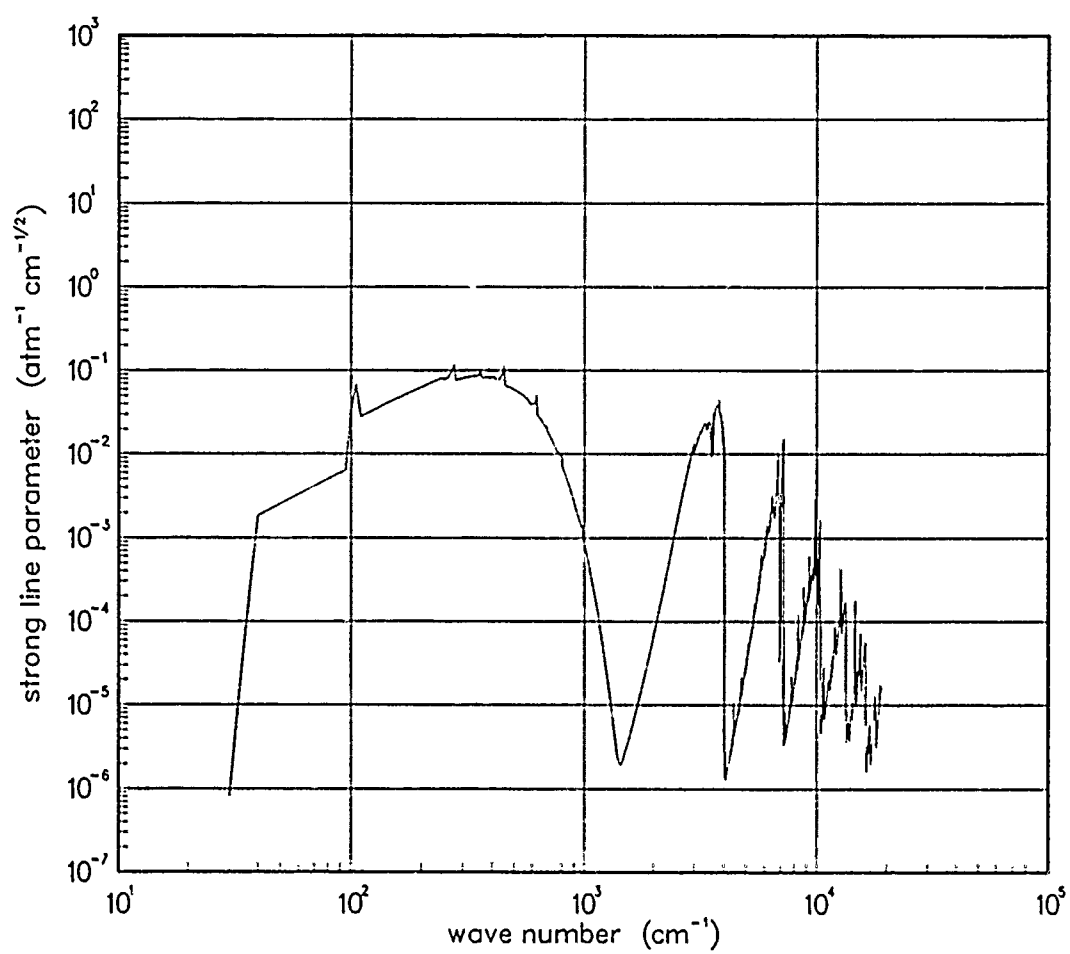


Figure 50. Strong-line parameter for OH at 1500°K.

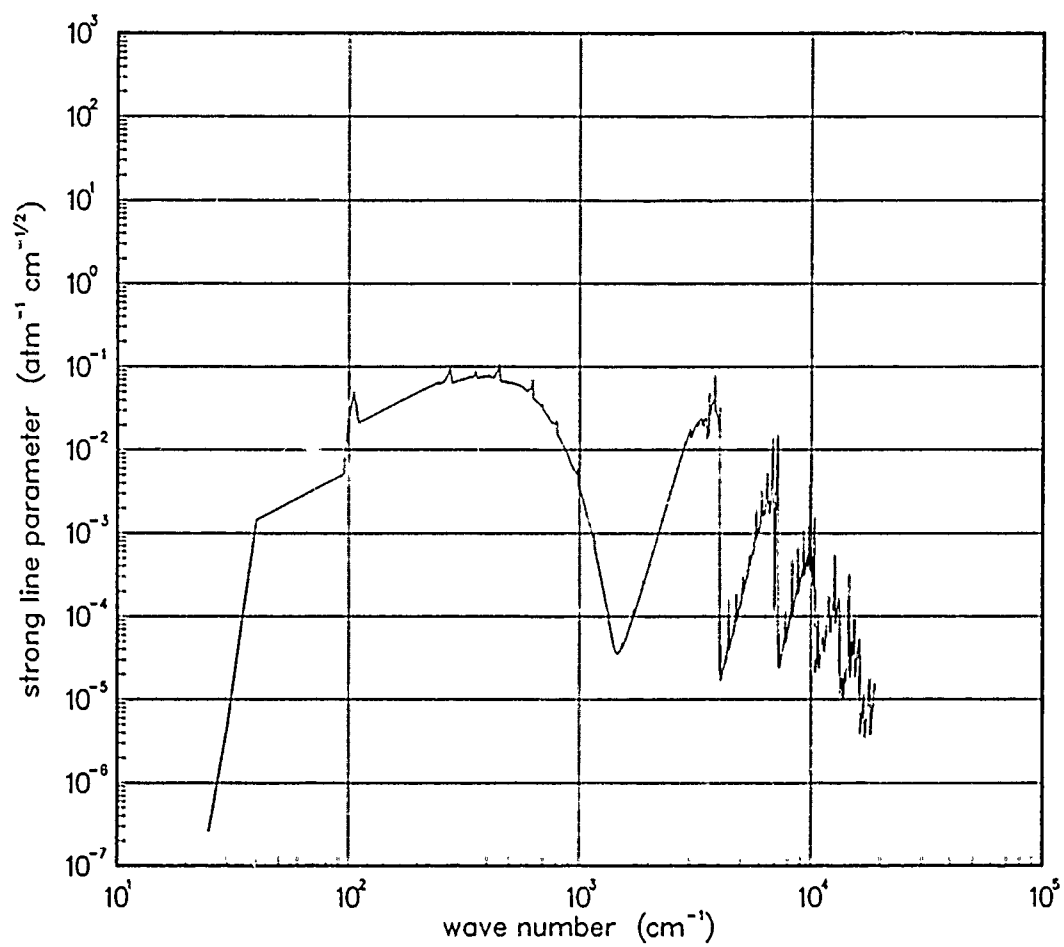


Figure 51. Strong-line parameter for OH at 2000°K.

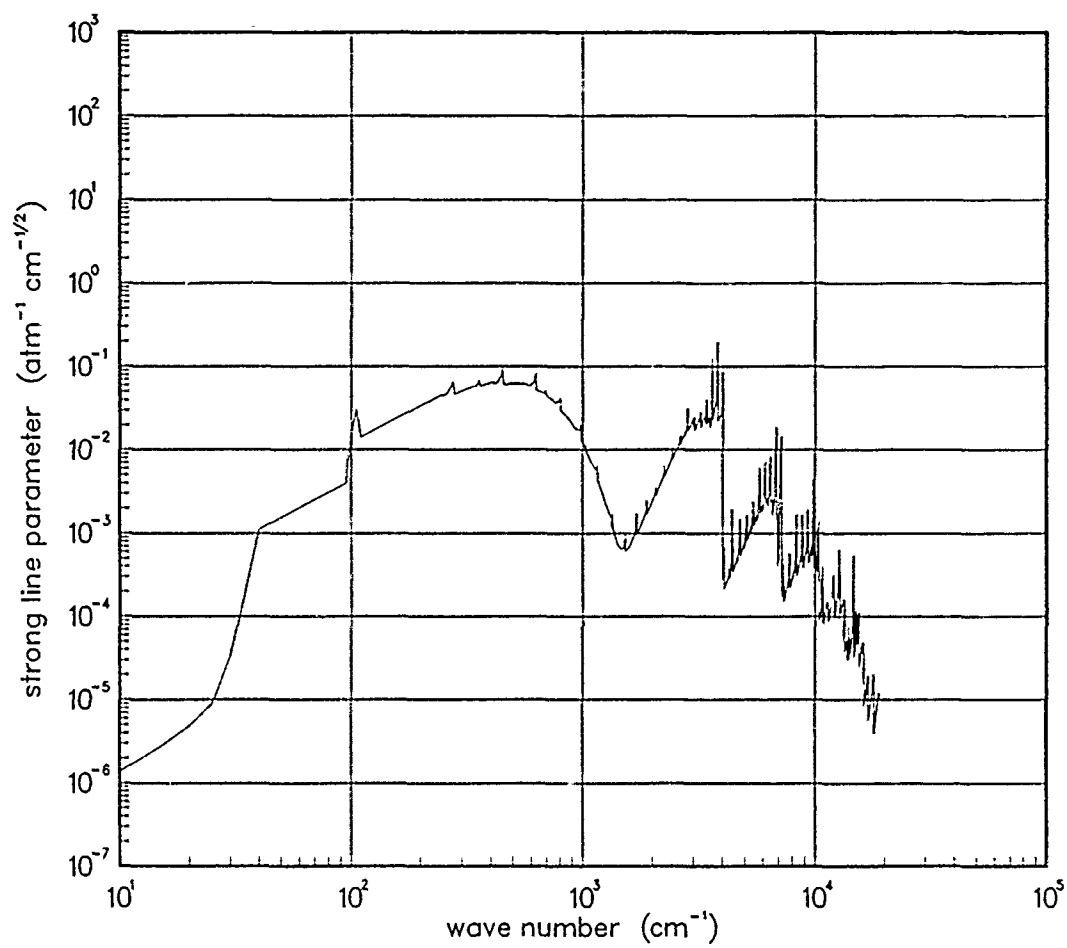


Figure 52. Strong-line parameter for OH at 3000°K.

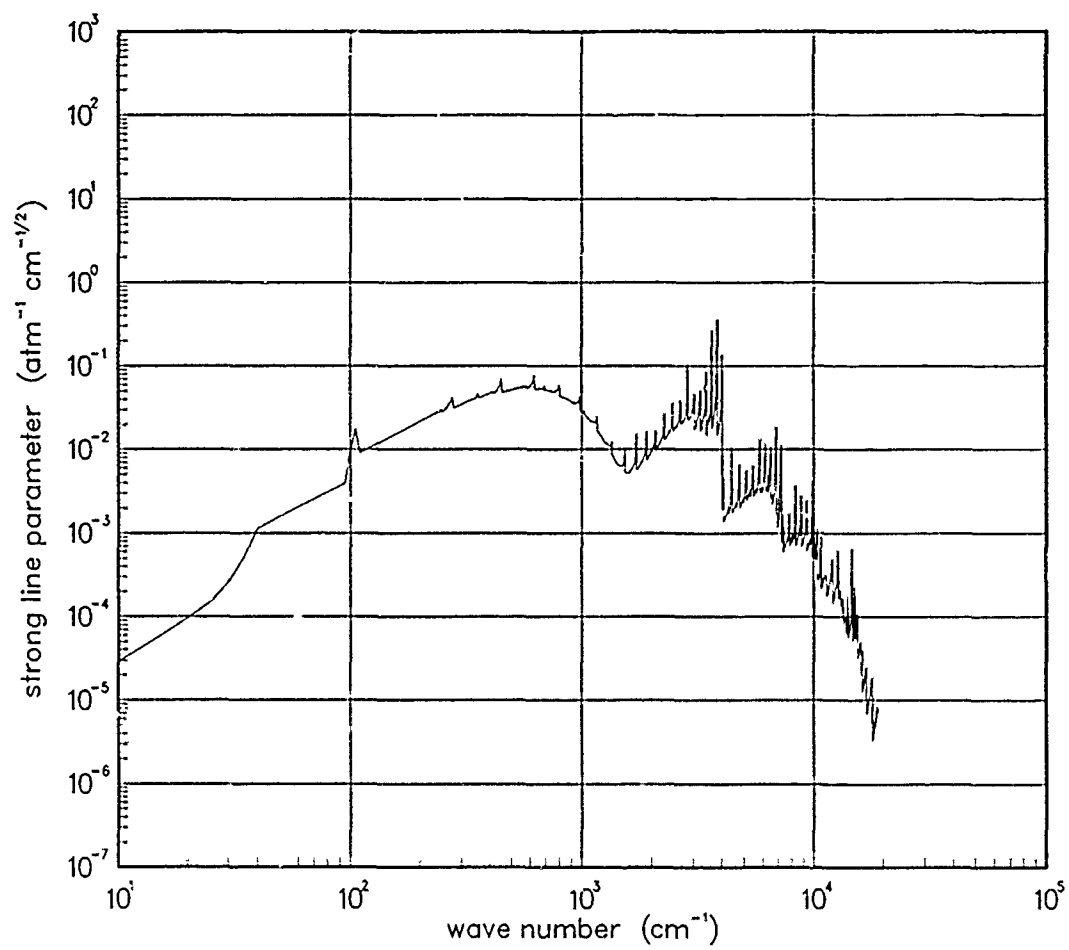


Figure 53. Strong-line parameter for OH at 5000°K.

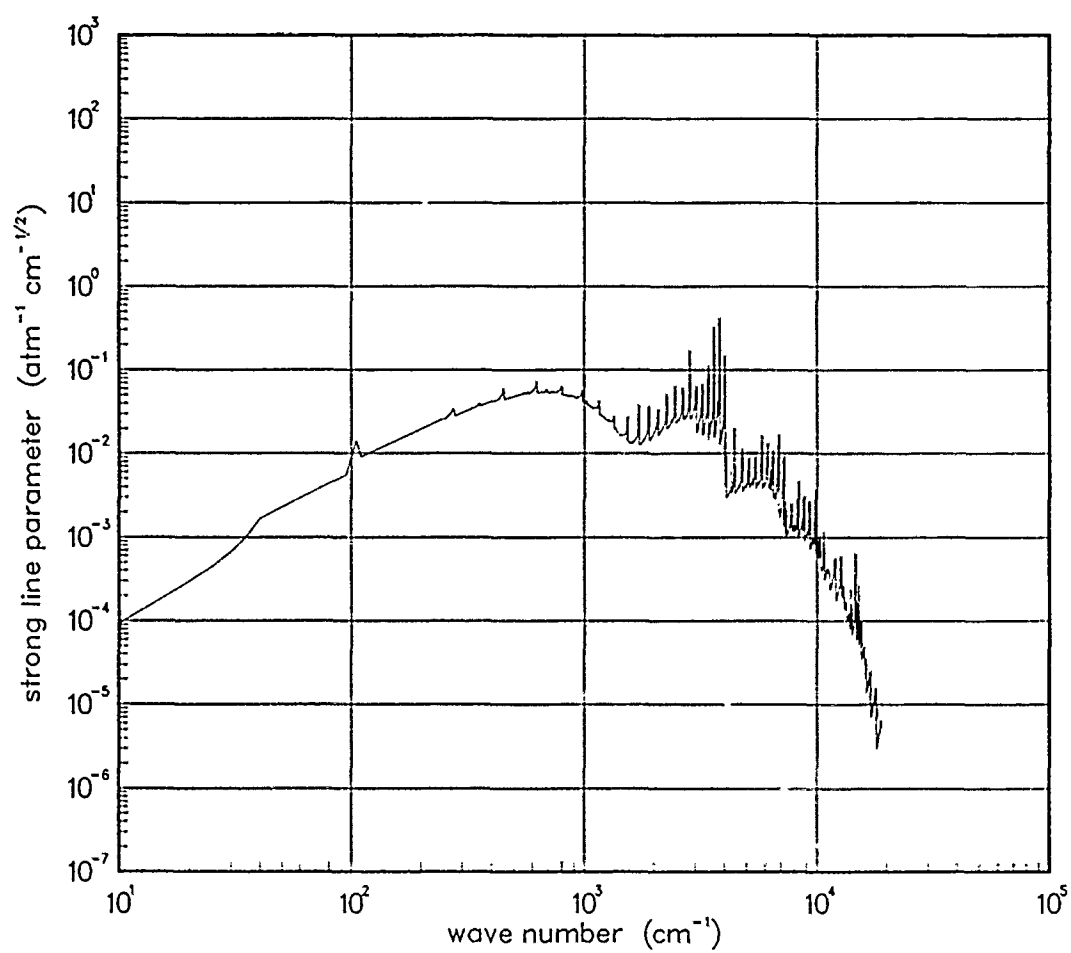


Figure 54. Strong-line parameter for OH at 7000°K.

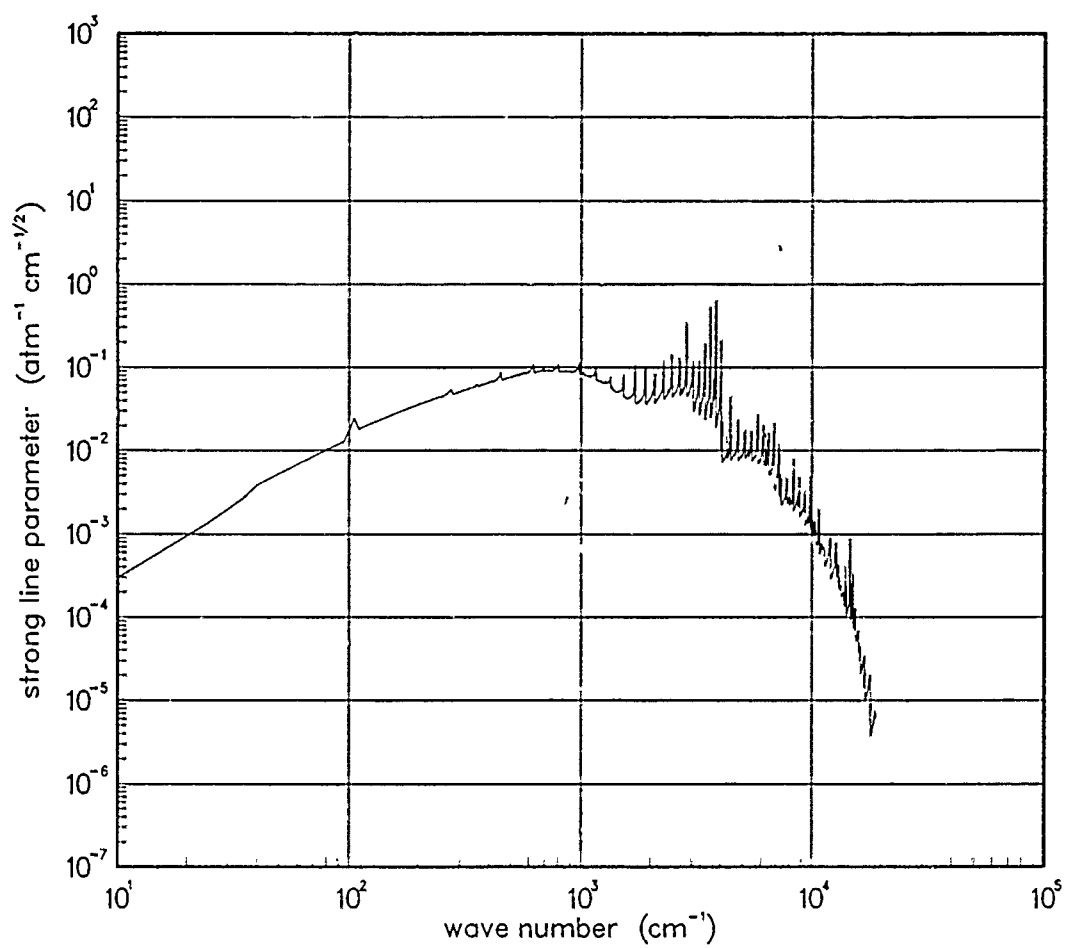


Figure 55. Strong-line parameter for OH at 10000°K.

4.3 NITROGEN (N₂).

The Nitrogen species were calculated by the VisiDyne* Corporation from the RADFLO opacity data base developed by the Air Force Weapons Laboratory in the late sixties. Data for the weak-line parameter for N₂ and N₂⁺ in the visible region (5,000 cm⁻¹ - 100,000 cm⁻¹) is available. There is no inverse line spacing information available in this region.

Data Source:

*H. Smith, T. Keneshea, VisiDyne Corporation, private communication (1986).

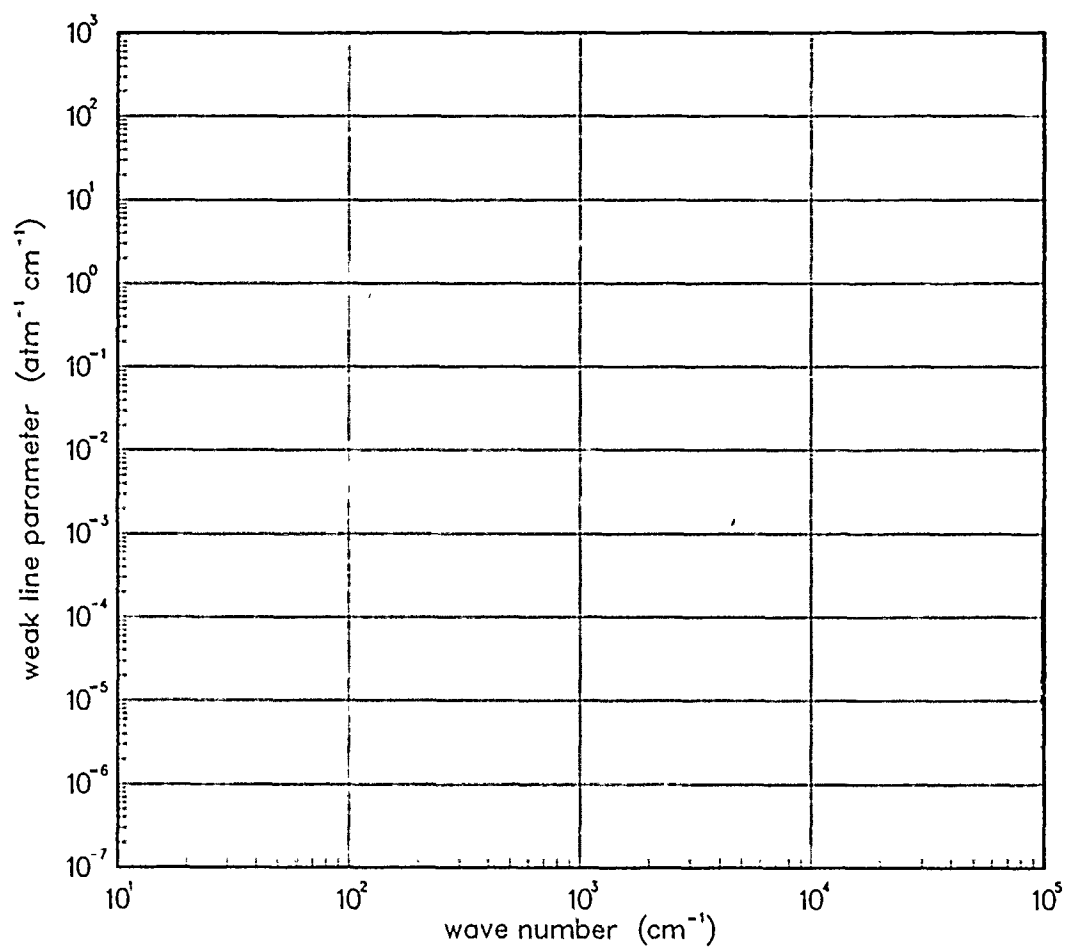


Figure 56. Weak-line parameter for N₂ at 500°K.

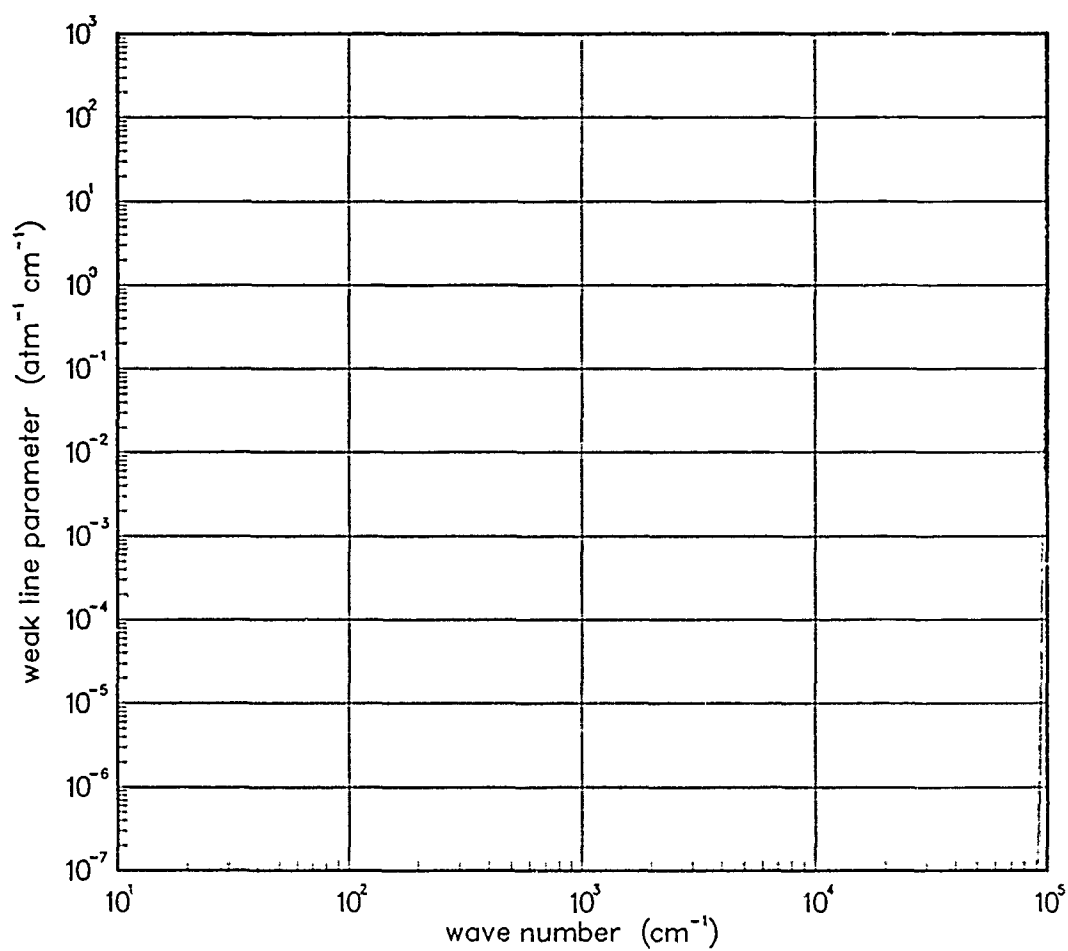


Figure 57. Weak-line parameter for N₂ at 750°K.

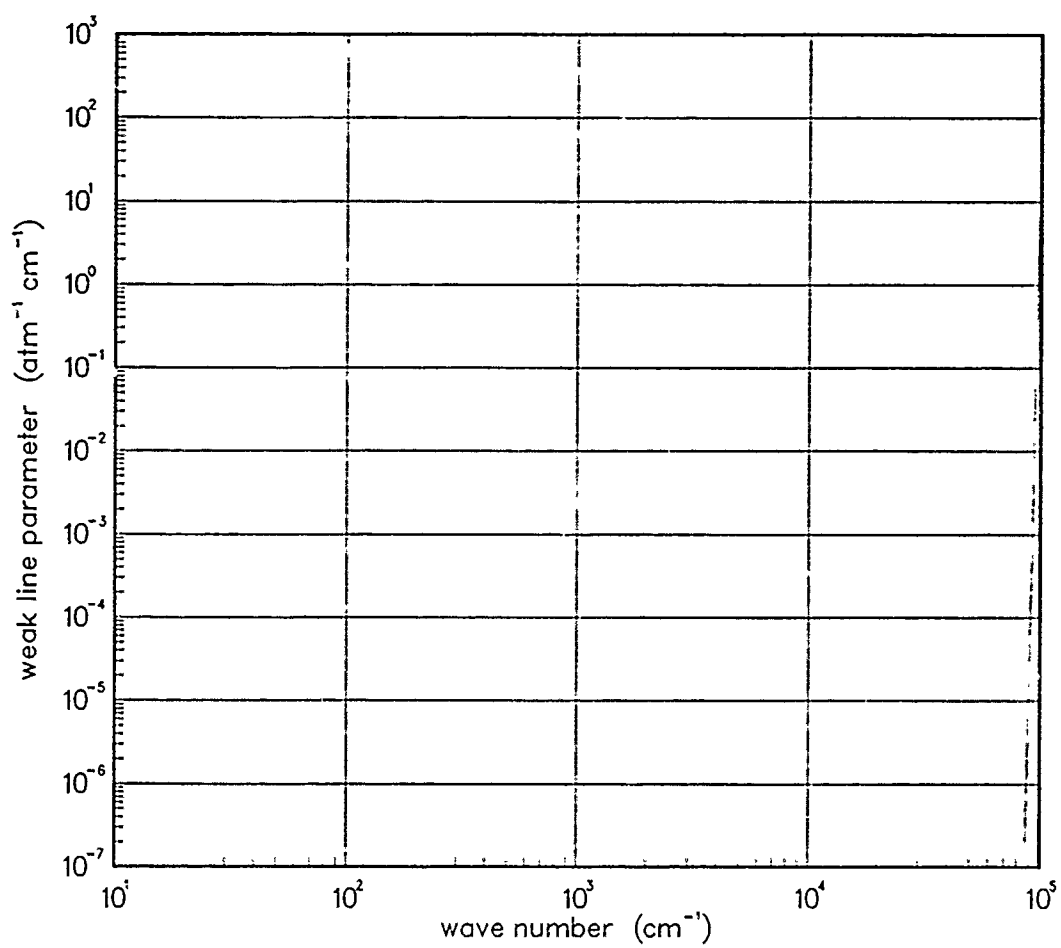


Figure 58. Weak-line parameter for N₂ at 1000°K.

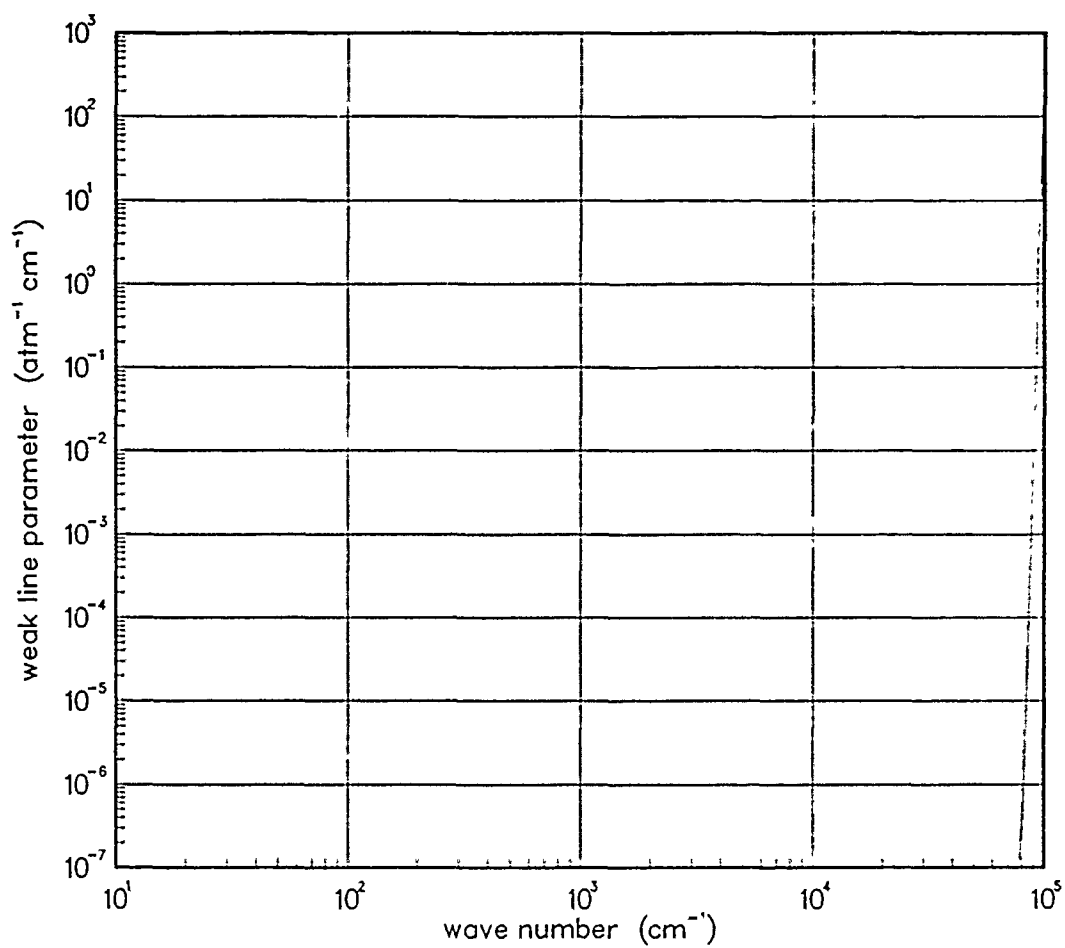


Figure 59. Weak-line parameter for N₂ at 1500°K.

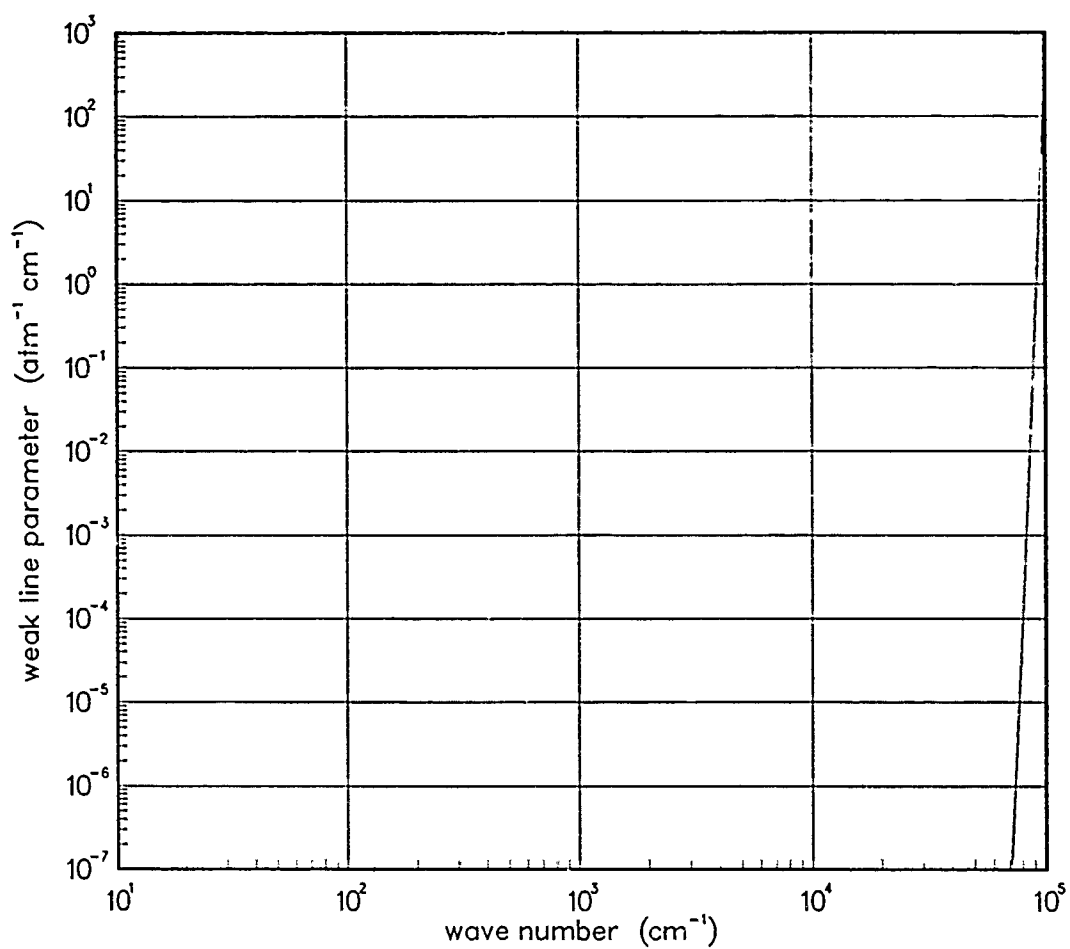


Figure 60. Weak-line parameter for N₂ at 2000°K.

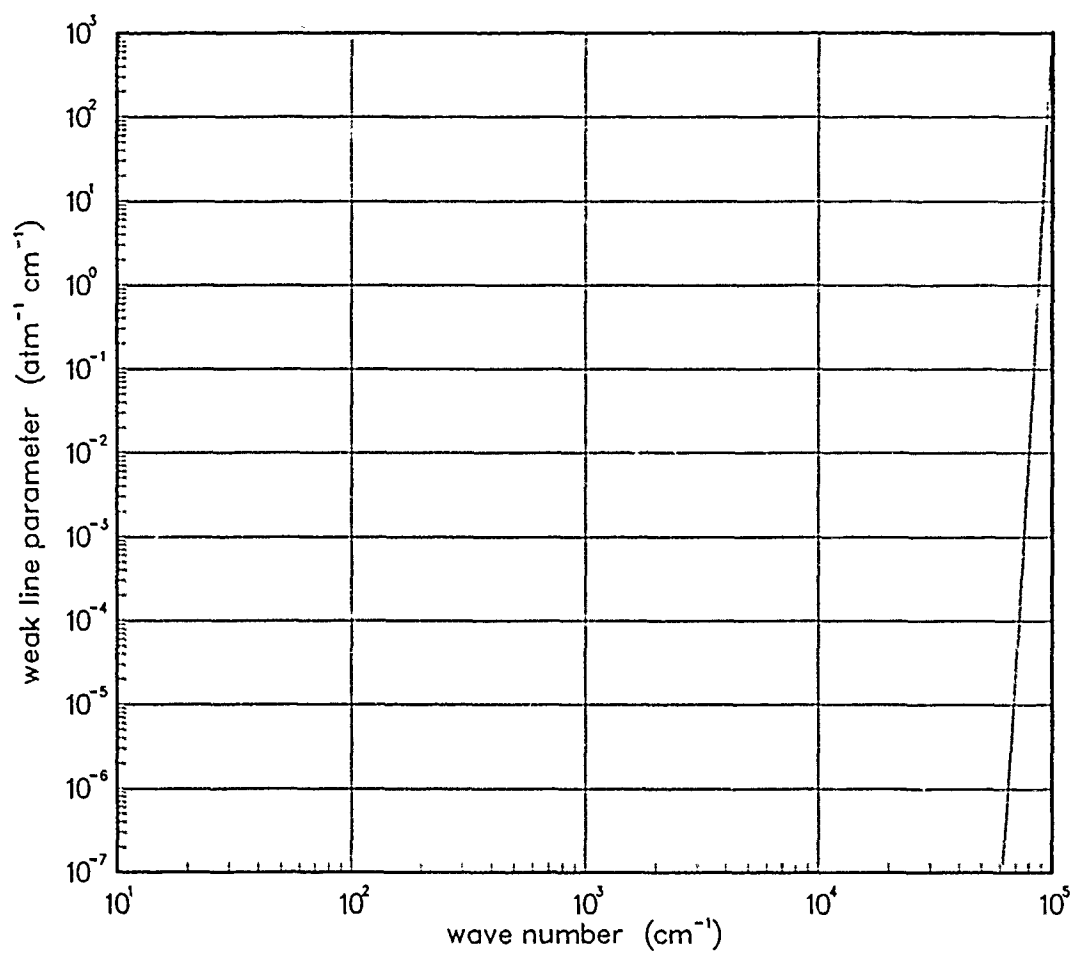


Figure 61. Weak-line parameter for N₂ at 3000°K.

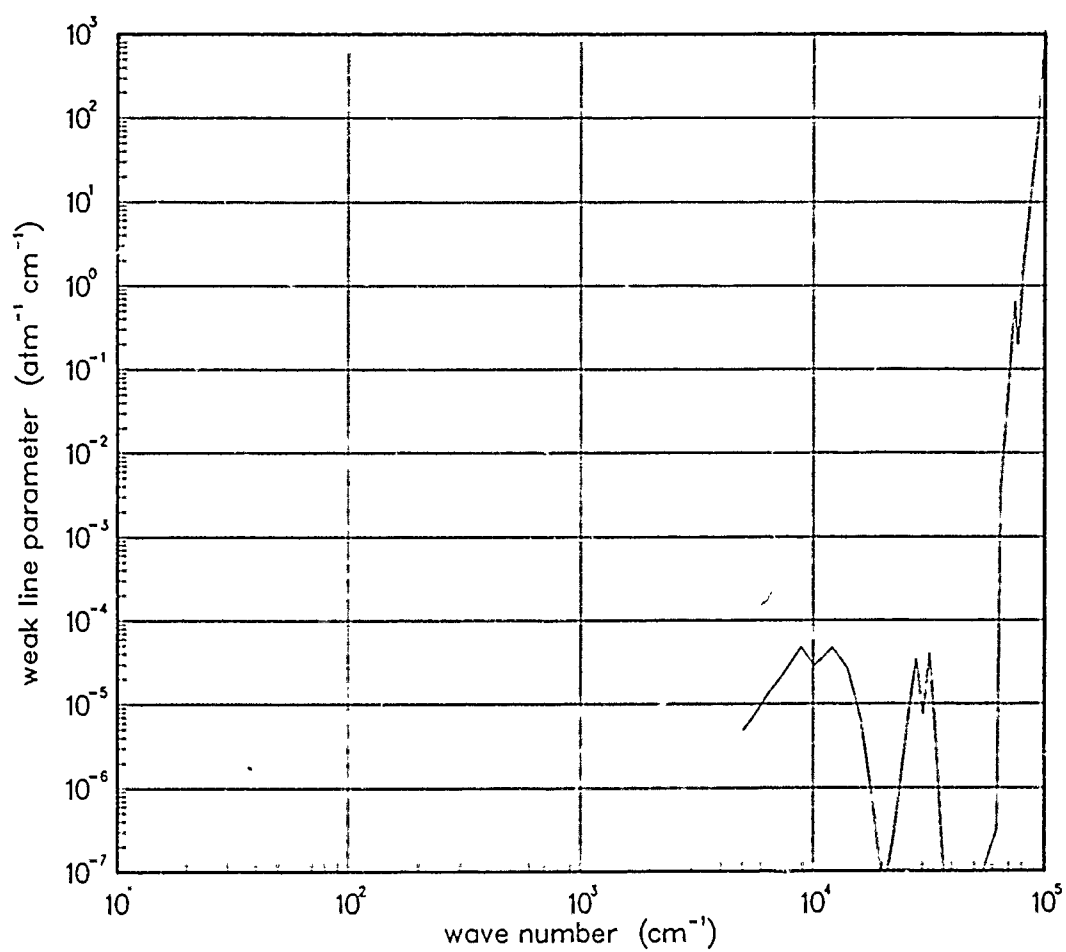


Figure 62. Weak-line parameter for N₂ at 5000°K.

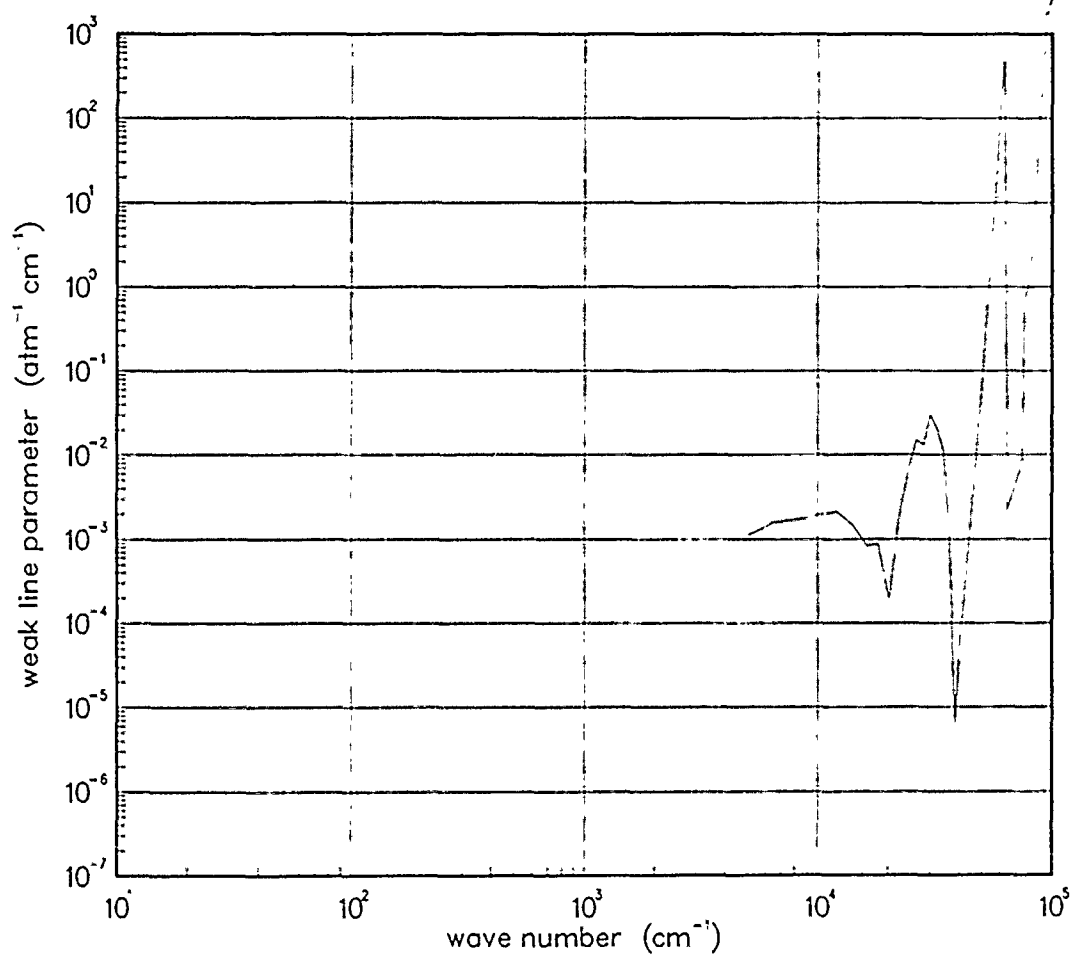


Figure 63. Weak-line parameter for N_2 at $7000^\circ K$.

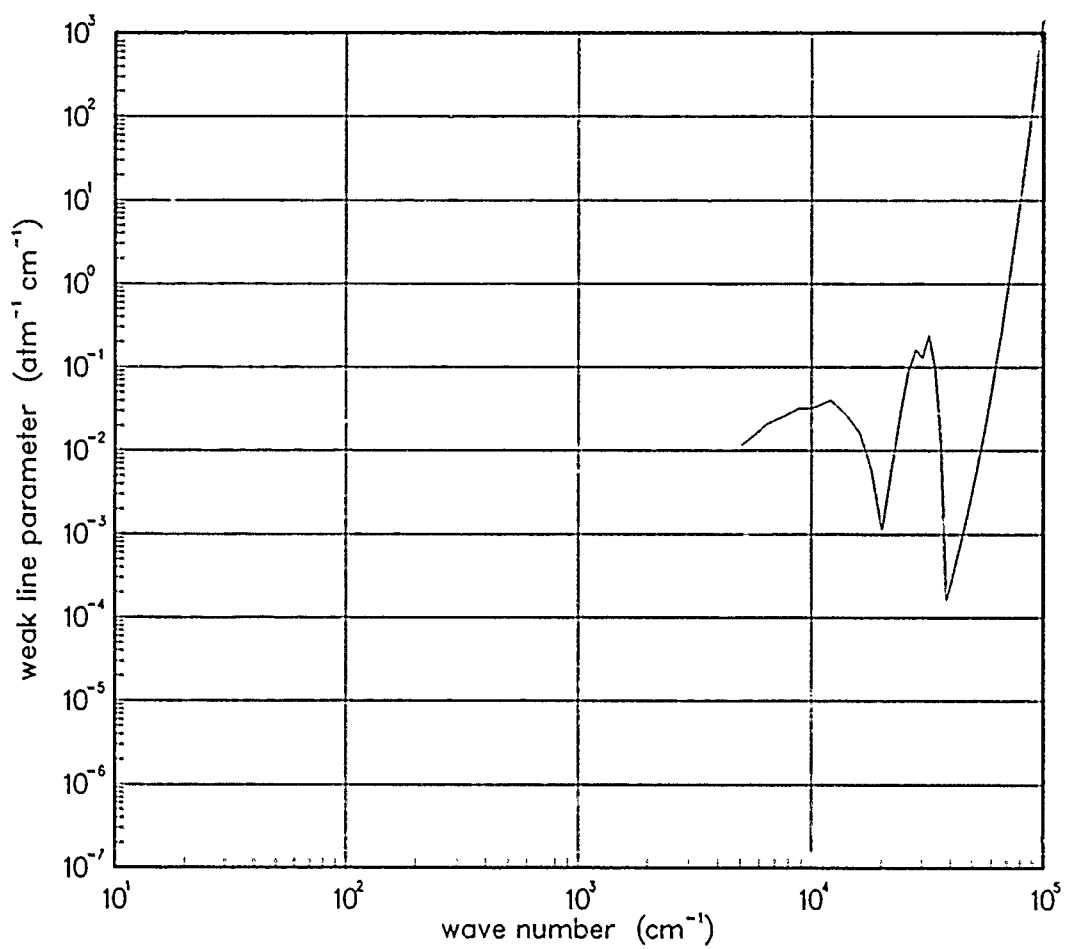


Figure 64. Weak-line parameter for N₂ at 10000°K.

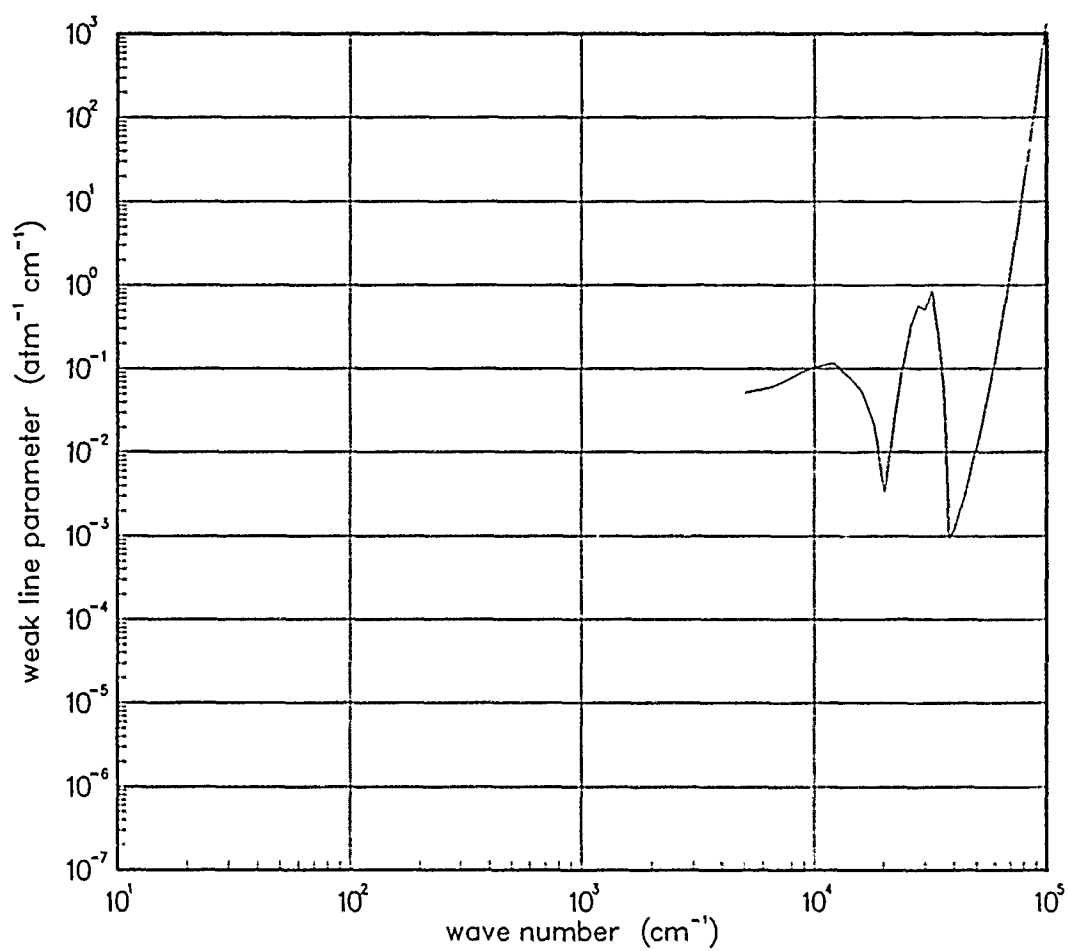


Figure 65. Weak-line parameter for N₂ at 12000°K.

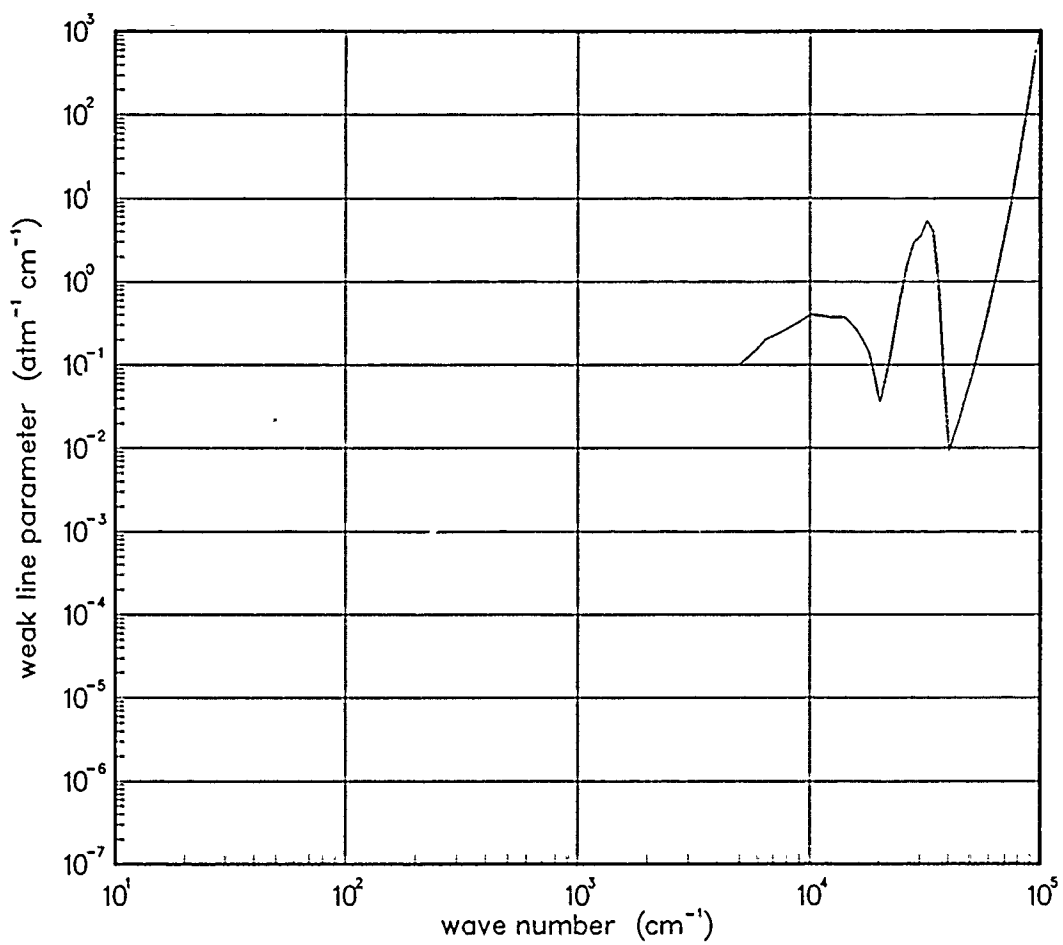


Figure 66. Weak-line parameter for N_2 at $18000^\circ K$.

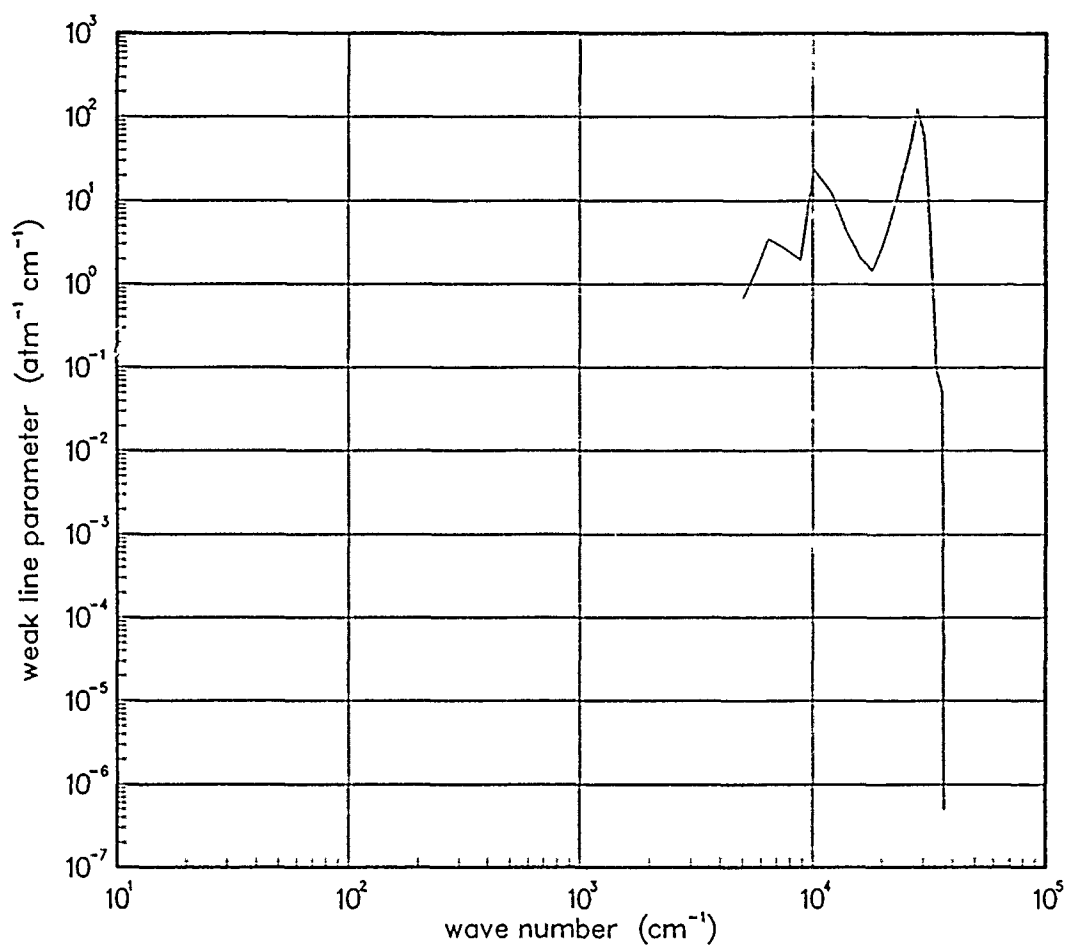


Figure 67. Weak-line parameter for N_2^+ at $5000^\circ K$.

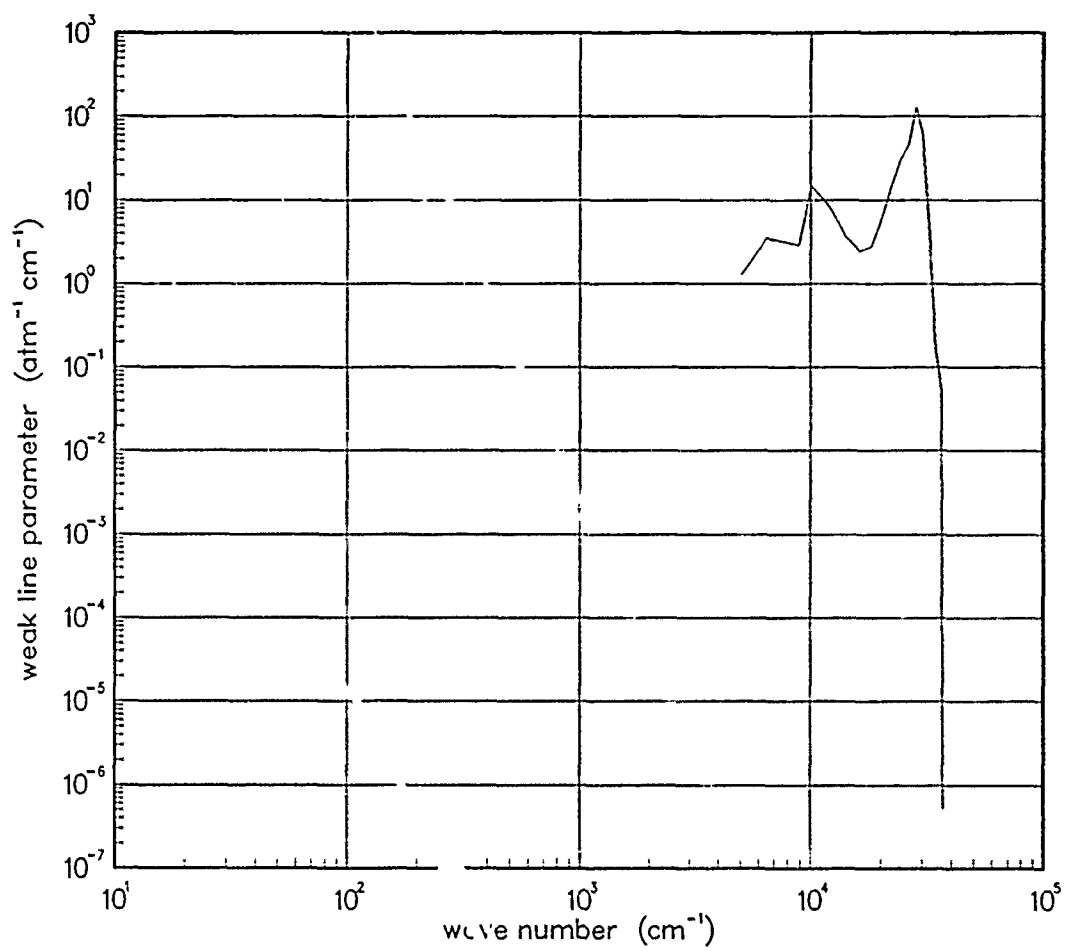


Figure 68. Weak-line parameter for N_2^+ at 7000°K.

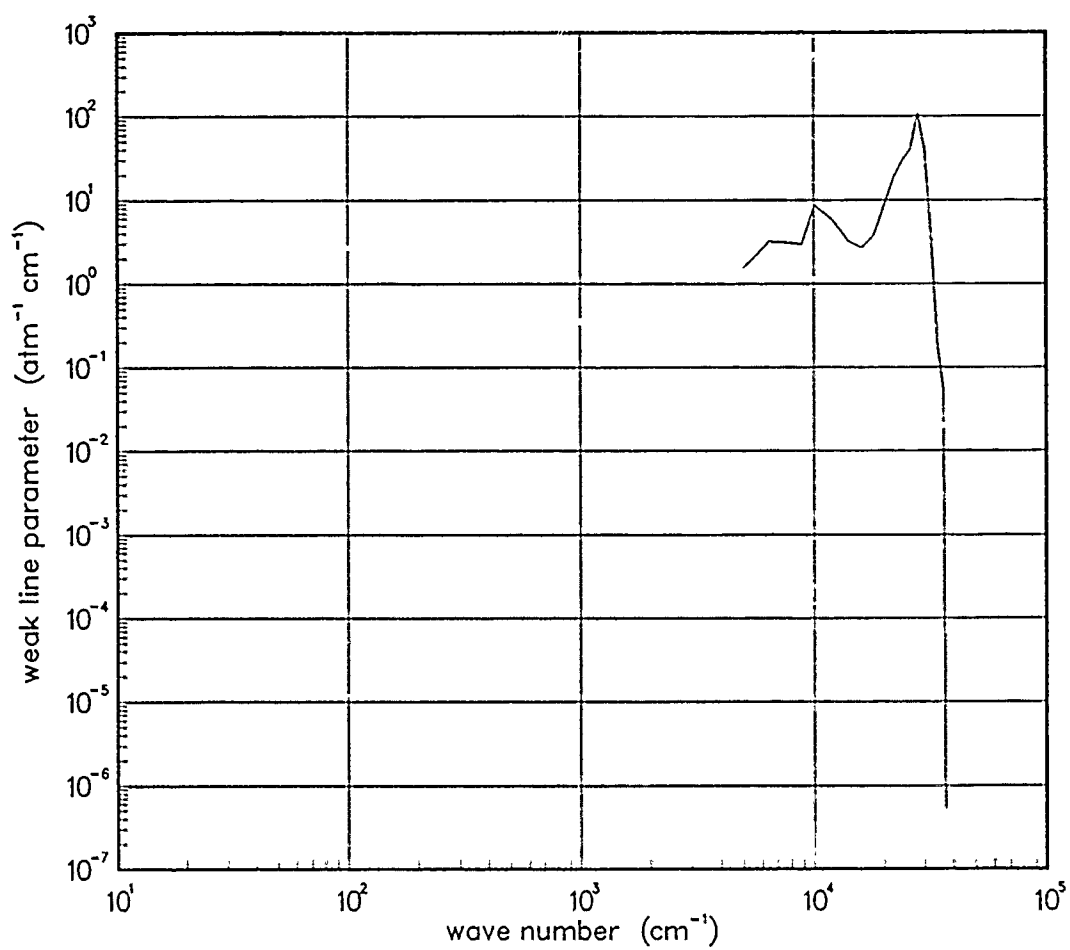


Figure 69. Weak-line parameter for N_2^+ at $10000^\circ K$.

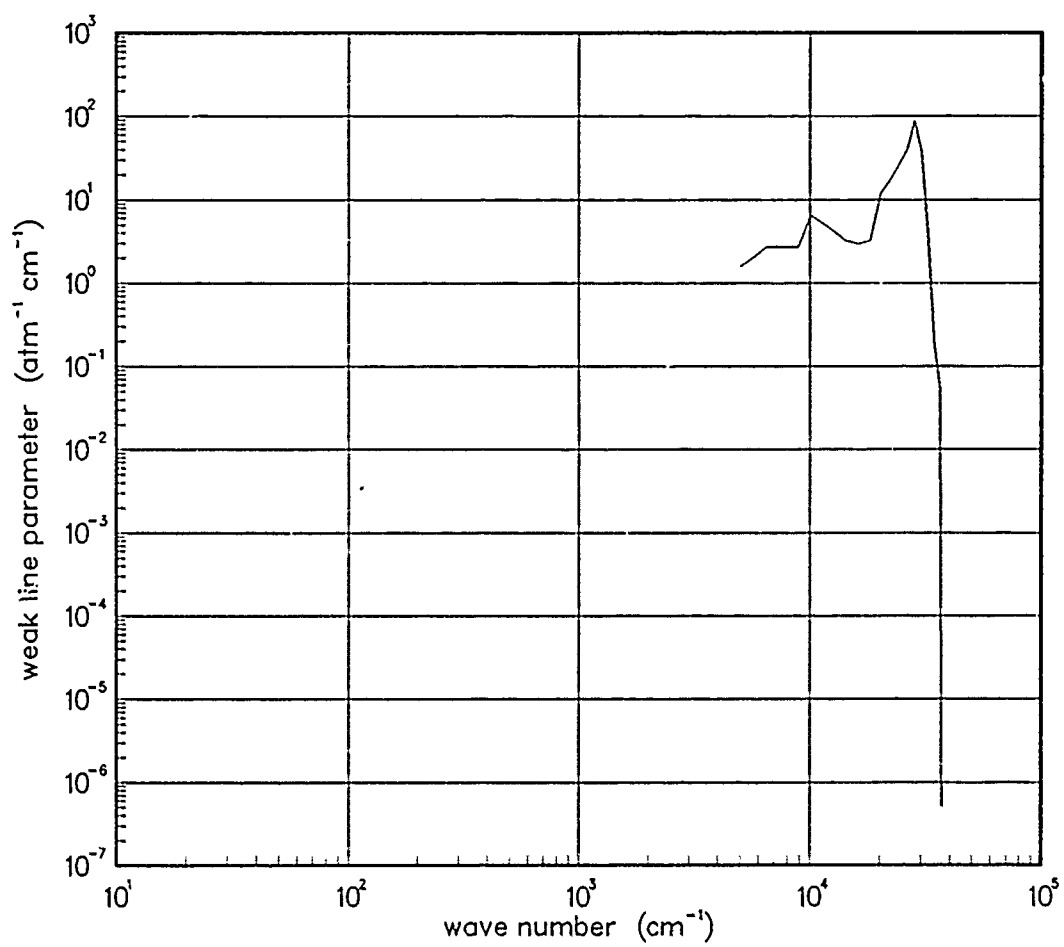


Figure 70. Weak-line parameter for N_2^+ at $12000^\circ K$.

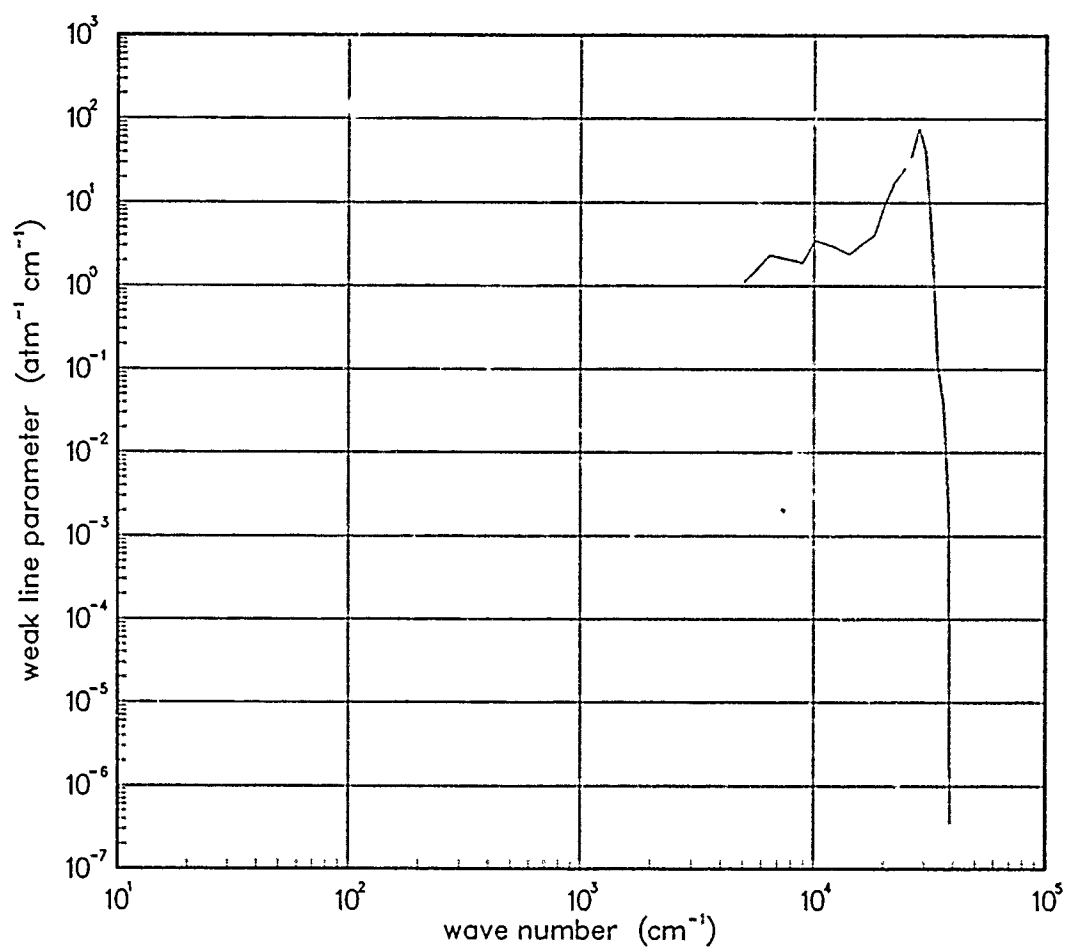


Figure 71. Weak-line parameter for N_2^+ at 18000°K.

4.4 NITROGEN OXIDE (NO).

Data for the NO and NO⁺ molecule in the spectral range 10 - 12,000 cm⁻¹ has been computed using the DATE code.

The Nitrogen oxide was also calculated by the VisiDyne Corporation^{||} from the RADFLO opacity data base developed by the Air Force Weapons Laboratory in the late sixties. Data is available for the weak-line parameter in the visible region (5,000 cm⁻¹ - 100,000 cm⁻¹). The inverse line spacing is not available in this region.

Table 3. Spectroscopic data for NO.

X ²Π

$$\begin{array}{lll} \omega_e = 1904.087^* & \omega_e x_e = 14.044^* & \\ \alpha_e = 0.017612^\ddagger & B_e = 1.70509^\dagger & A_e = 123.61^* \end{array}$$

$$S_{10} = 125.0^* \quad S_{20} = 2.11^\ddagger \quad S_{30} = 0.0458^\ddagger$$

$$\gamma_\ell(300^\circ\text{K}) = 0.040^\S$$

Data Source:

*M.D. Olman, M.D. McNelis, and C.D. Hause, J. Mol. Spectrosc., 14, 62 (1964)

†U.P. Oppenheim, Y. Aviv, and A. Goldman, Appl. Opt. 6, 1305 (1967).

‡B. Schurin, and R.E. Ellis, J.Chem. Phys., 45, 2528 (1966).

§Fit to the data of: L.L. Abels, and J.H. Shaw, J. Mol. Spectrosc., 20, 11, (1966).

||H. Smith, T. Keneshea, VisiDyne Corporation, private communication (1986).

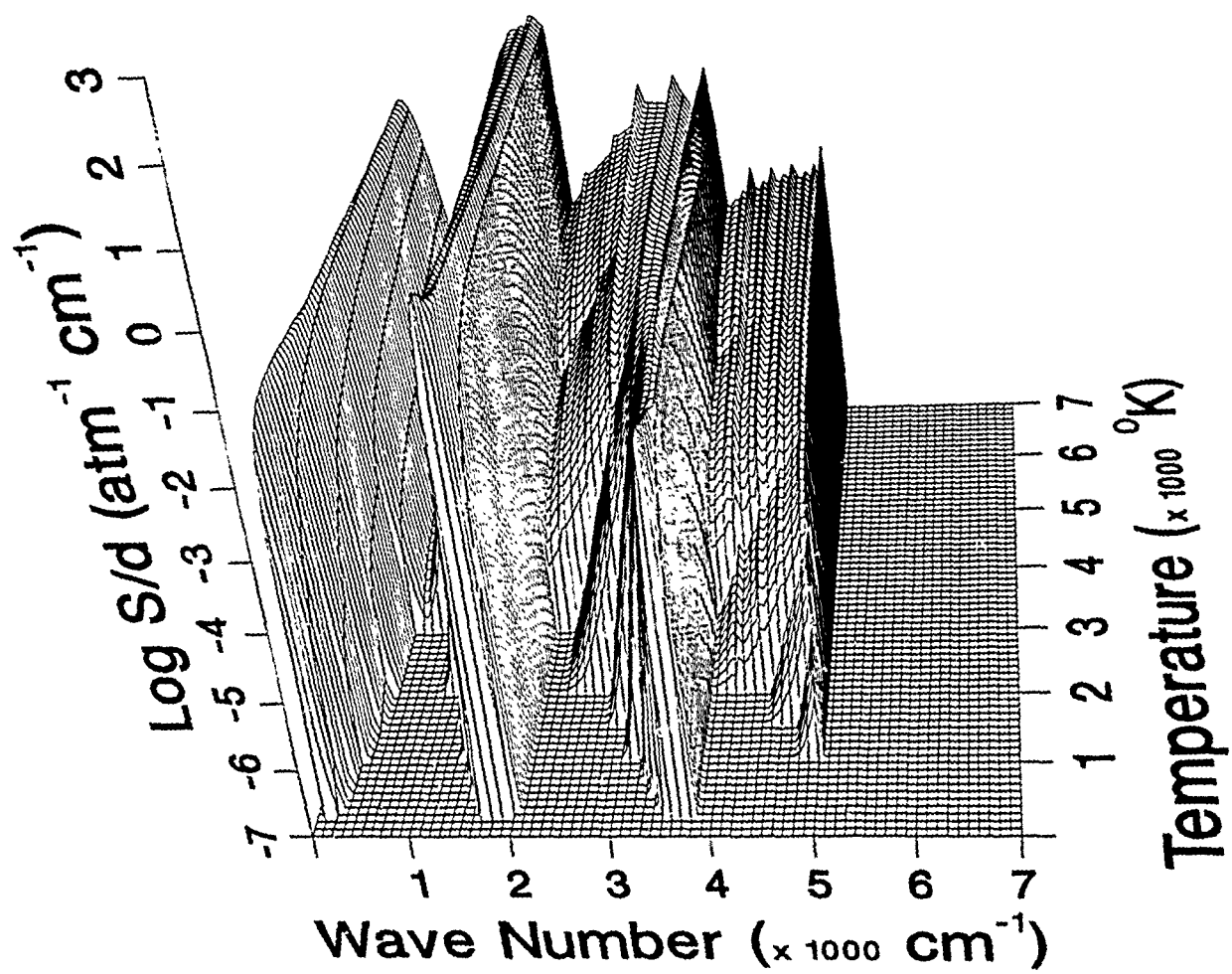


Figure 72. Weak-line parameter for NO.

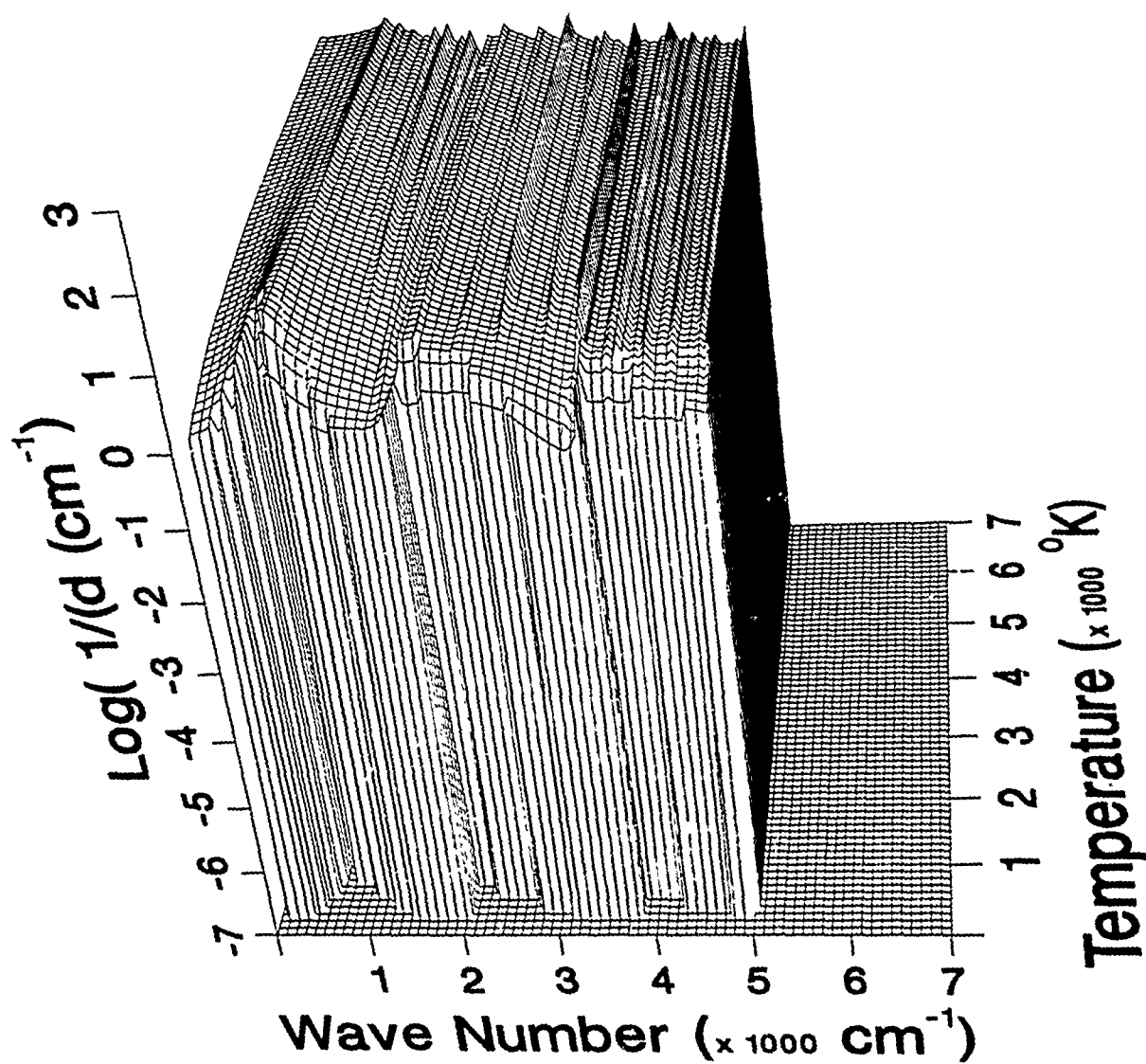


Figure 73. Inverse line spacing for NO.

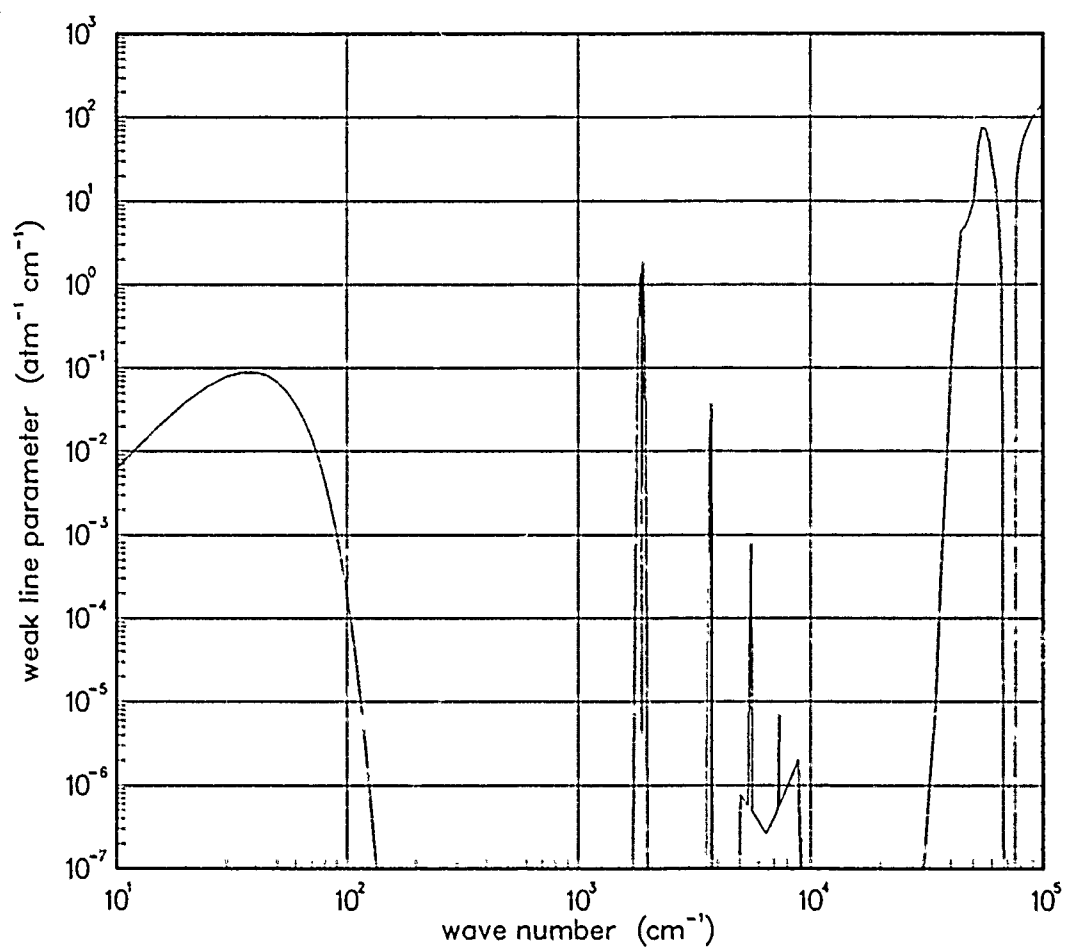


Figure 74. Weak-line parameter for NO at 200°K.

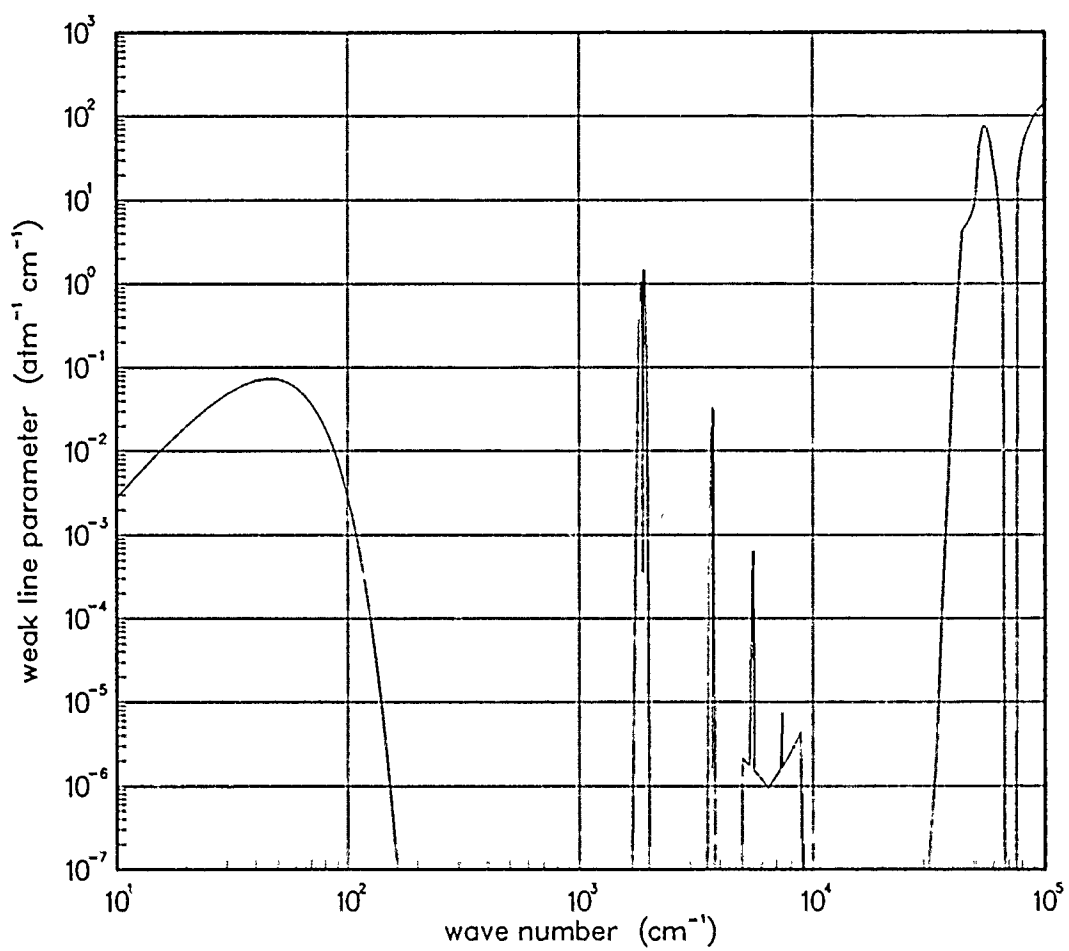


Figure 75. Weak-line parameter for NO at 300°K.

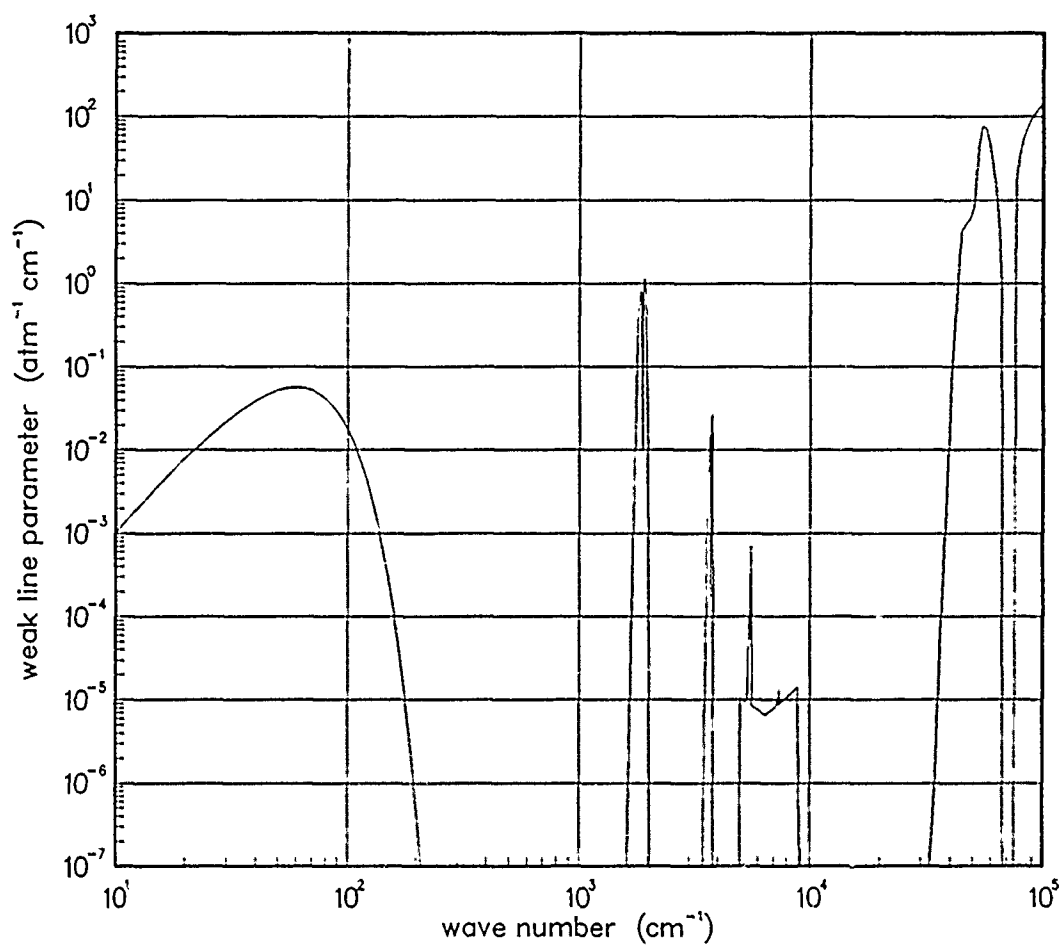


Figure 76. Weak-line parameter for NO at 500°K.

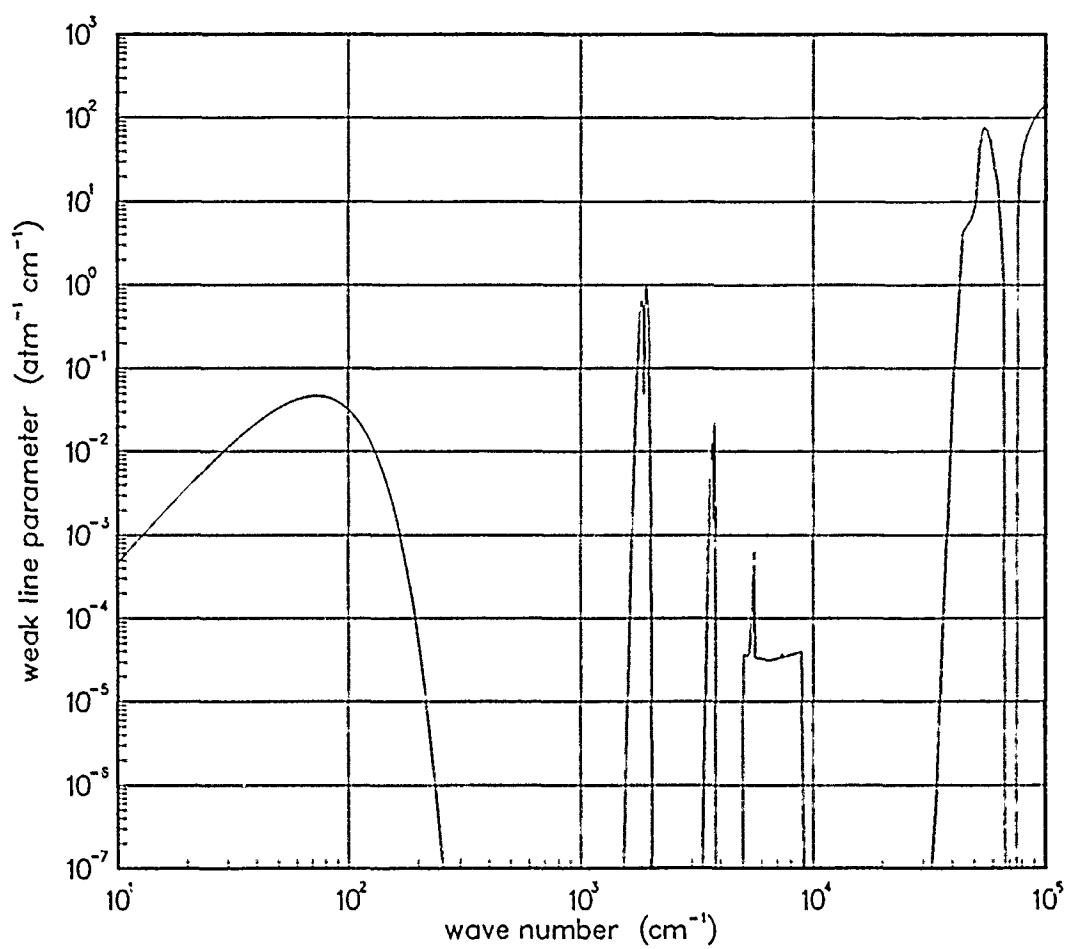


Figure 77. Weak-line parameter for NO at 750°K.

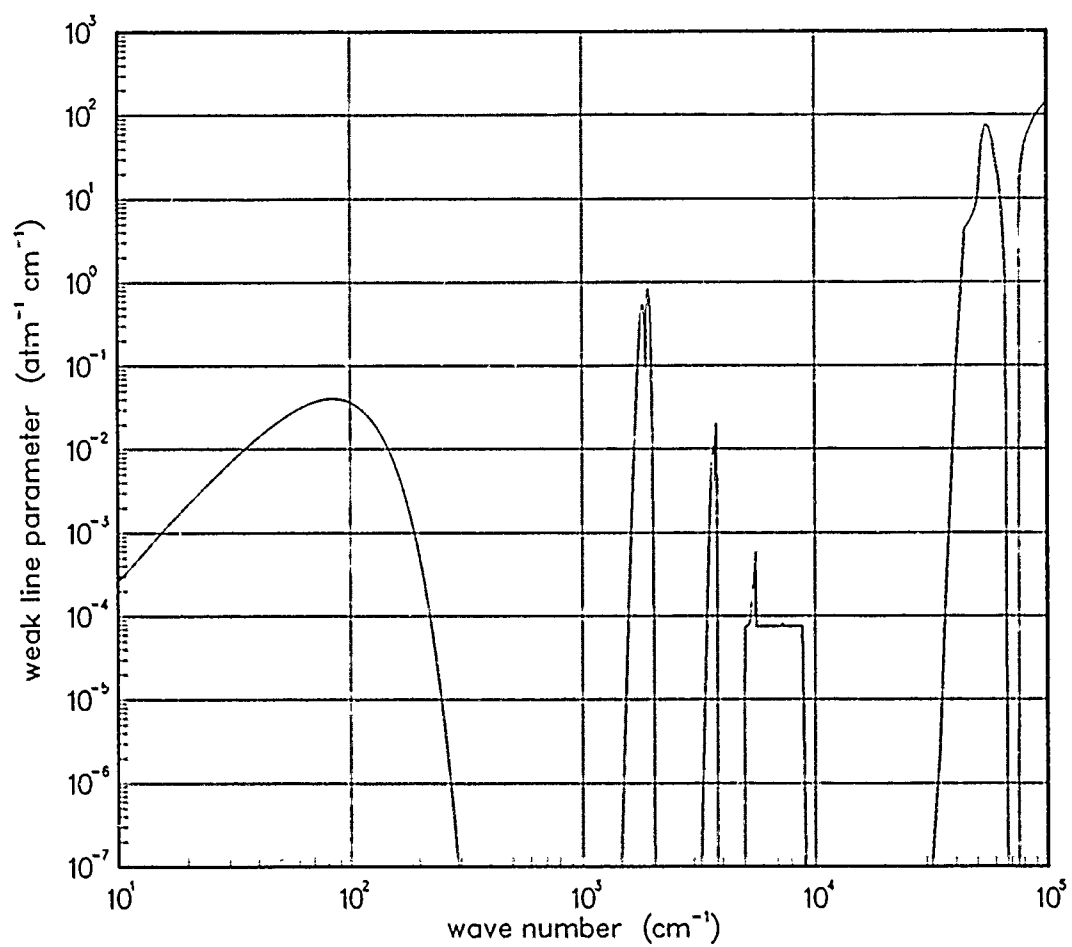


Figure 78. Weak-line parameter for NO at 1000°K.

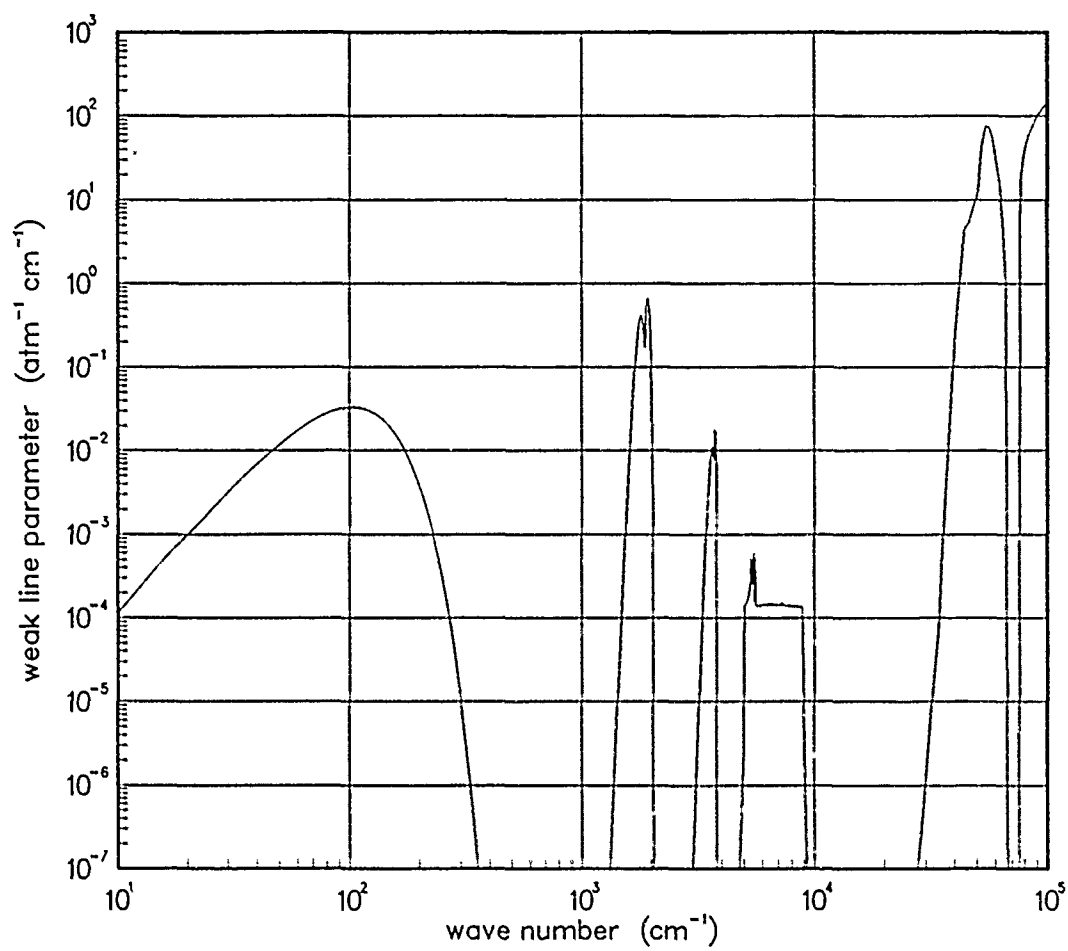


Figure 79. Weak-line parameter for NO at 1500°K.

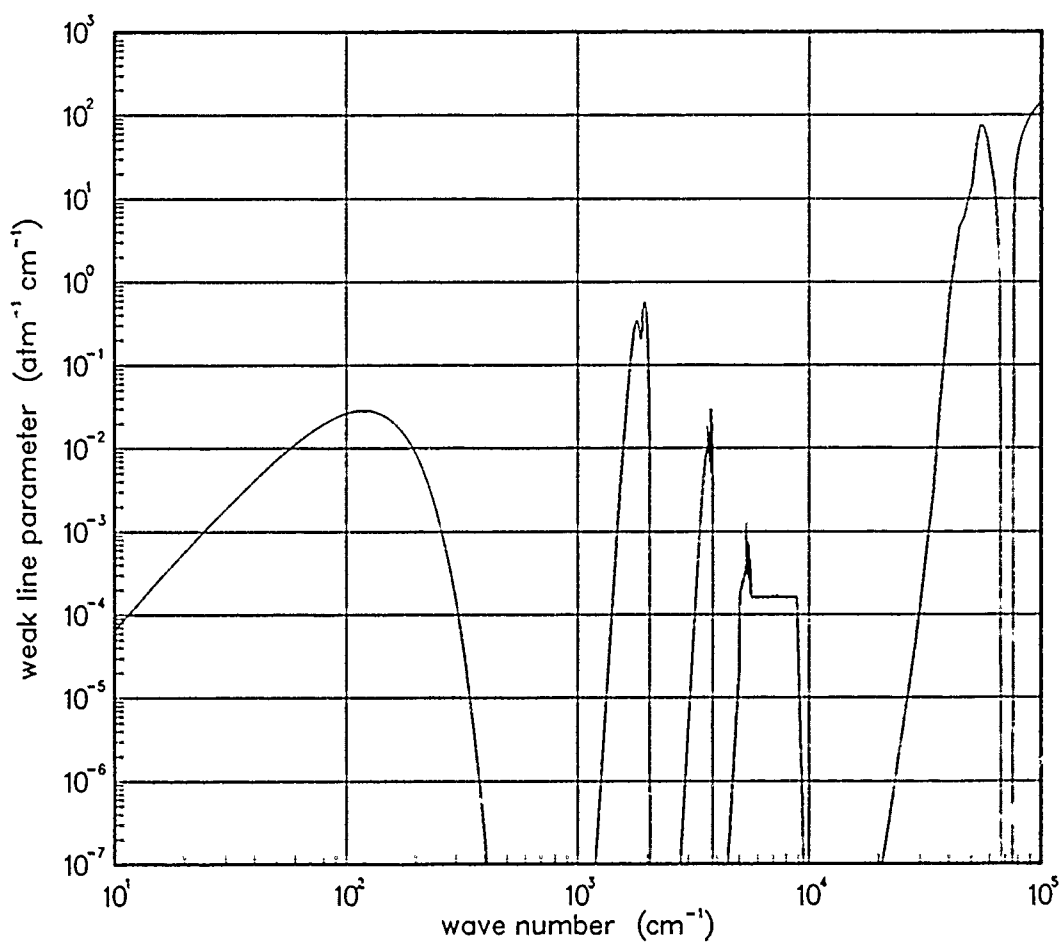


Figure 80. Weak-line parameter for NO at 2000°K.

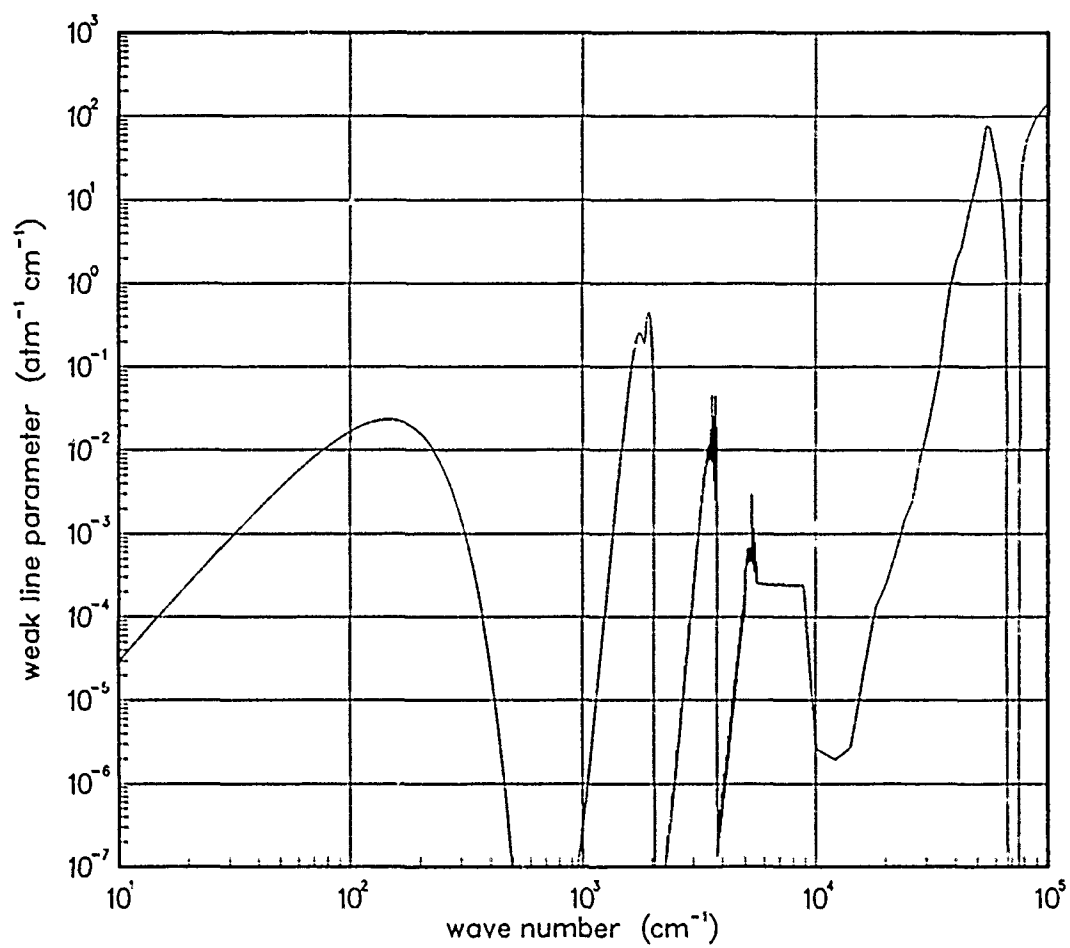


Figure 81. Weak-line parameter for NO at 3000°K.

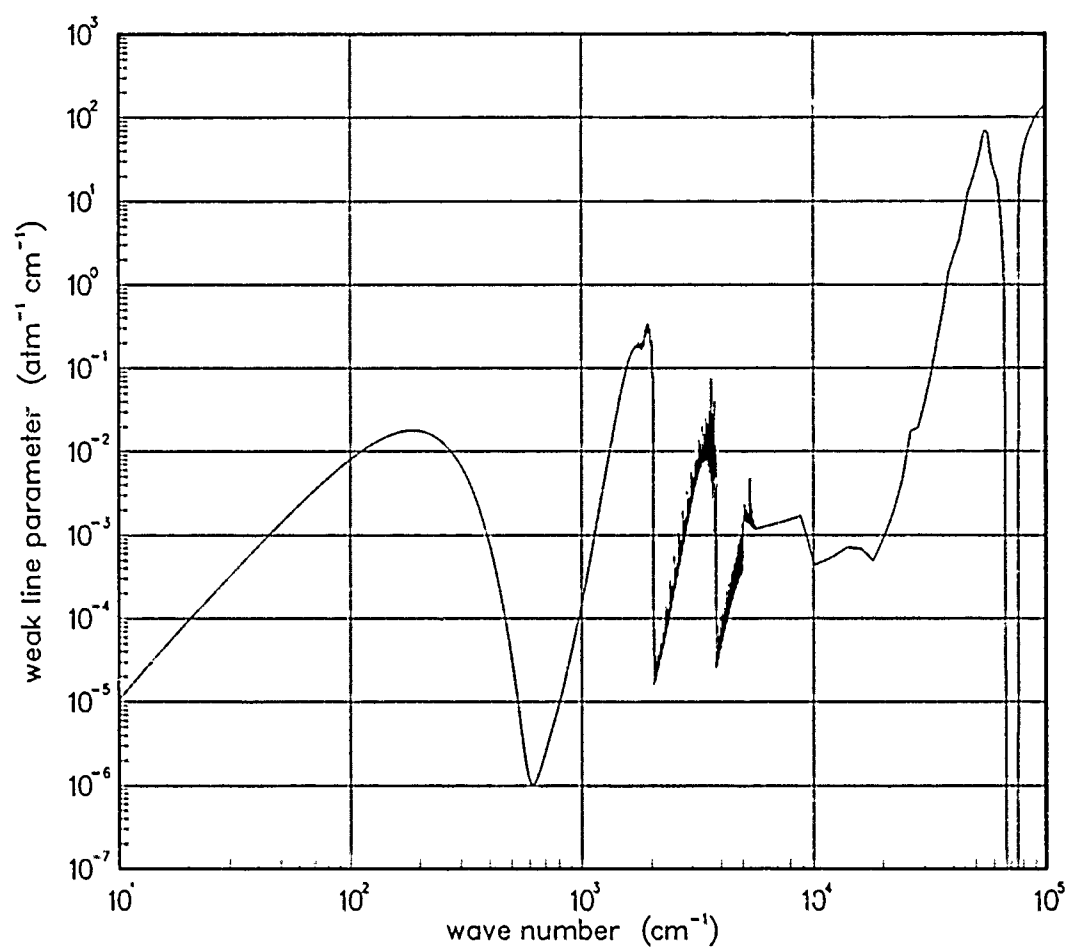


Figure 82. Weak-line parameter for NO at 5000°K.

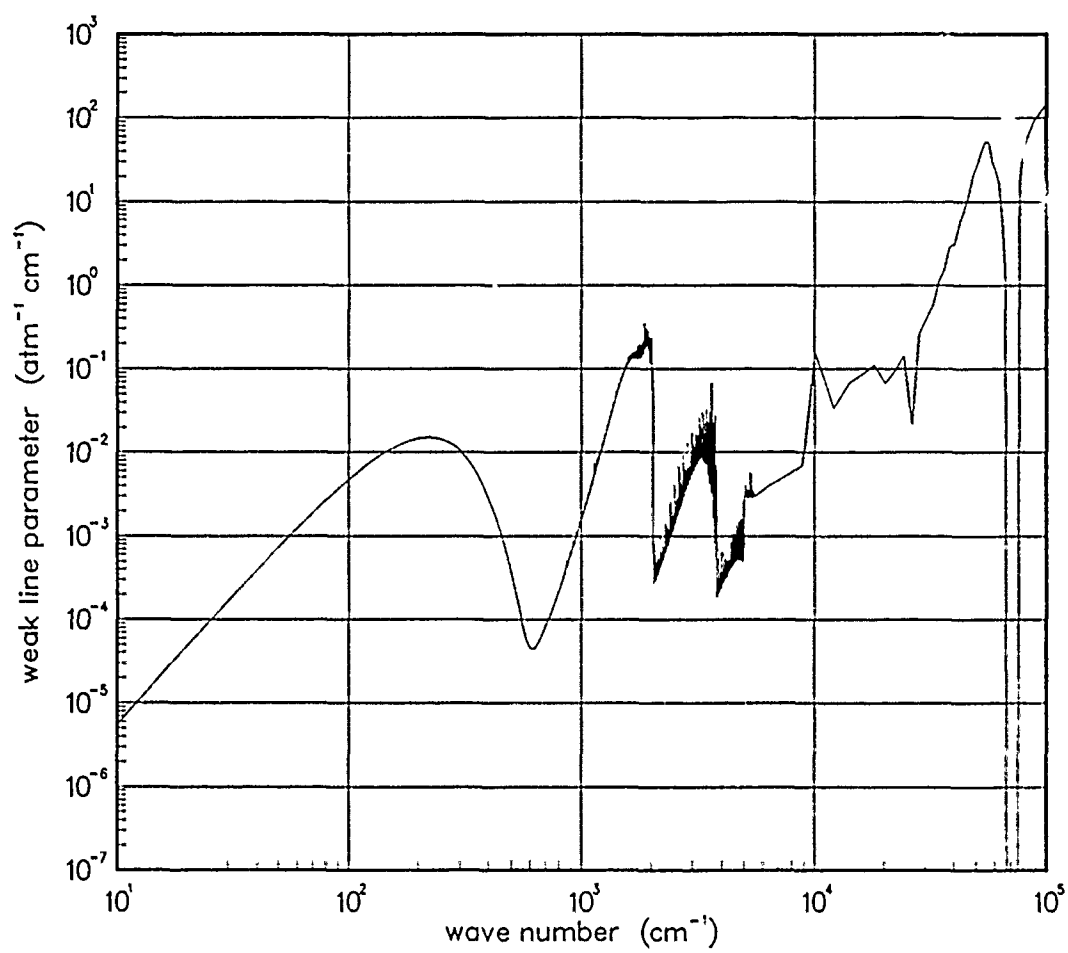


Figure 83. Weak-line parameter for NO at 7000°K.

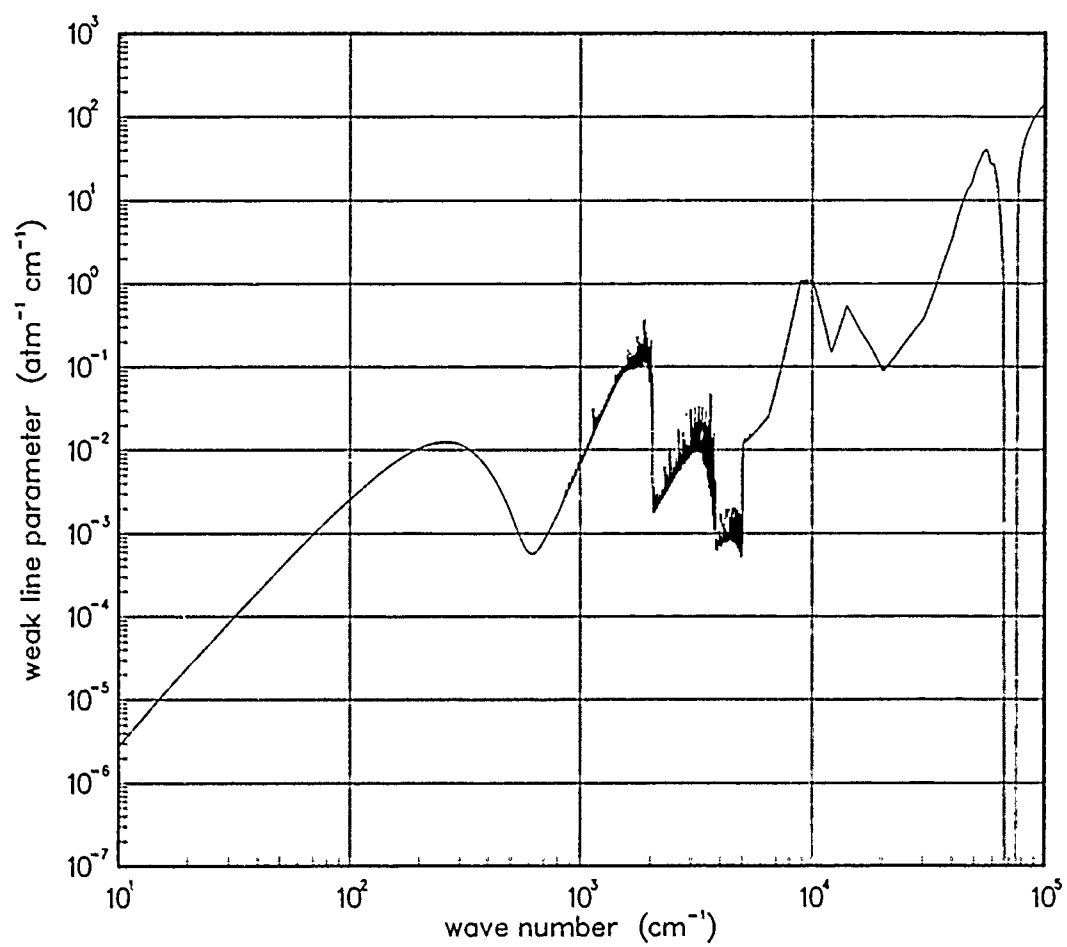


Figure 84. Weak-line parameter for NO at 10000°K.

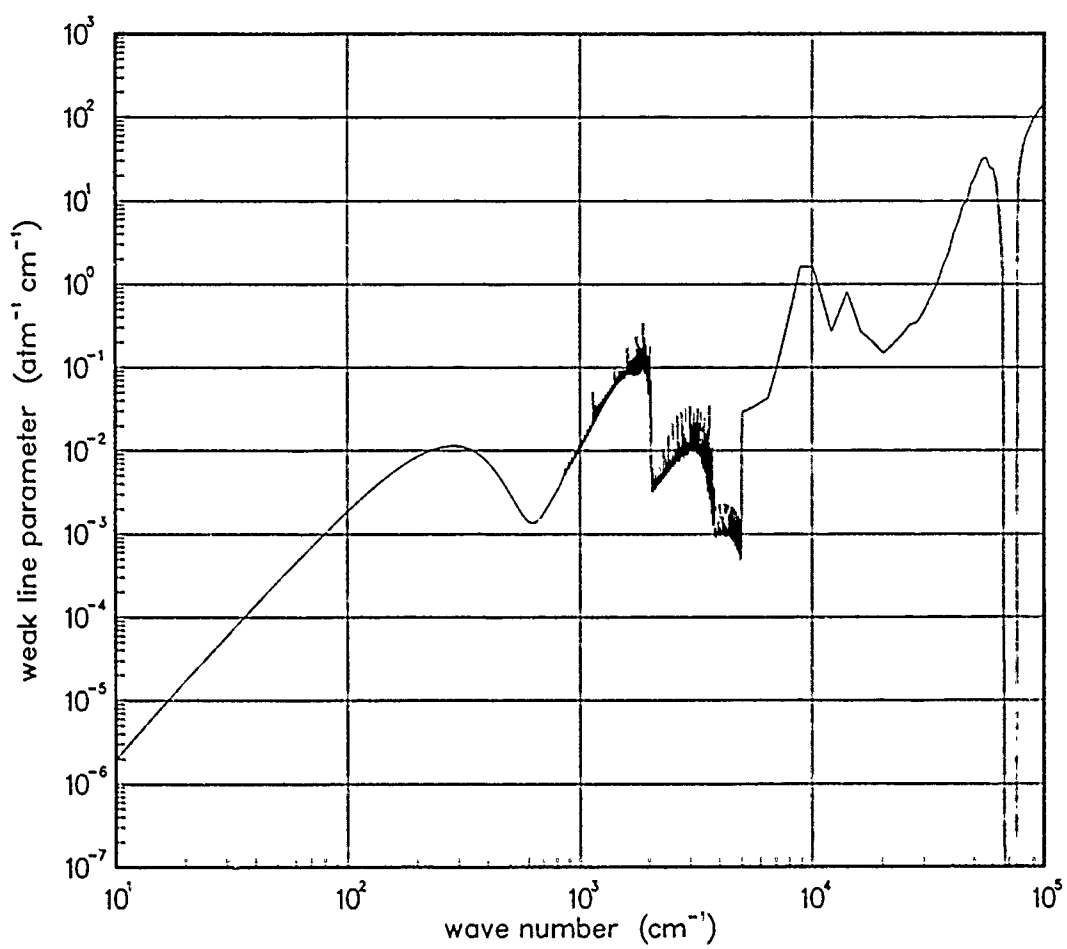


Figure 85. Weak-line parameter for NO at 12000°K.

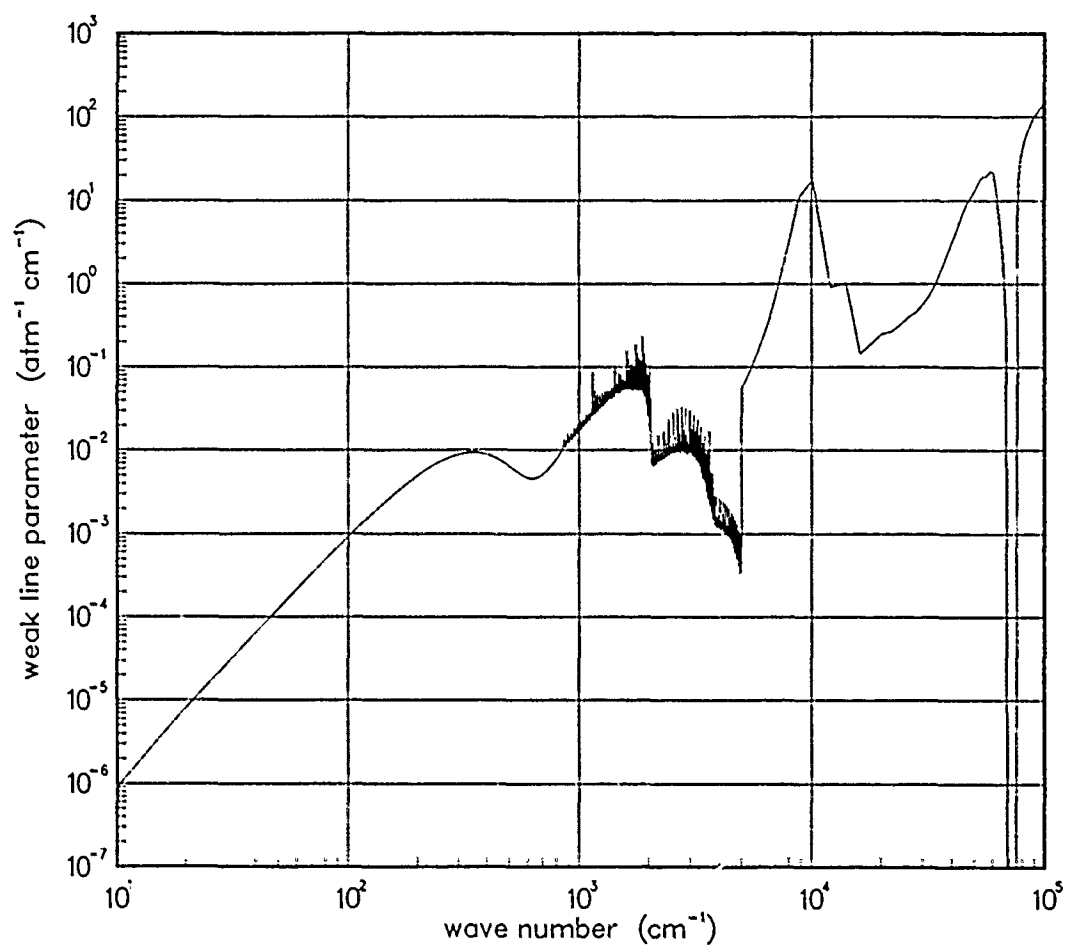


Figure 86. Weak-line parameter for NO at 18000°K.

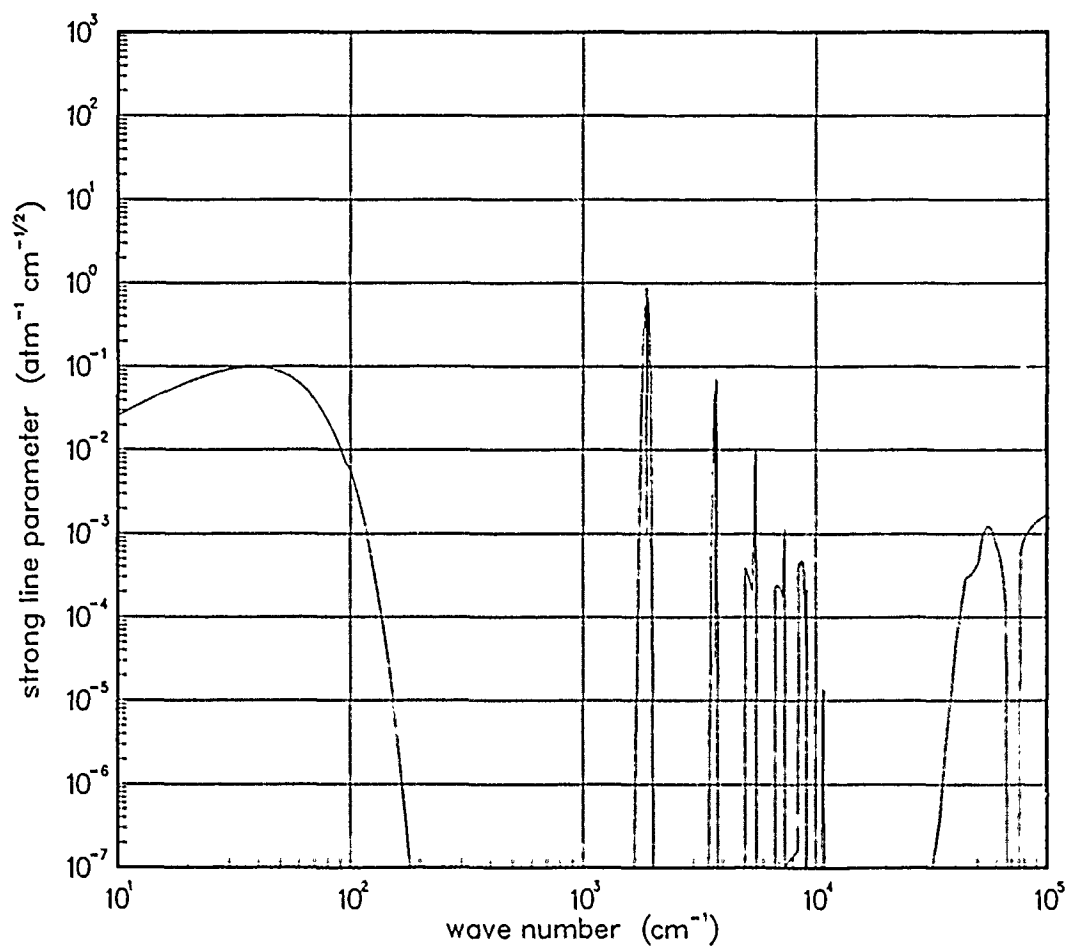


Figure 87. Strong-line parameter for NO at 200°K.

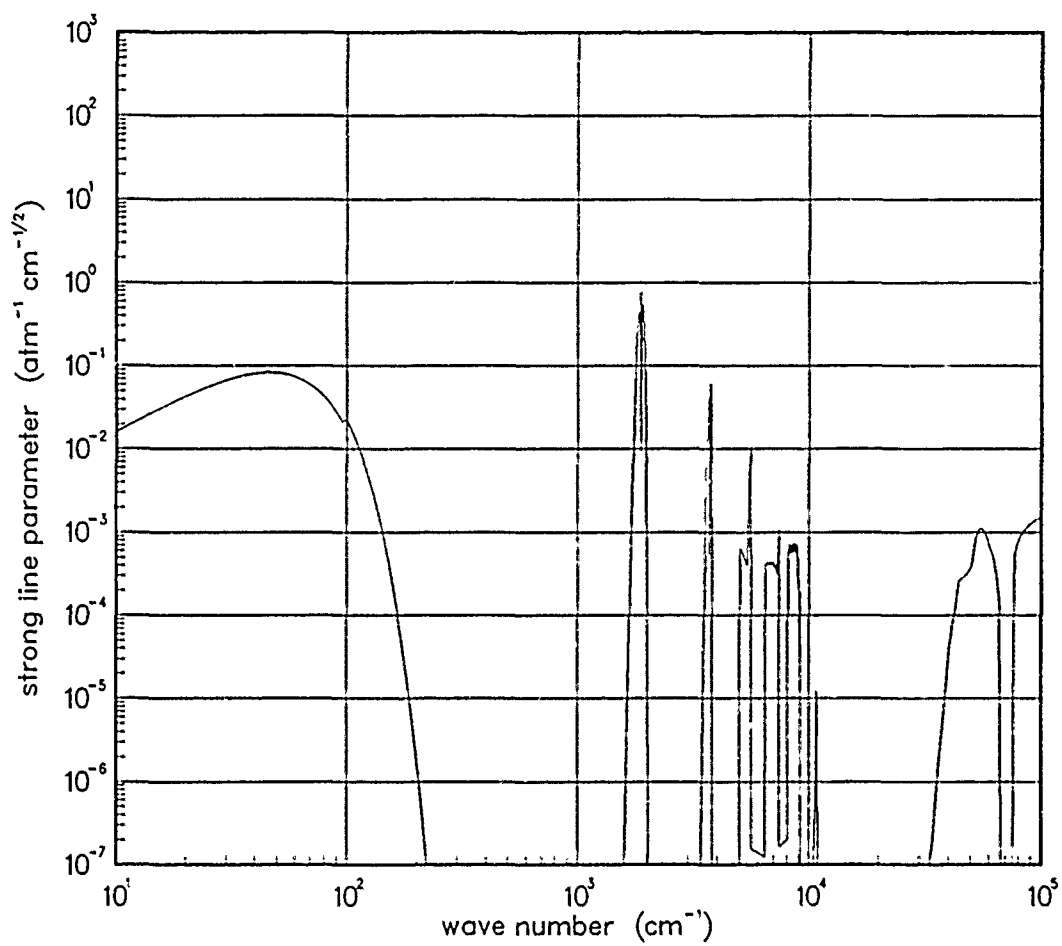


Figure 88. Strong-line parameter for NO at 300°K.

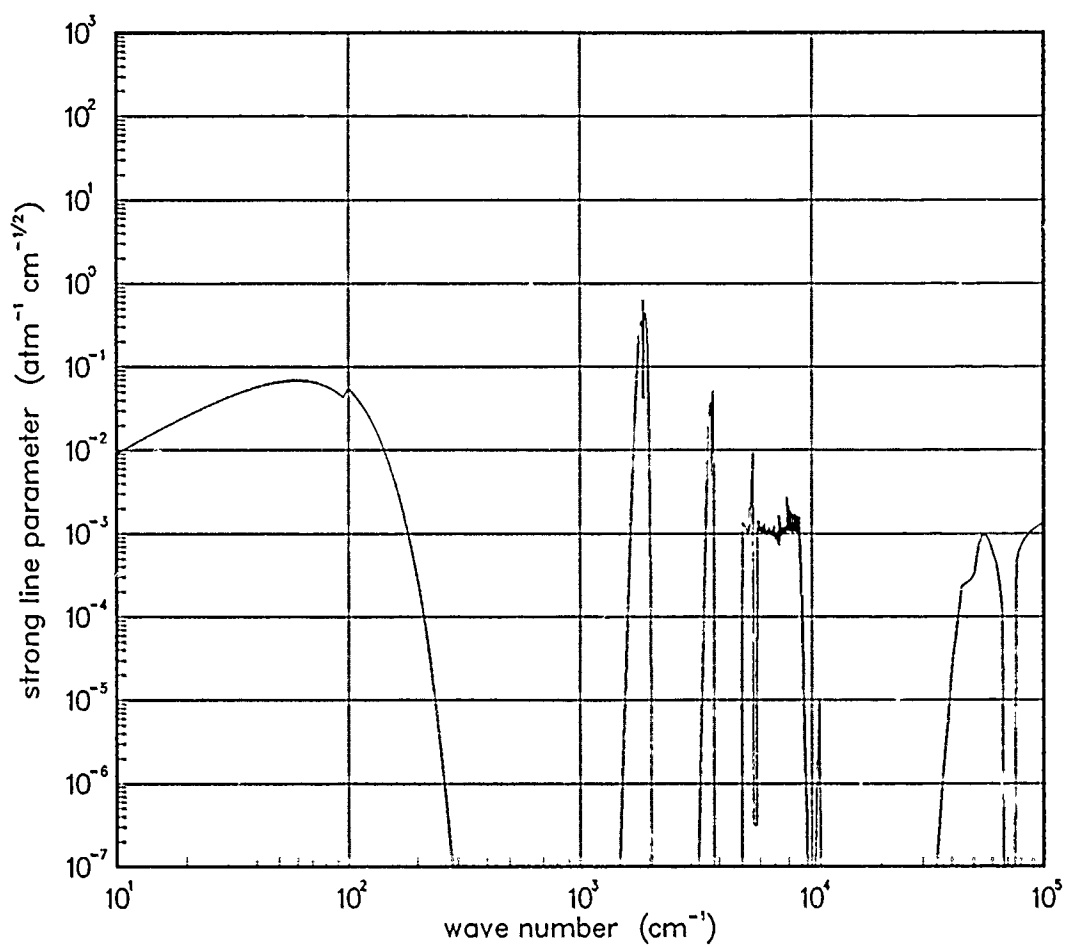


Figure 89. Strong-line parameter for NO at 500°K.

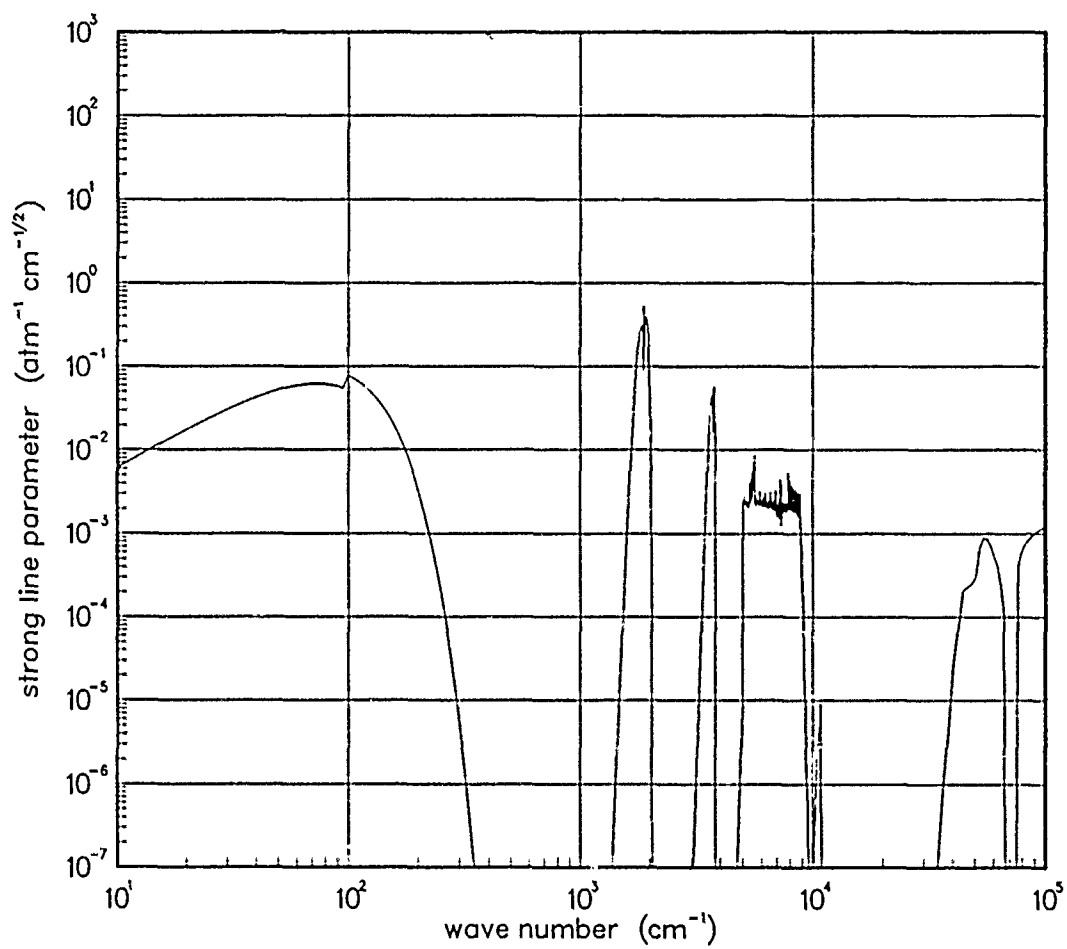


Figure 90. Strong-line parameter for NO at 750°K.

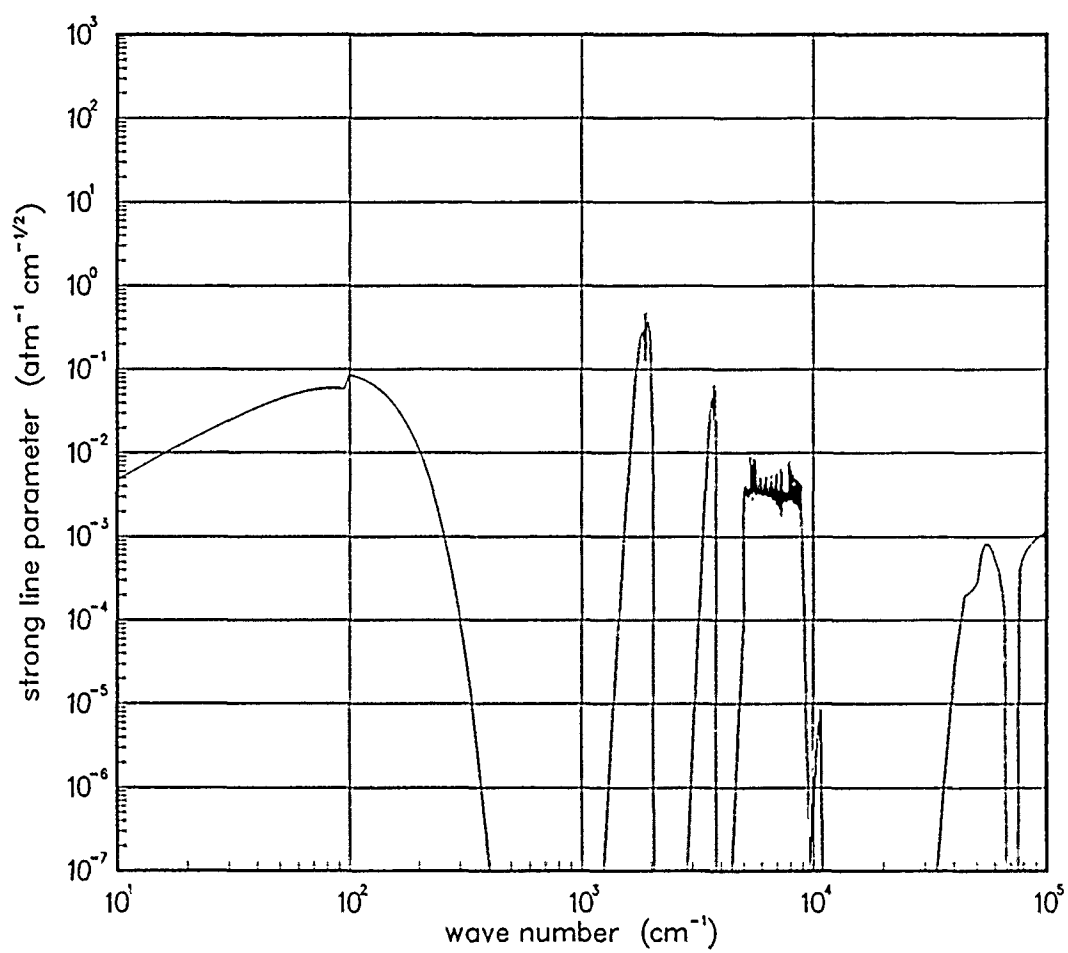


Figure 91. Strong-line parameter for NO at 1000°K.

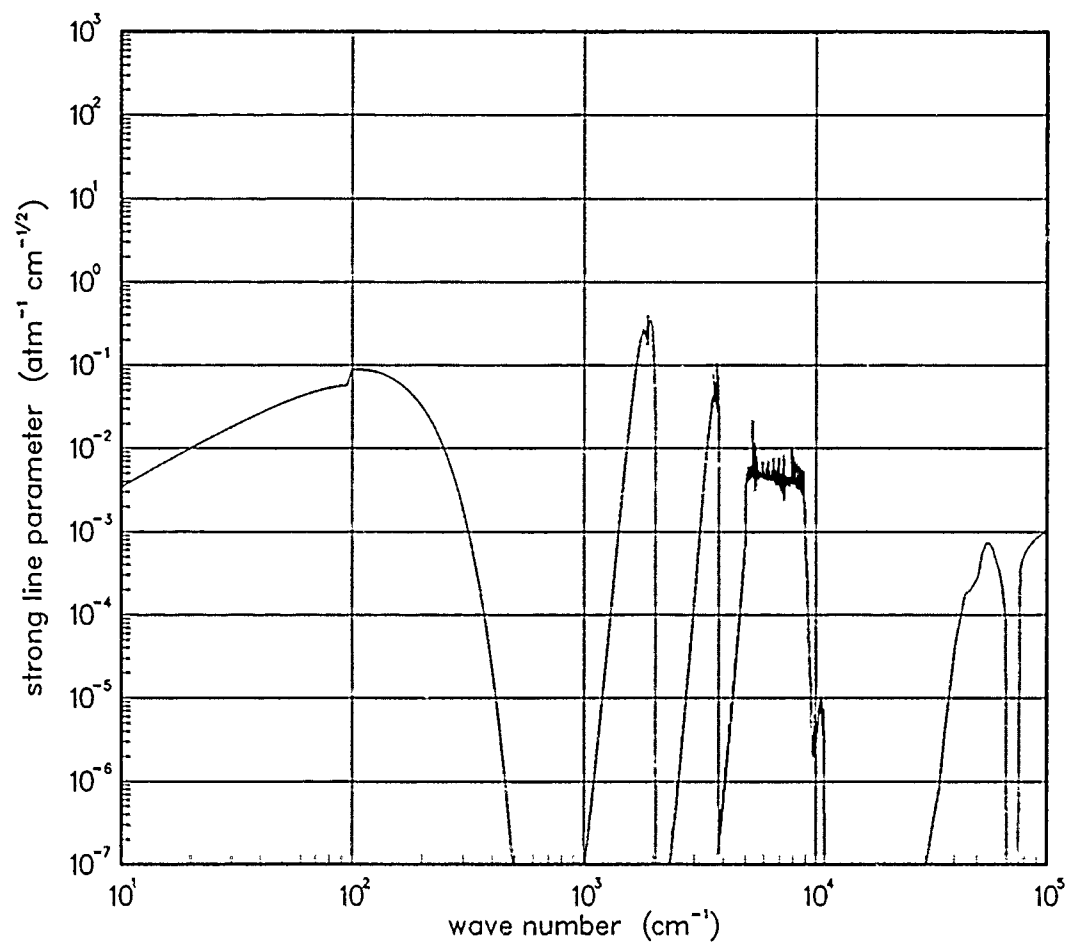


Figure 92. Strong-line parameter for NO at 1500°K.

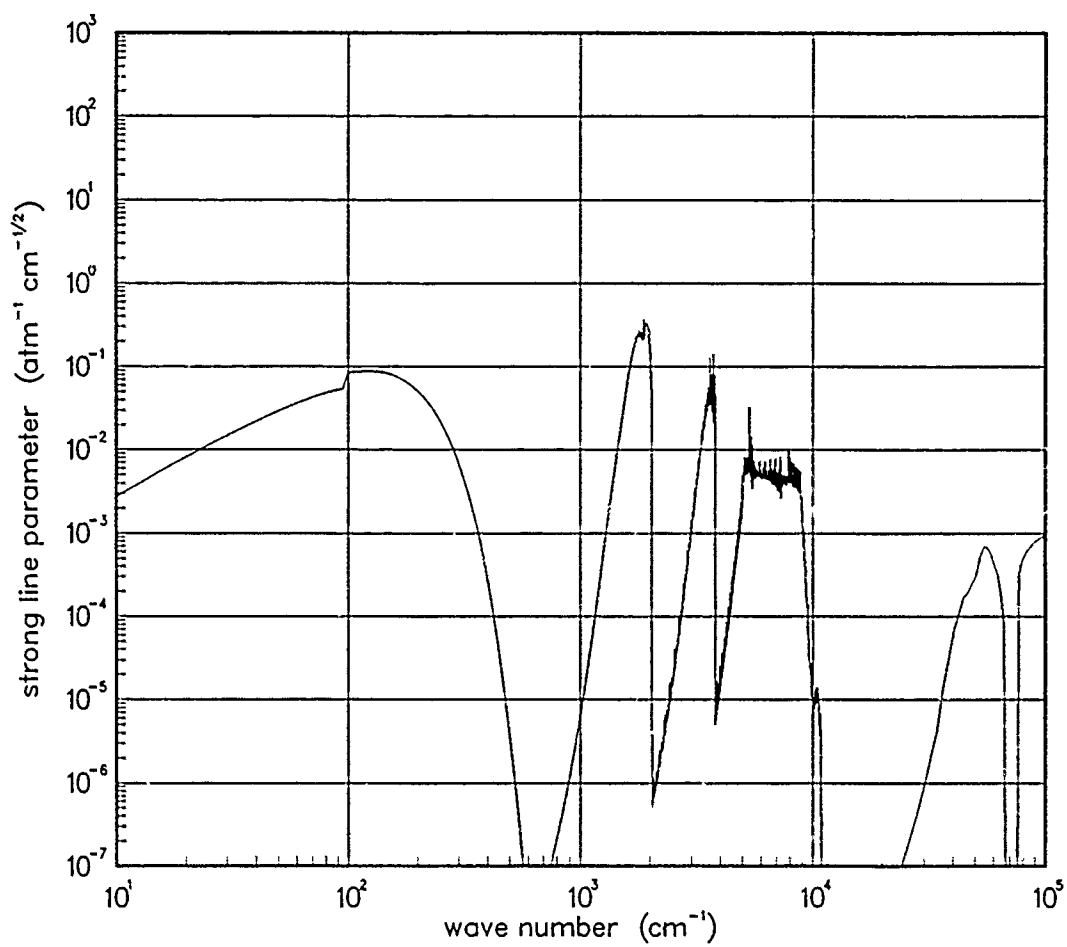


Figure 93. Strong-line parameter for NO at 2000°K.

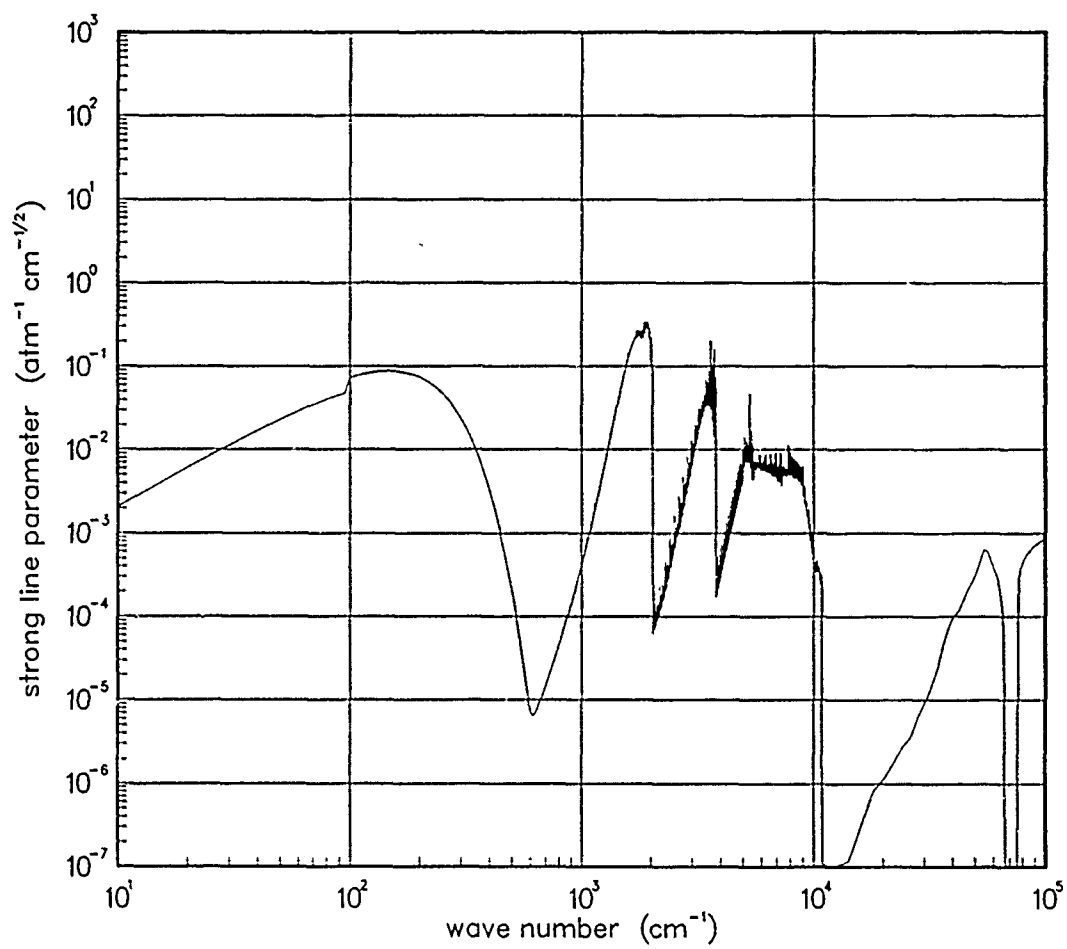


Figure 94. Strong-line parameter for NO at 3000°K.

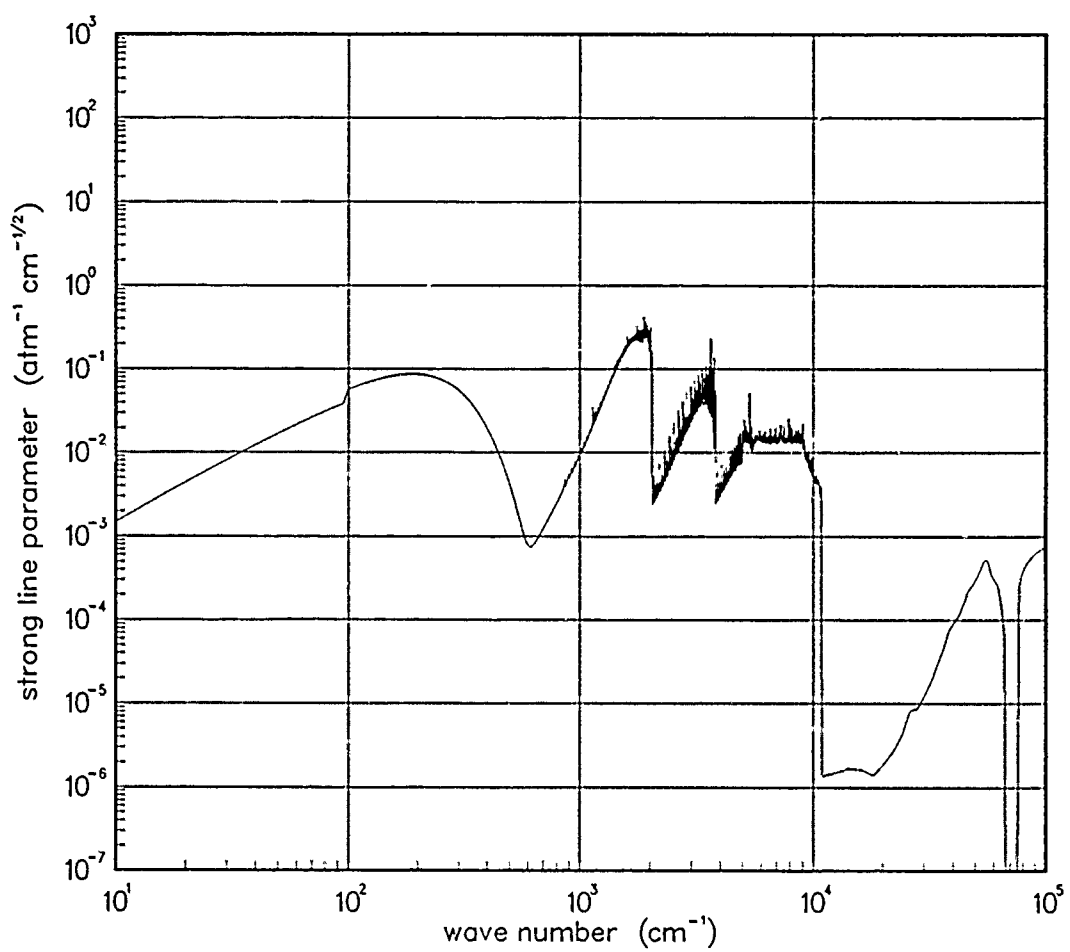


Figure 95. Strong-line parameter for NO at 5000°K.

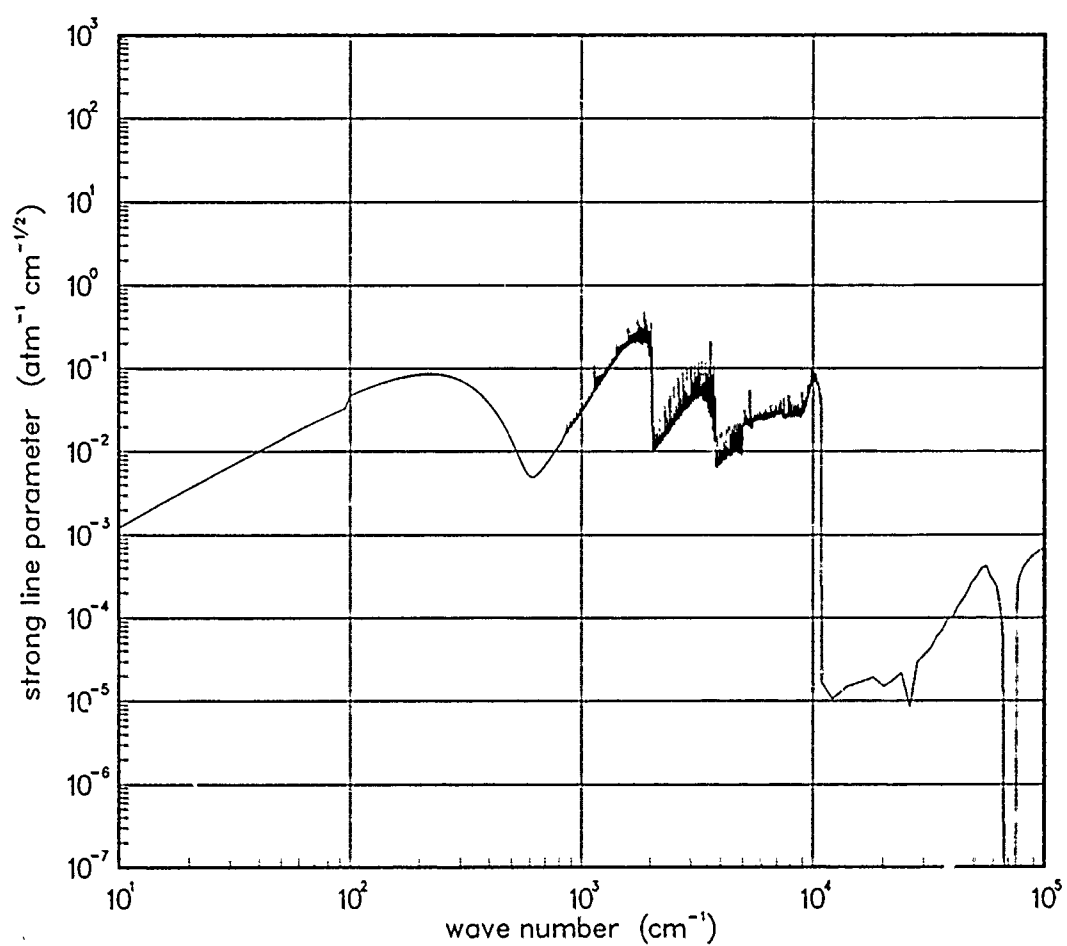


Figure 96. Strong-line parameter for NO at 7000°K.

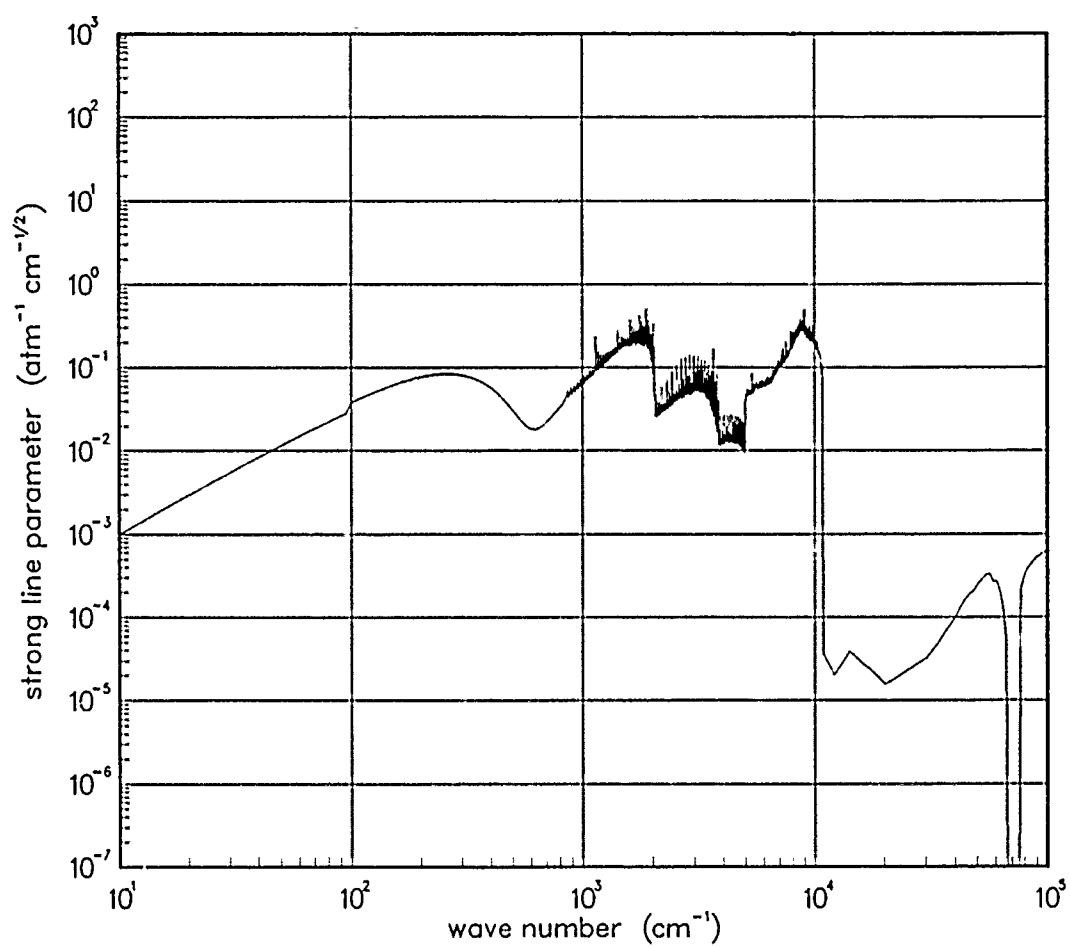


Figure 97. Strong-line parameter for NO at 10000°K.

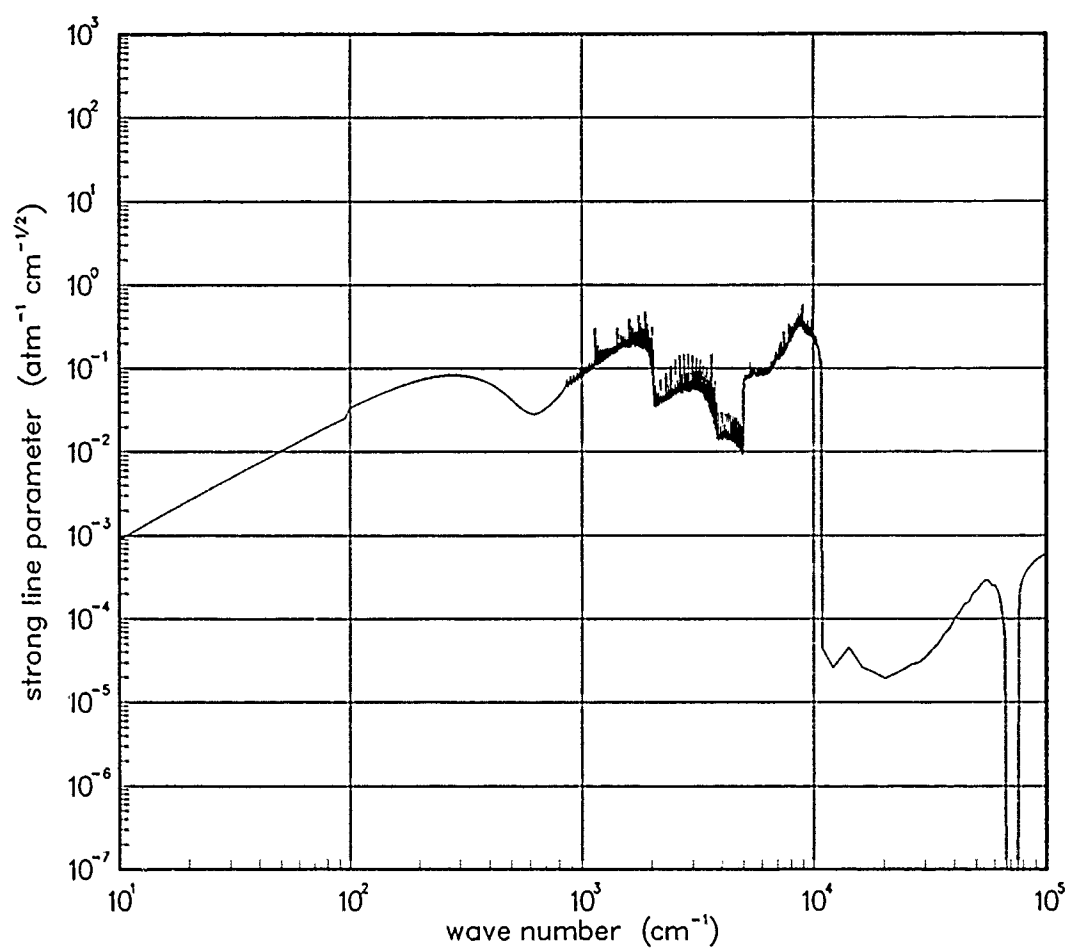


Figure 98. Strong-line parameter for NO at 12000°K.

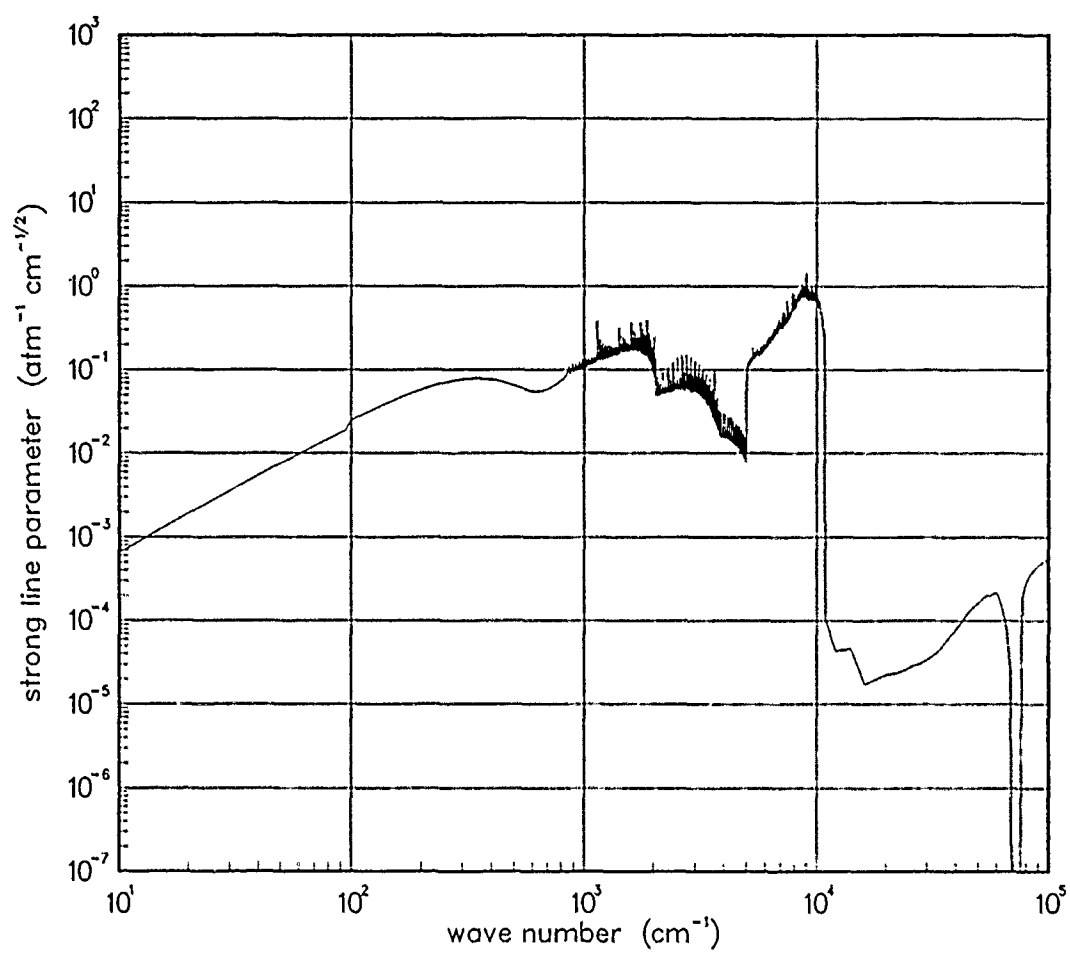


Figure 99. Strong-line parameter for NO at 18000°K.

Table 4. Spectroscopic data for NO⁺.

X ¹Σ⁺

$$\begin{array}{ll} \omega_e = 2377.1^* & \omega_e x_e = 16.35^* \\ \alpha_e = 0.0202^* & B_e = 2.002^* \end{array}$$

$$S_{10} = 70.83^\dagger$$

$$\gamma_t(300^\circ\text{K}) = 0.04^\ddagger$$

Data Source:

*E. Miescher, Helv. Phys. Acta., 29, 135, (1956).

†H.J. Werner, P. Rosmus, J. Mol. Spectrosc., 96, 362, (1982).

‡Estimate.

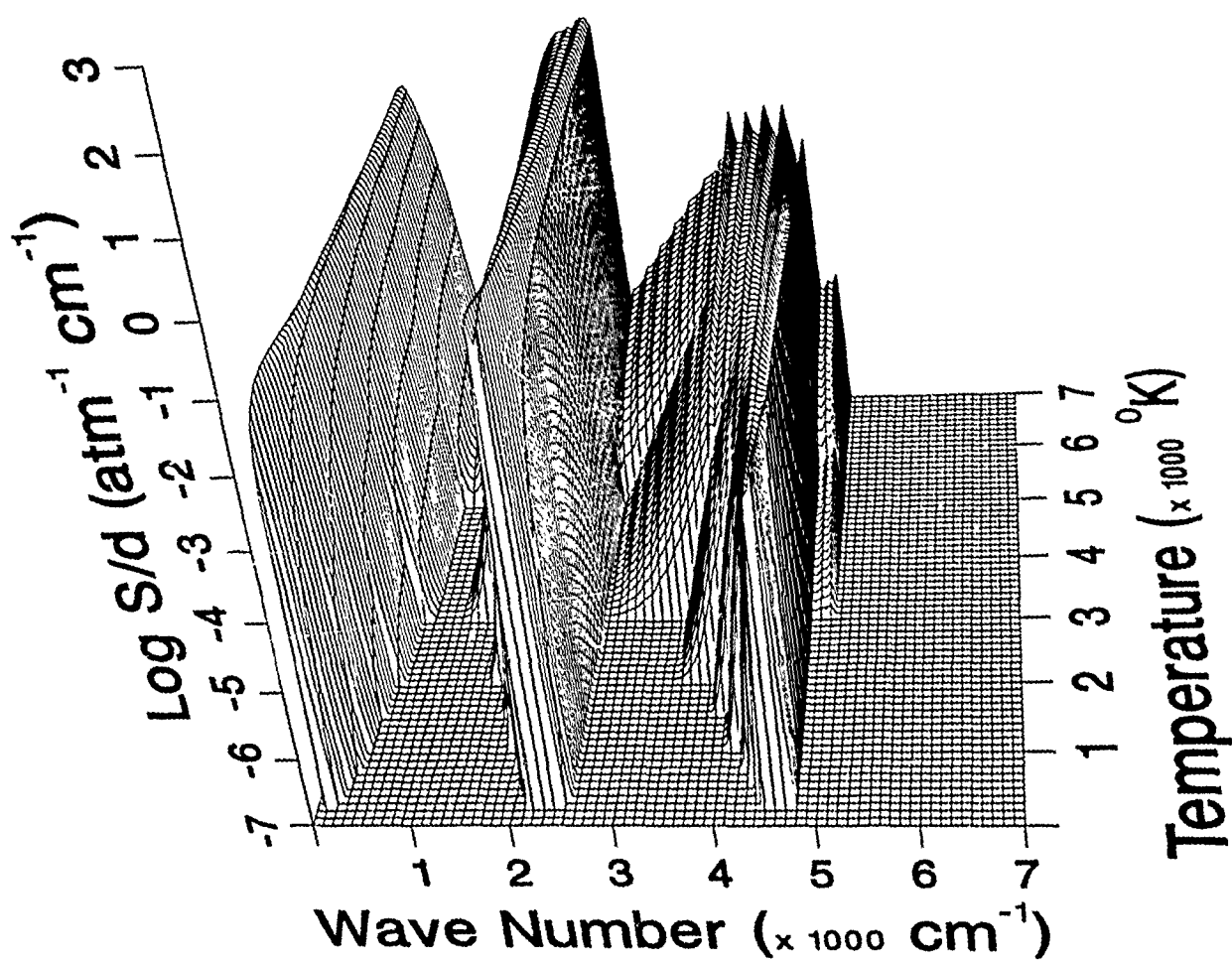


Figure 100. Weak-line parameter for NO^+ .

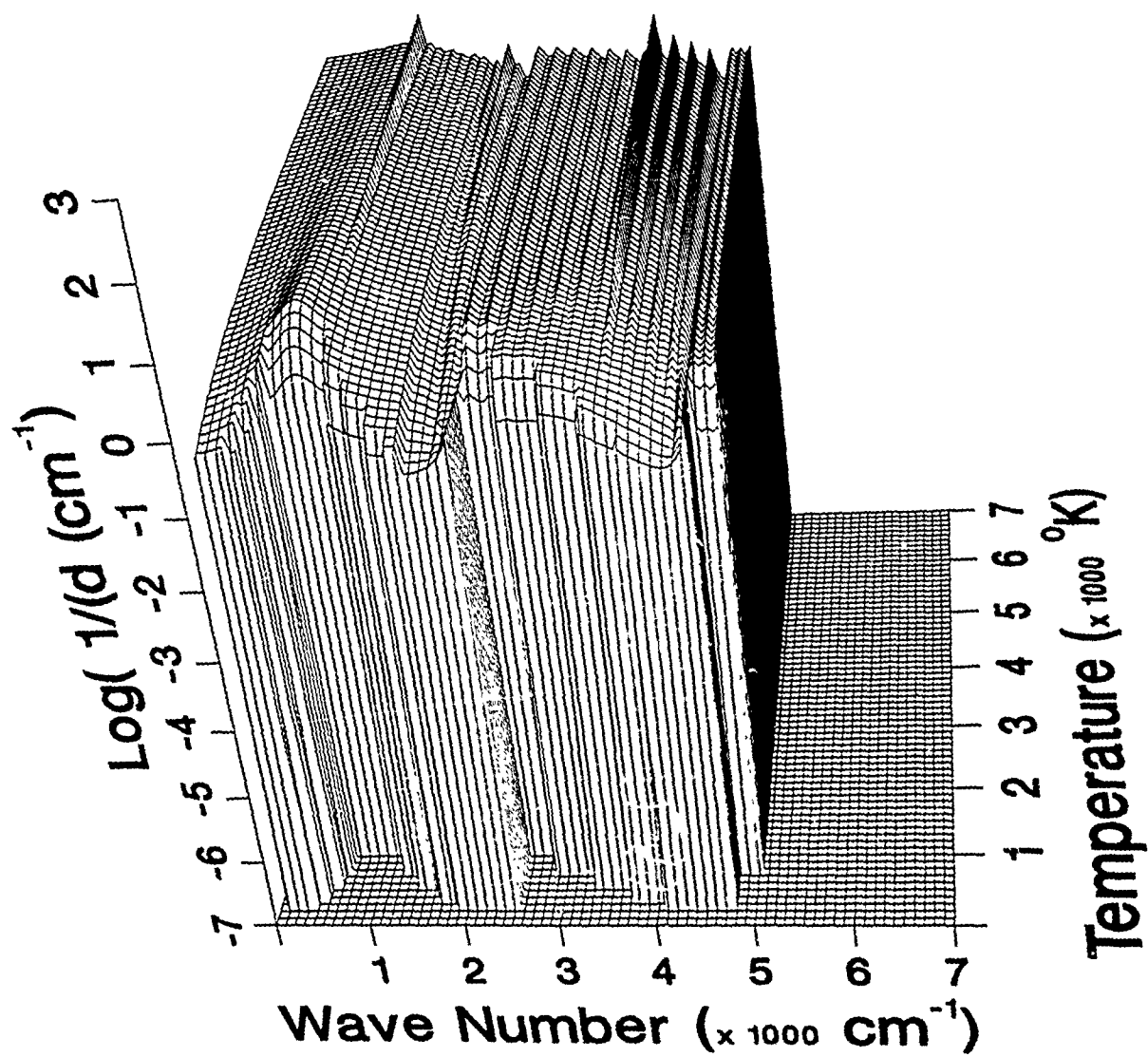


Figure 101. Inverse line spacing for NO^+ .

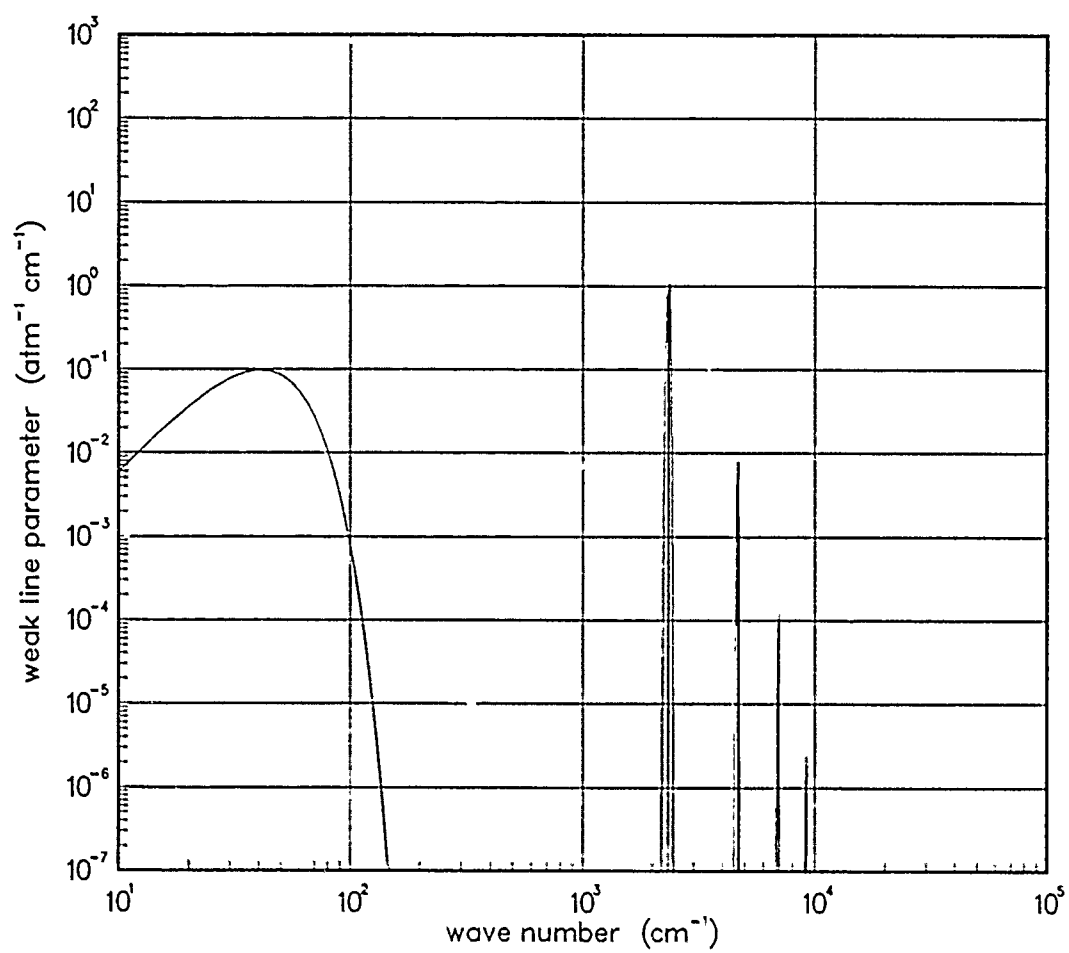


Figure 102. Weak-line parameter for NO⁺ at 200°K.

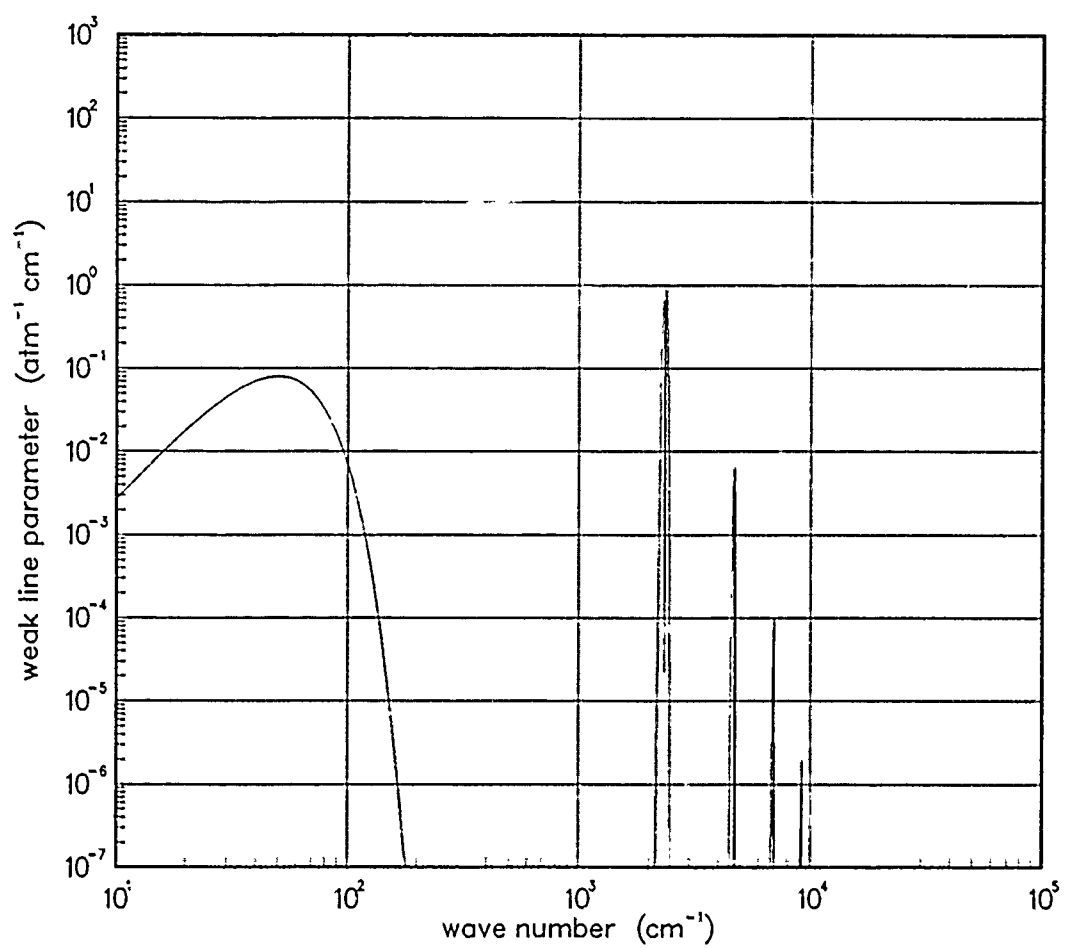


Figure 103. Weak-line parameter for NO⁺ at 300°K.

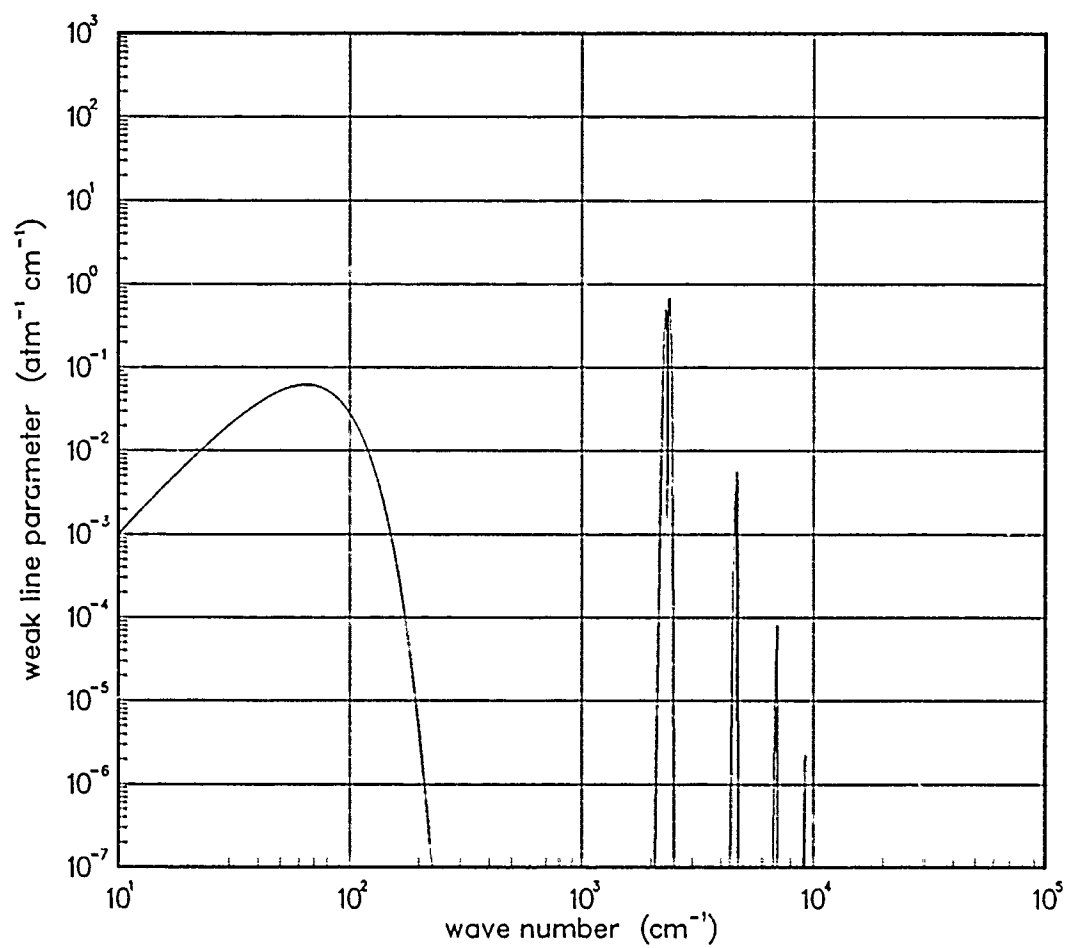


Figure 104. Weak-line parameter for NO⁺ at 500°K.

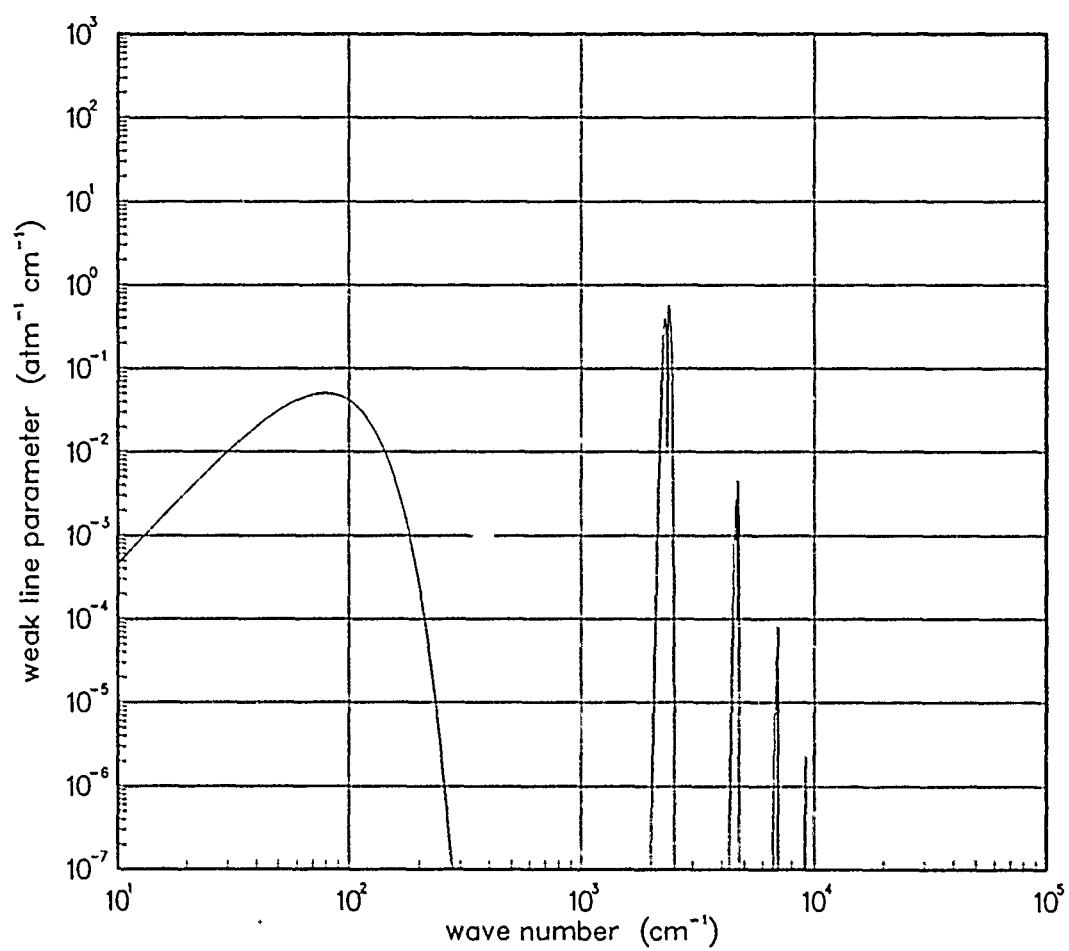


Figure 105. Weak-line parameter for NO⁺ at 750°K.

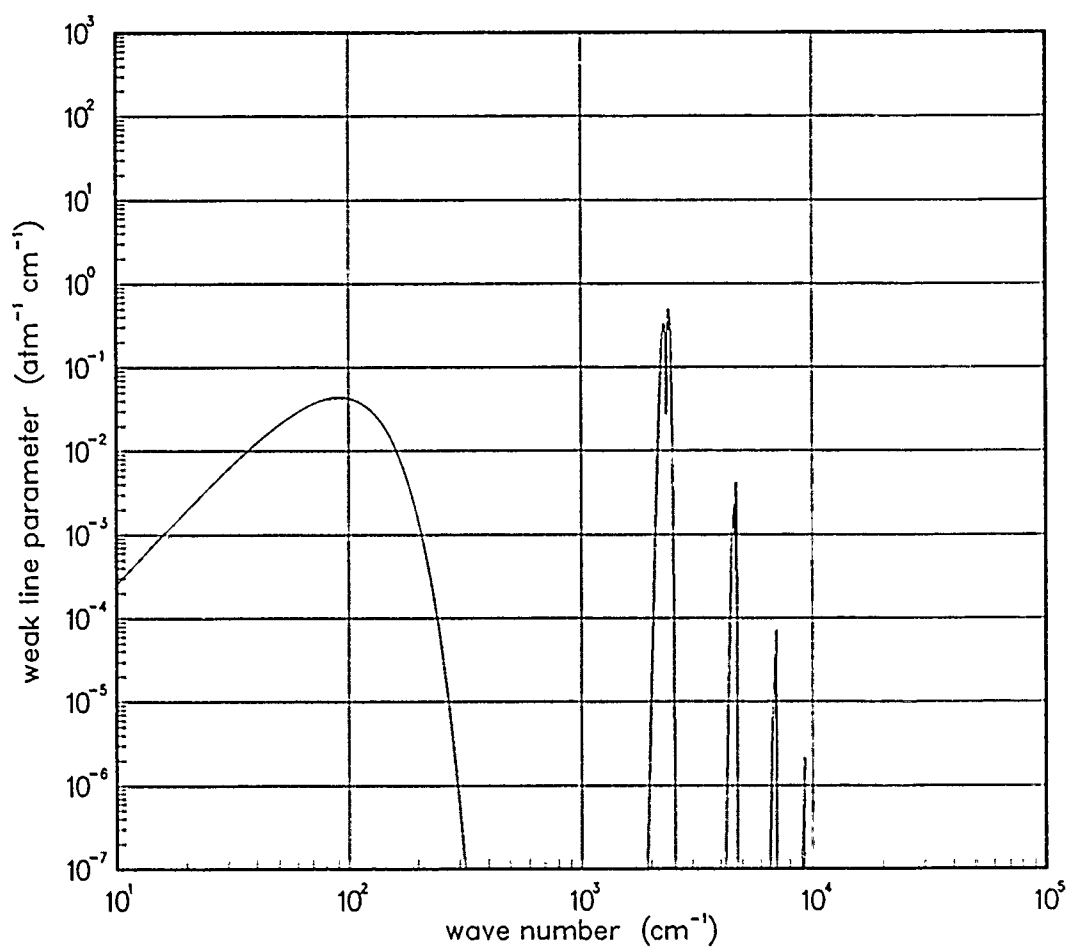


Figure 106. Weak-line parameter for NO⁺ at 1000°K.

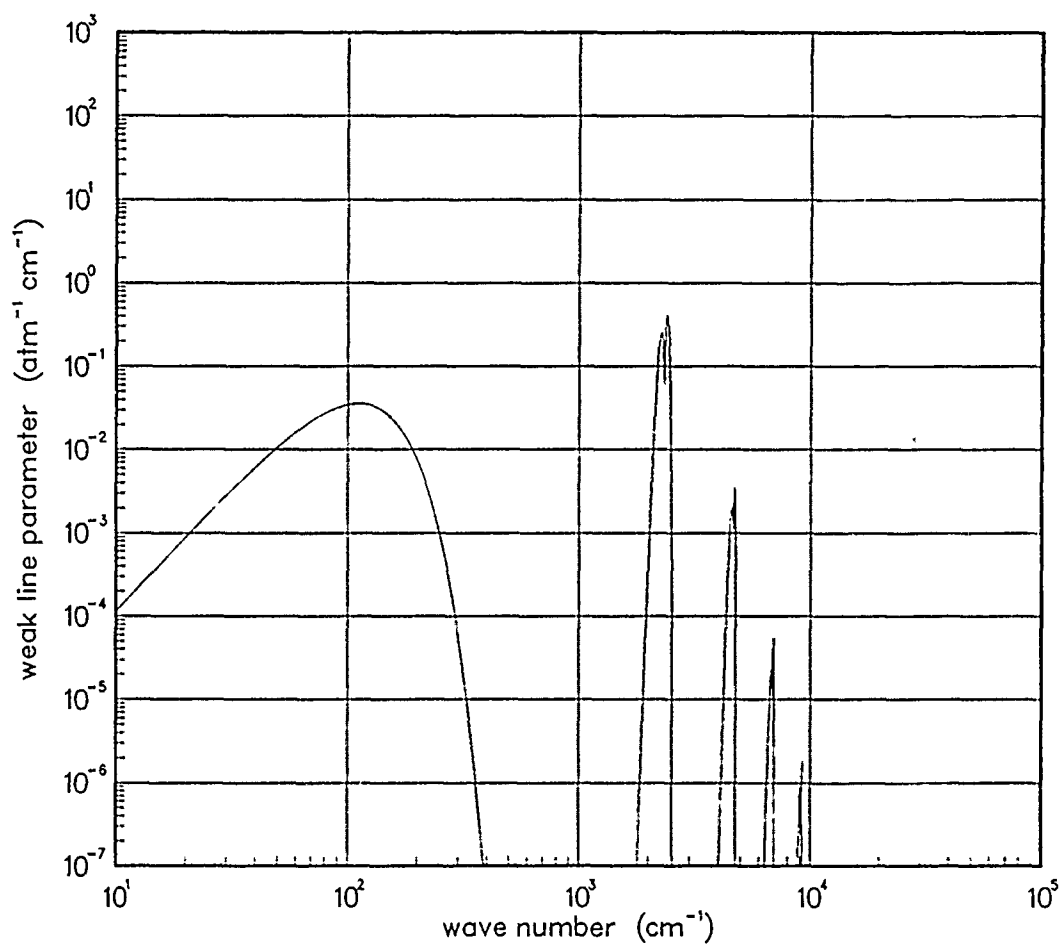


Figure 107. Weak-line parameter for NO⁺ at 1500°K.

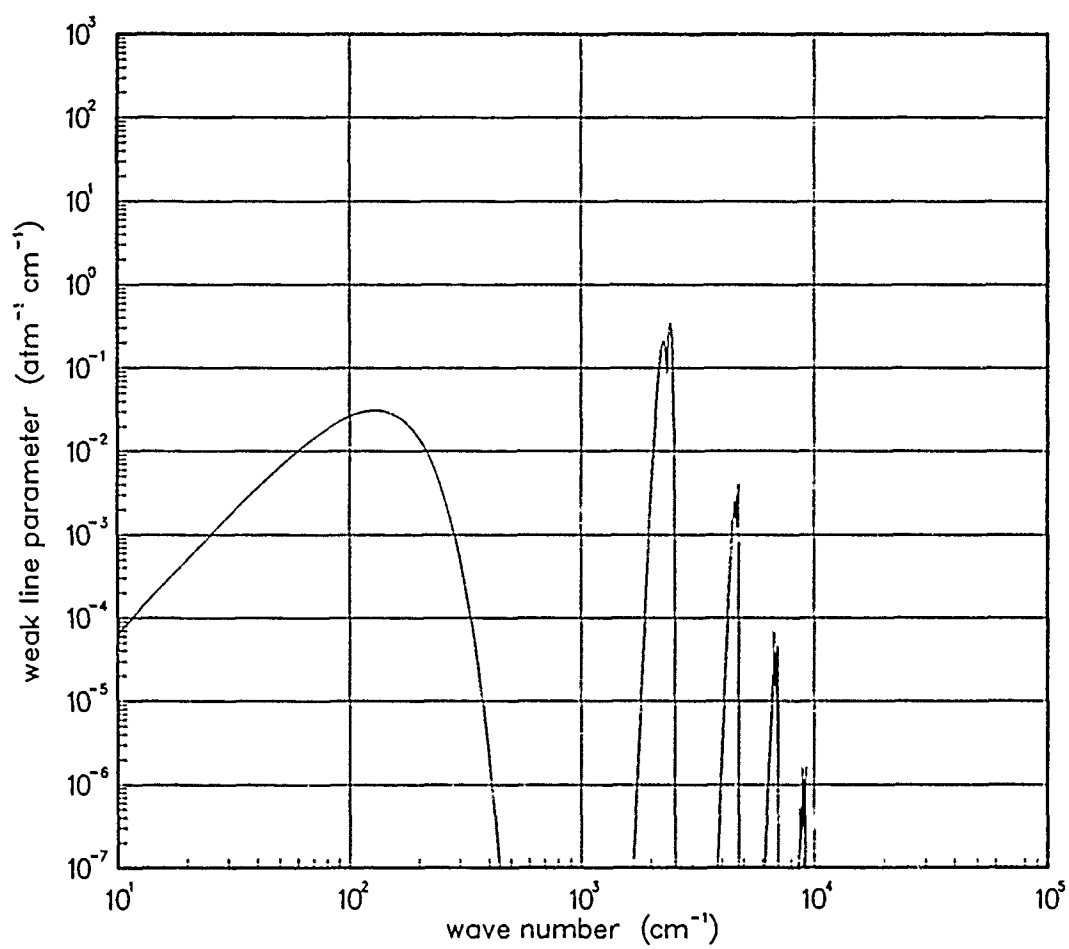


Figure 108. Weak-line parameter for NO⁺ at 2000°K.

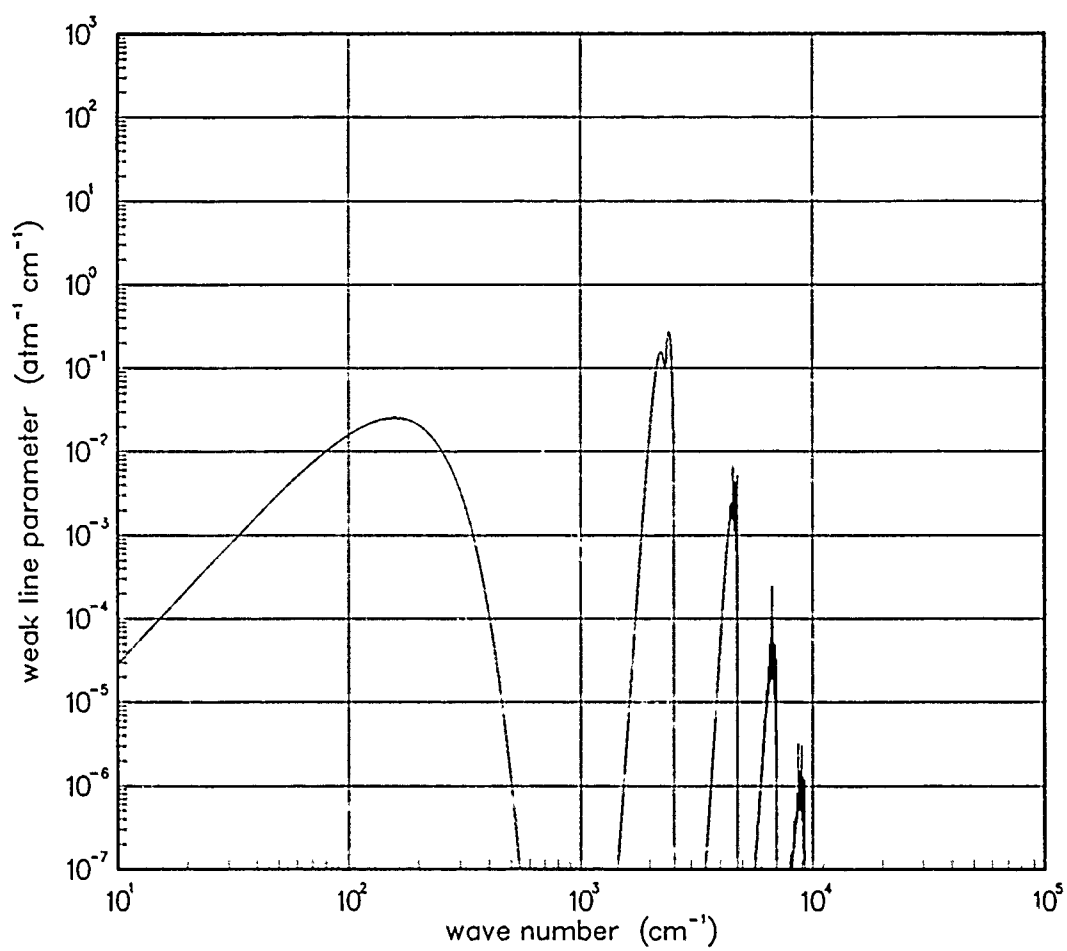


Figure 109. Weak-line parameter for NO⁺ at 3000°K.

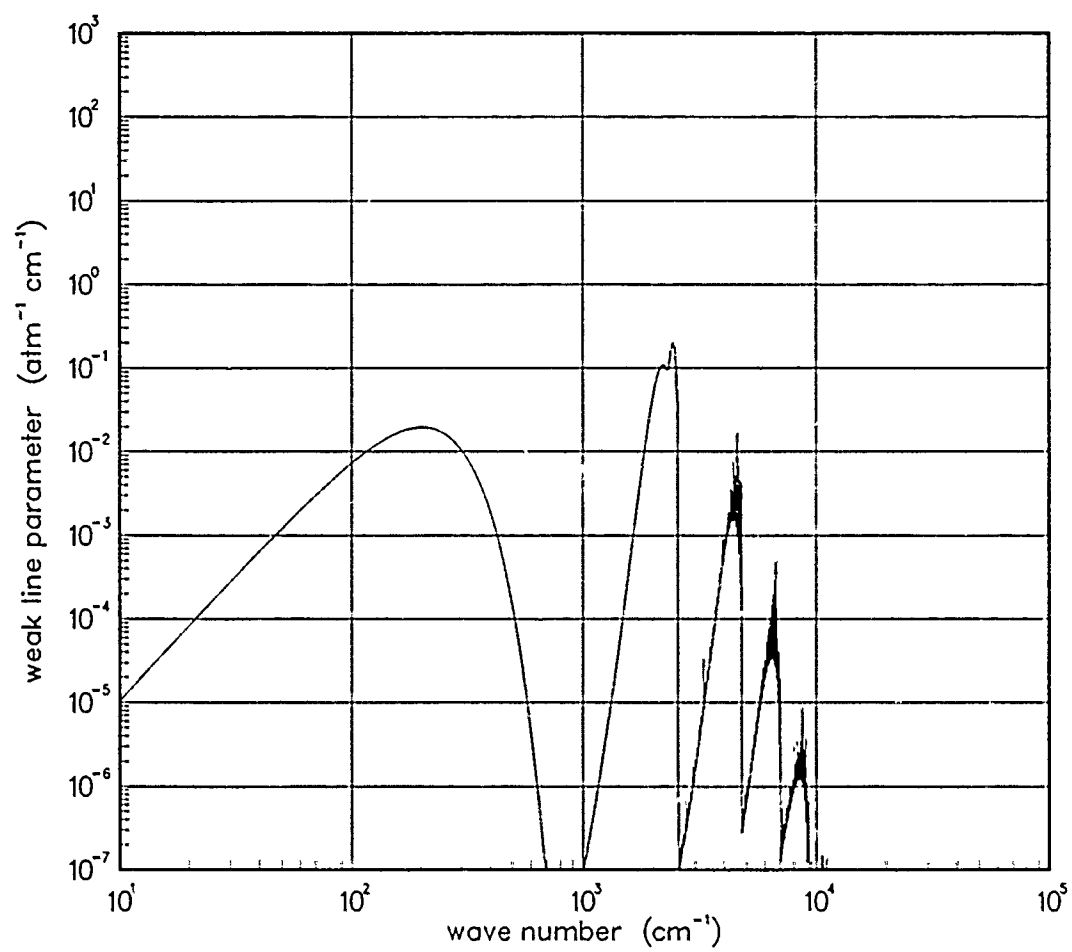


Figure 110. Weak-line parameter for NO⁺ at 5000°K.

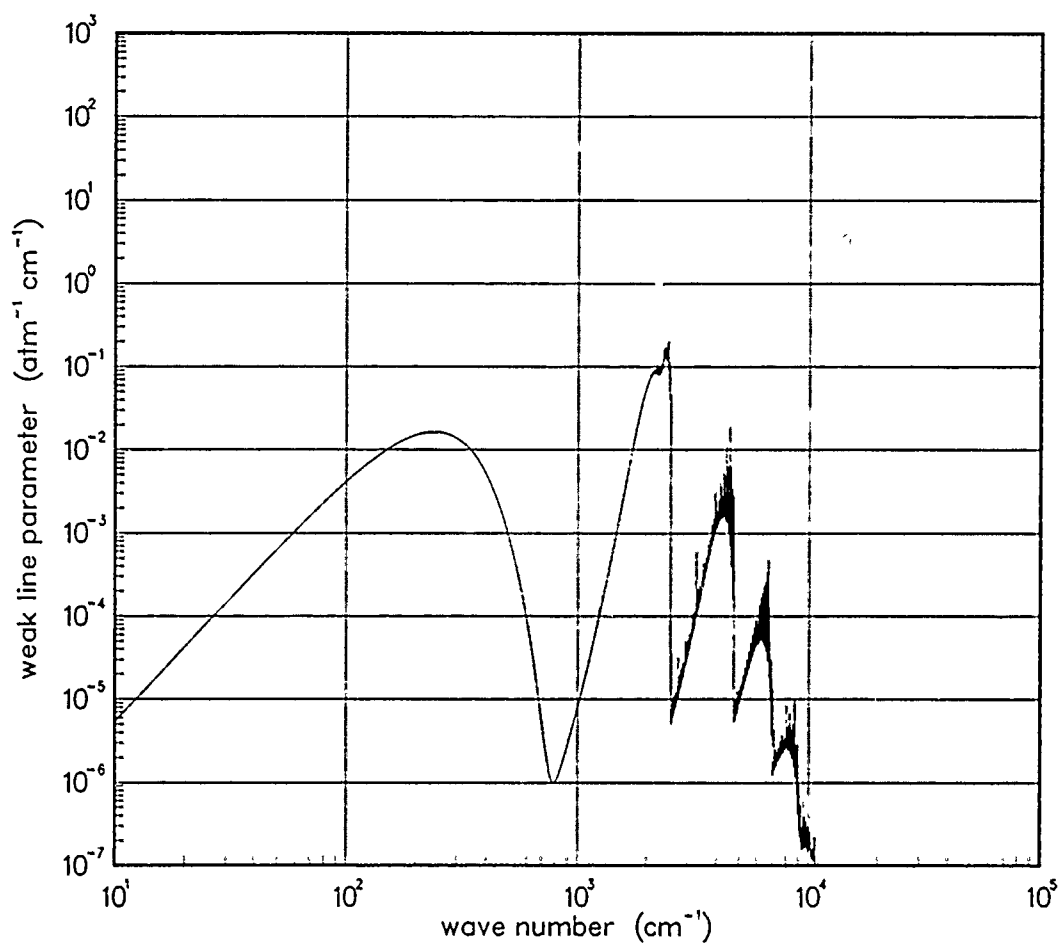


Figure 111. Weak-line parameter for NO⁺ at 7000°K.

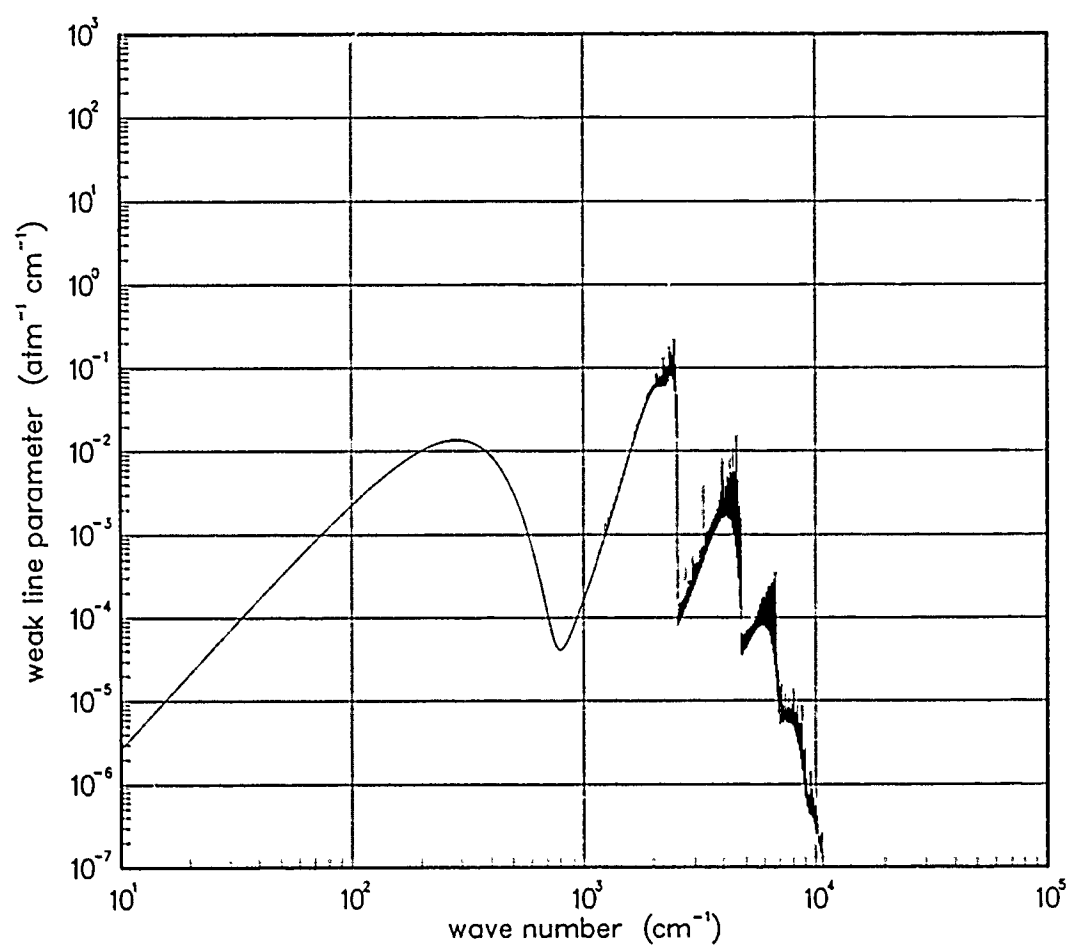


Figure 112. Weak-line parameter for NO^+ at 10000°K .

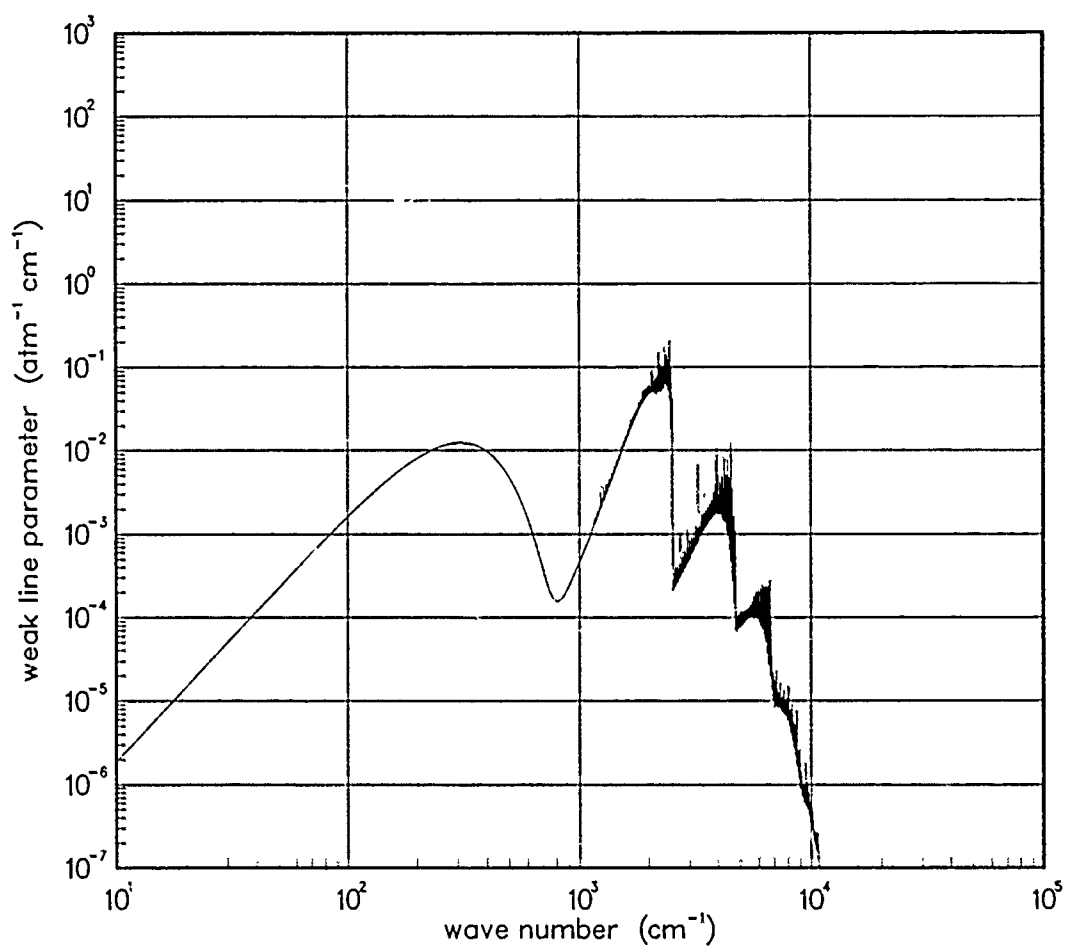


Figure 113. Weak-line parameter for NO⁺ at 12000°K.

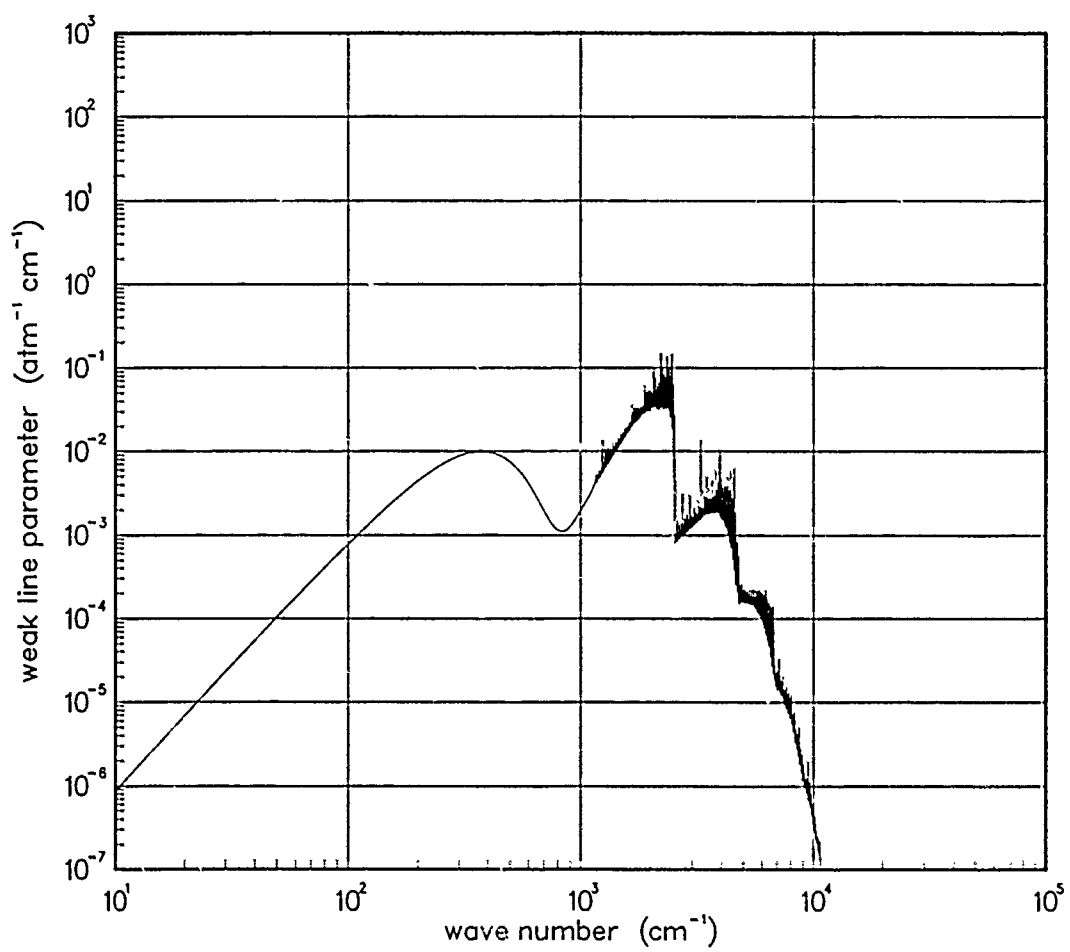


Figure 114. Weak-line parameter for NO⁺ at 18000°K.

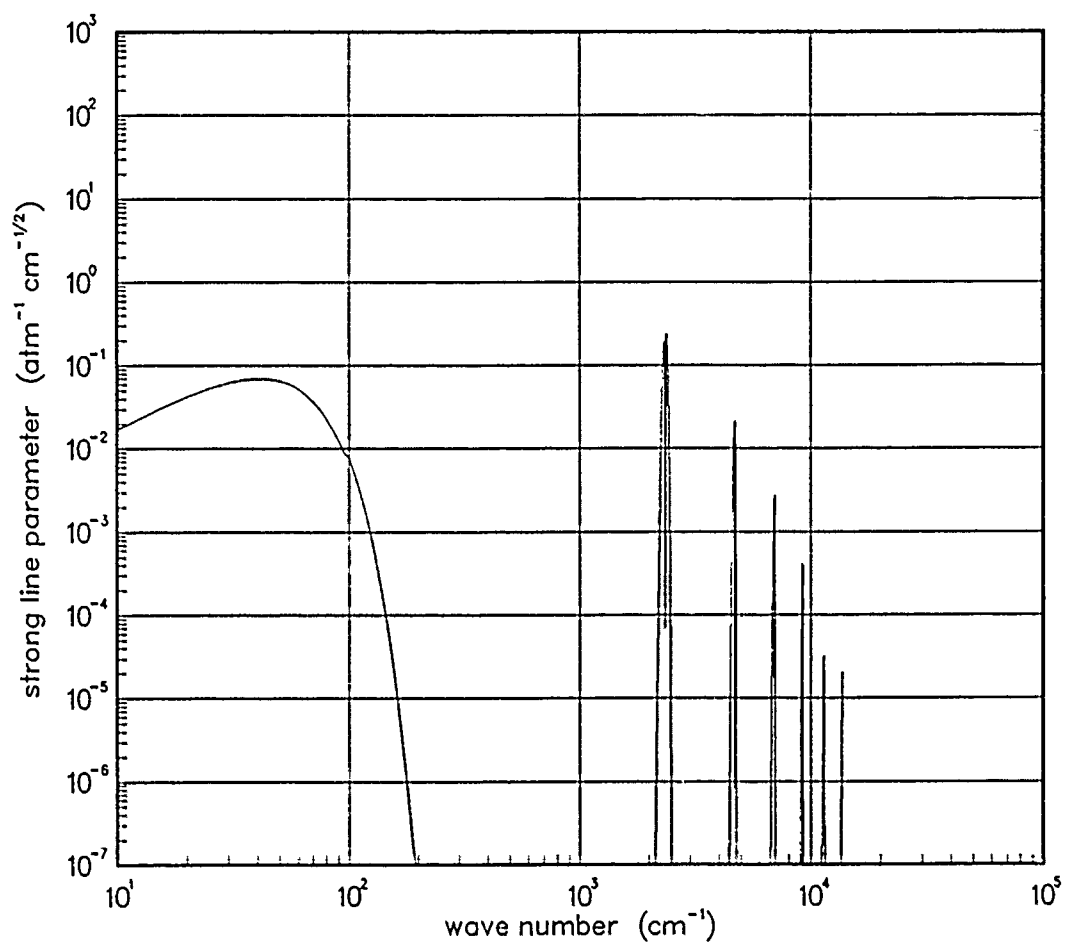


Figure 115. Strong-line parameter for NO⁺ at 200°K.

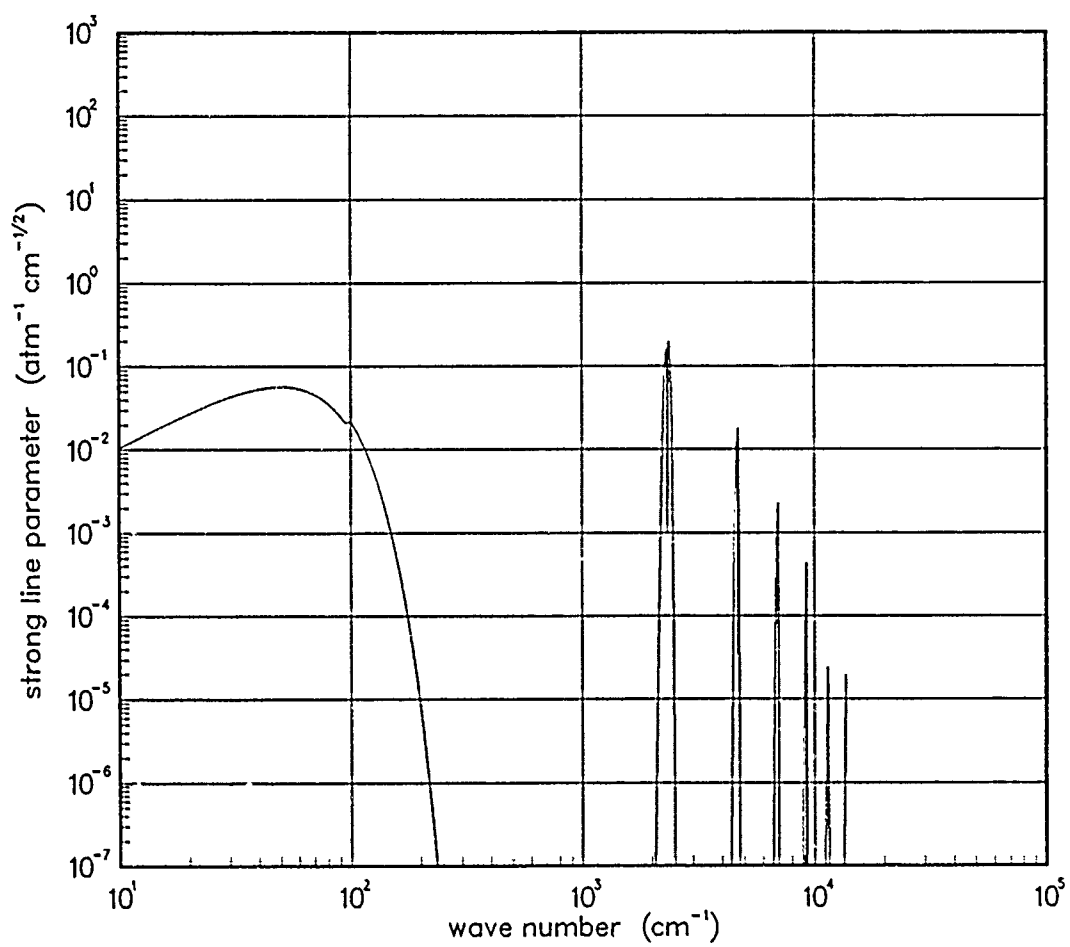


Figure 116. Strong-line parameter for NO⁺ at 300°K.

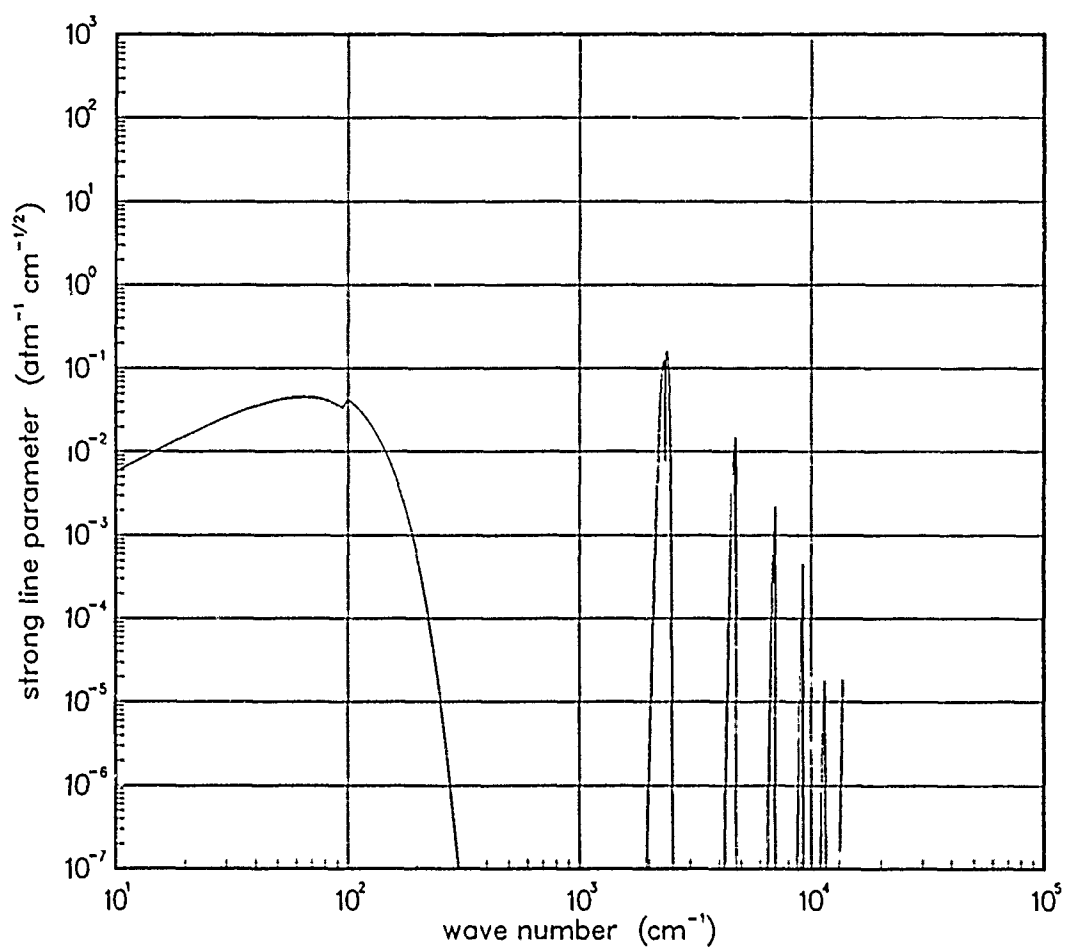


Figure 117. Strong-line parameter for NO⁺ at 500°K.

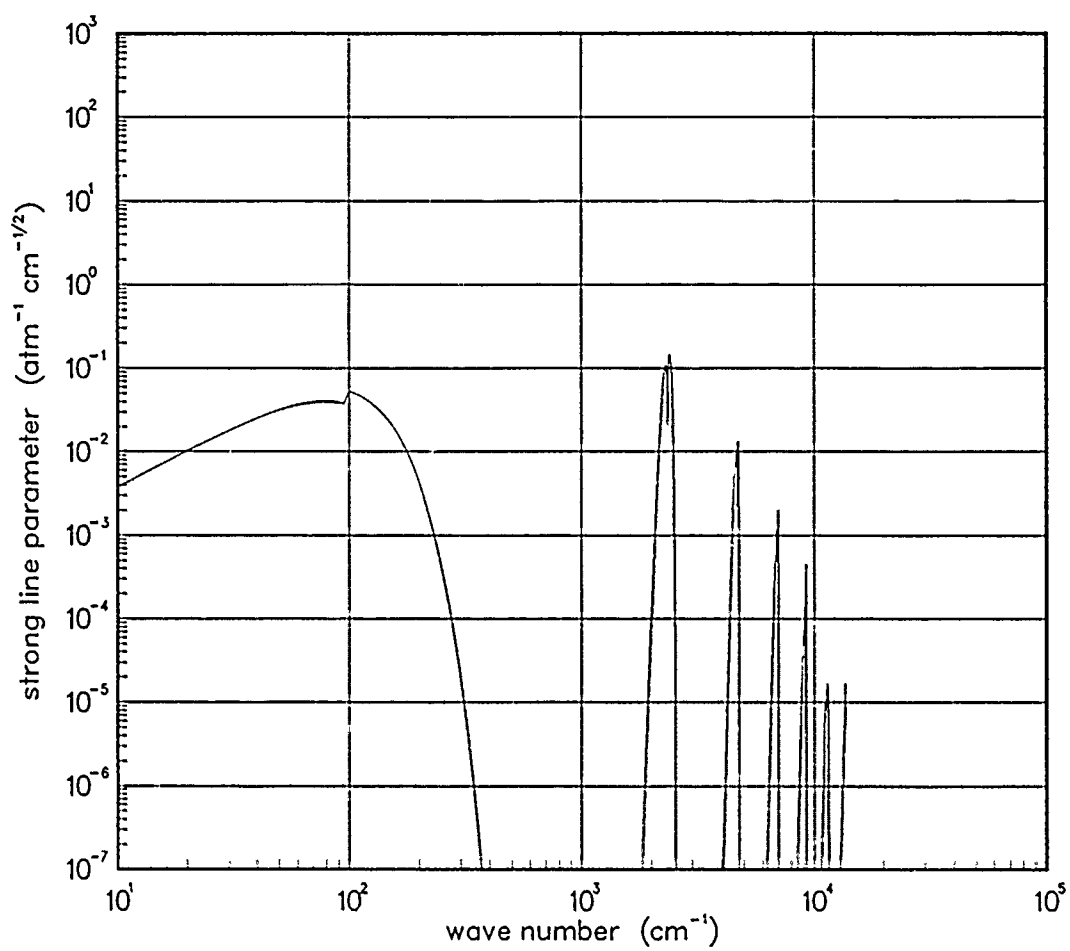


Figure 118. Strong-line parameter for NO⁺ at 750°K.

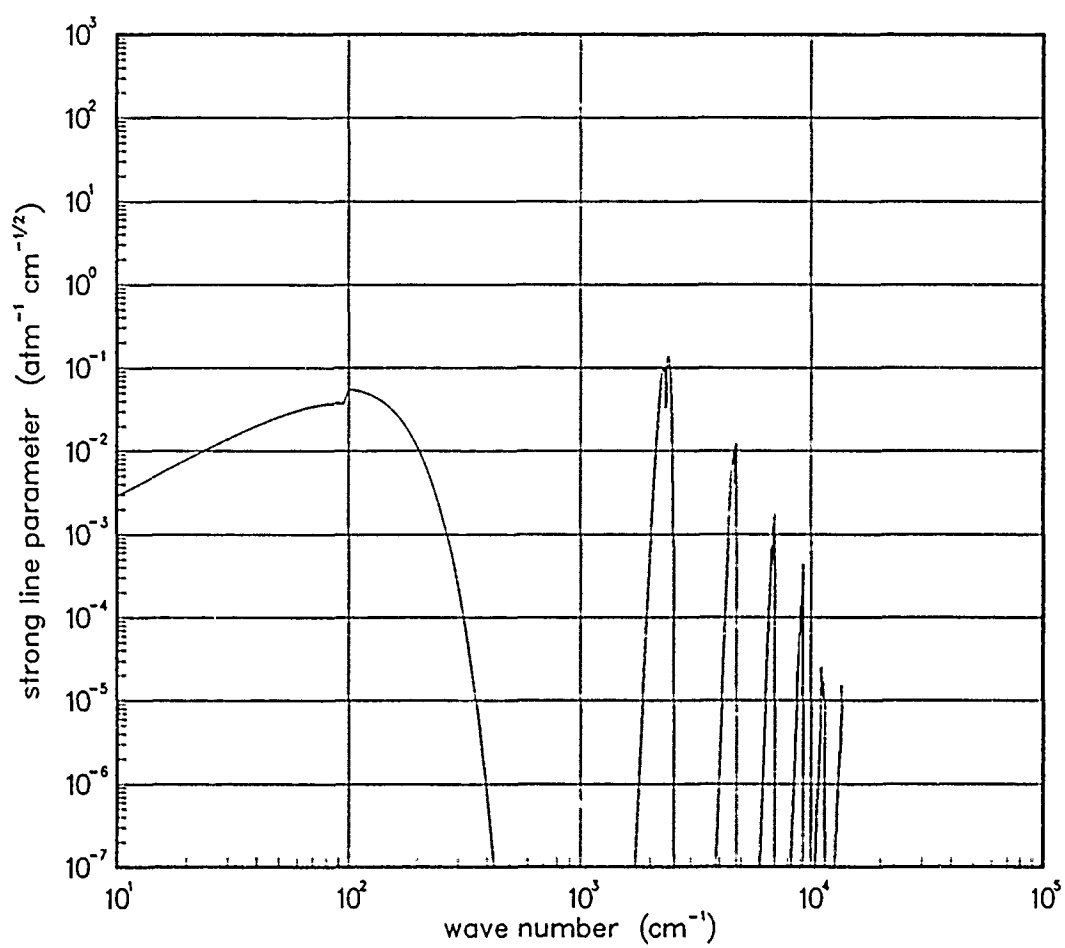


Figure 119. Strong-line parameter for NO⁺ at 1000°K.

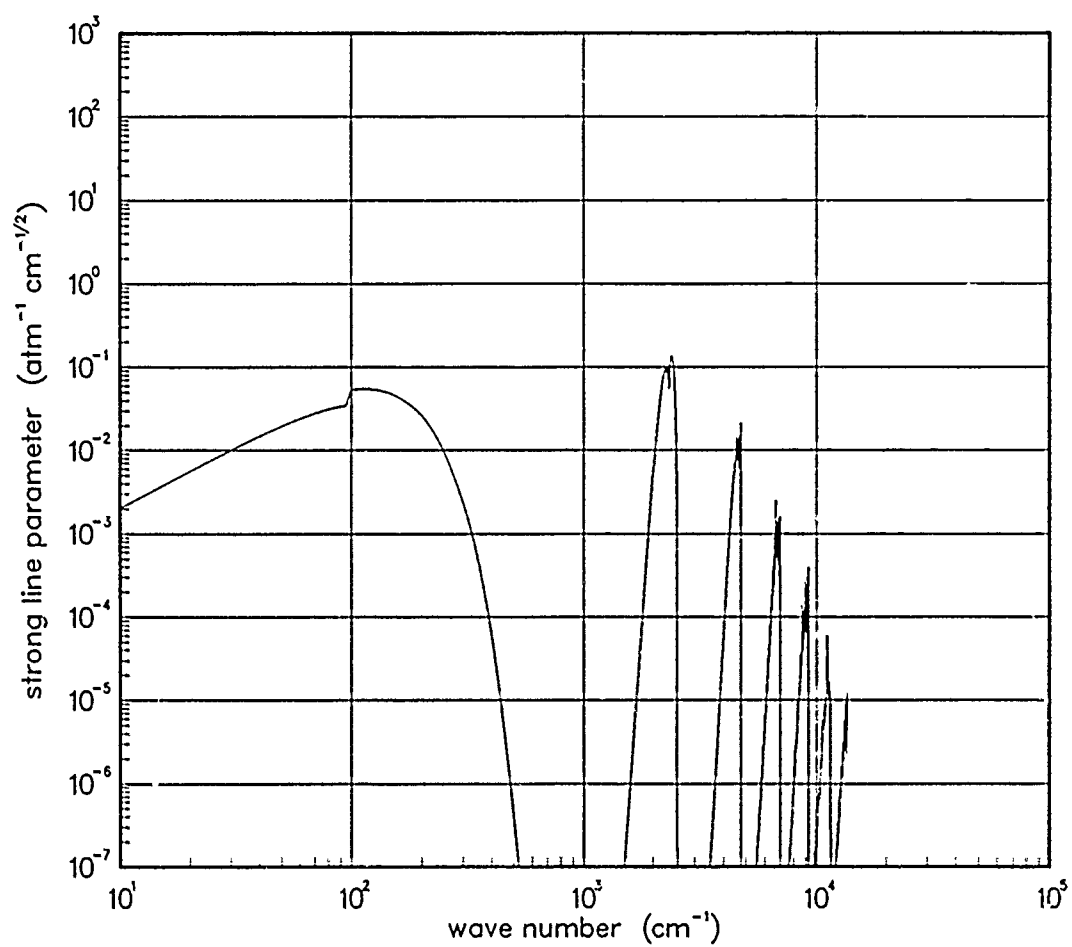


Figure 120. Strong-line parameter for NO⁺ at 1500°K.

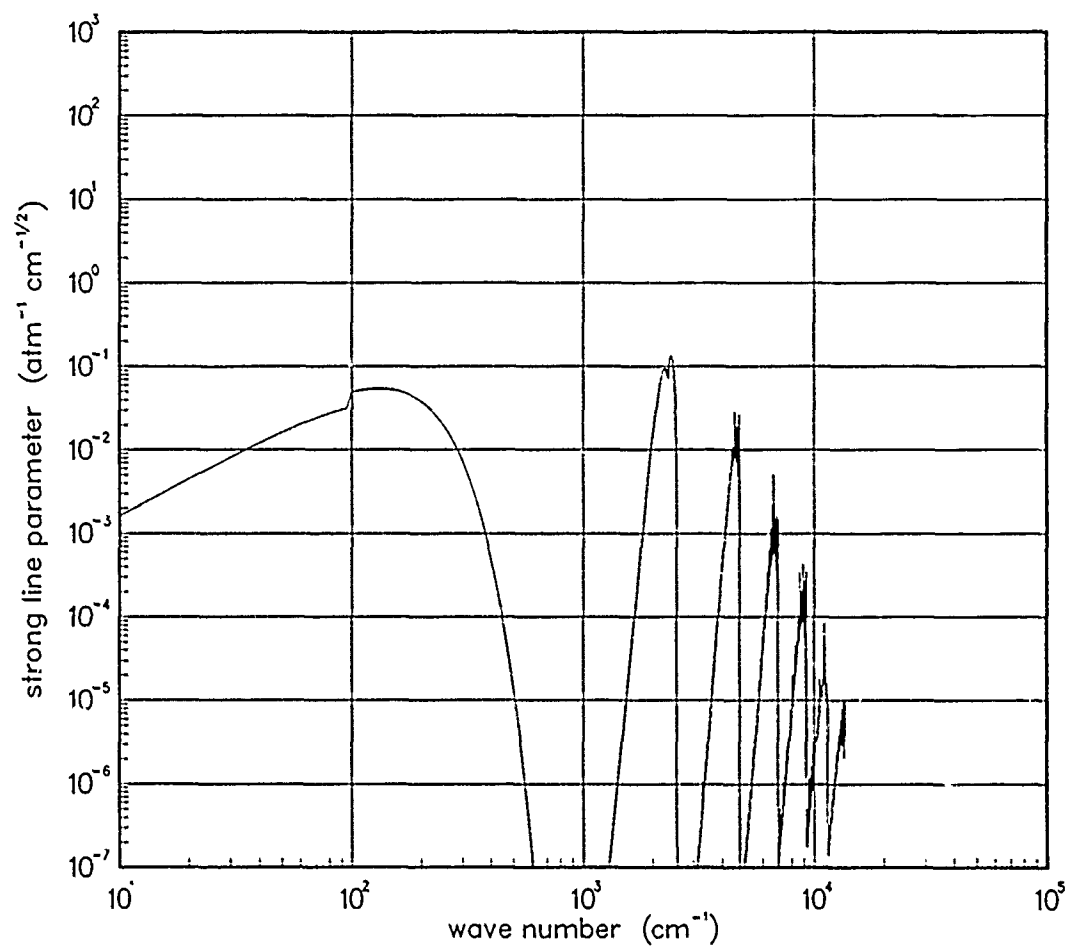


Figure 121. Strong-line parameter for NO⁺ at 2000°K.

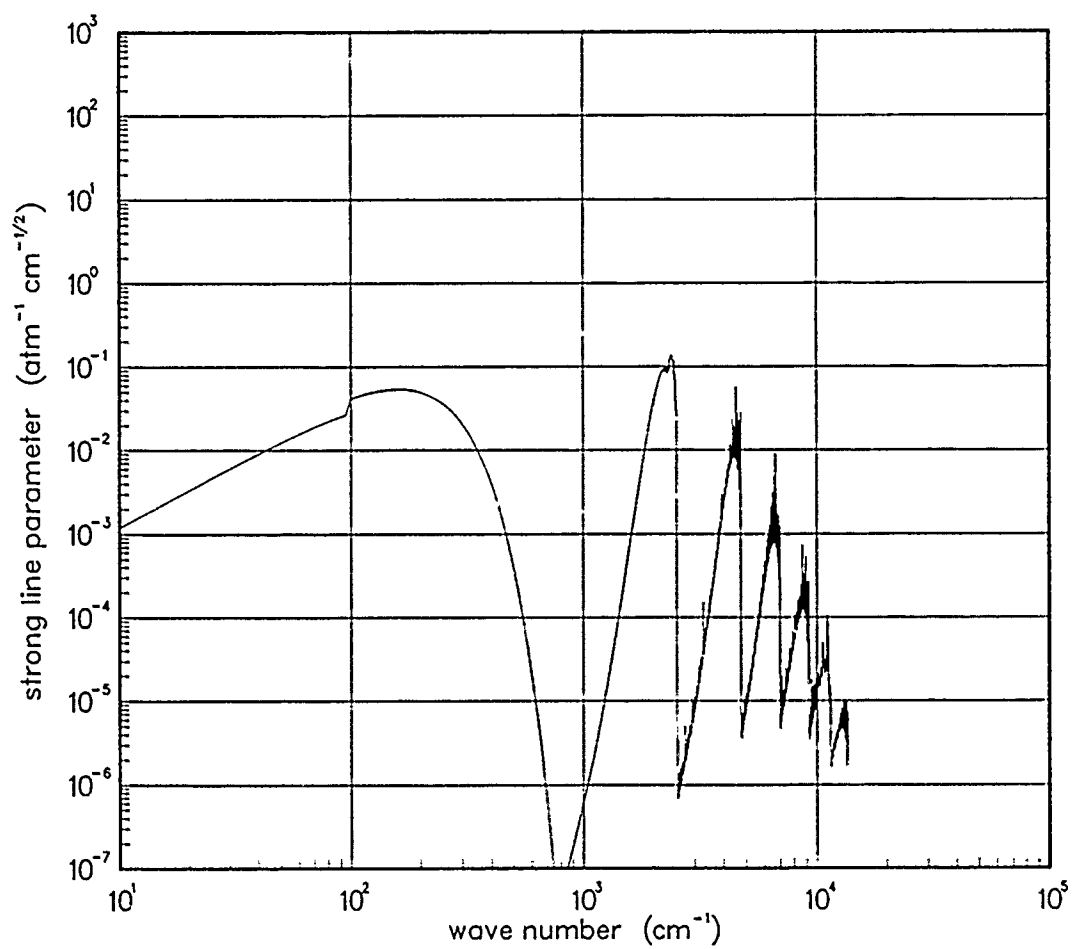


Figure 122. Strong-line parameter for NO⁺ at 3000°K.

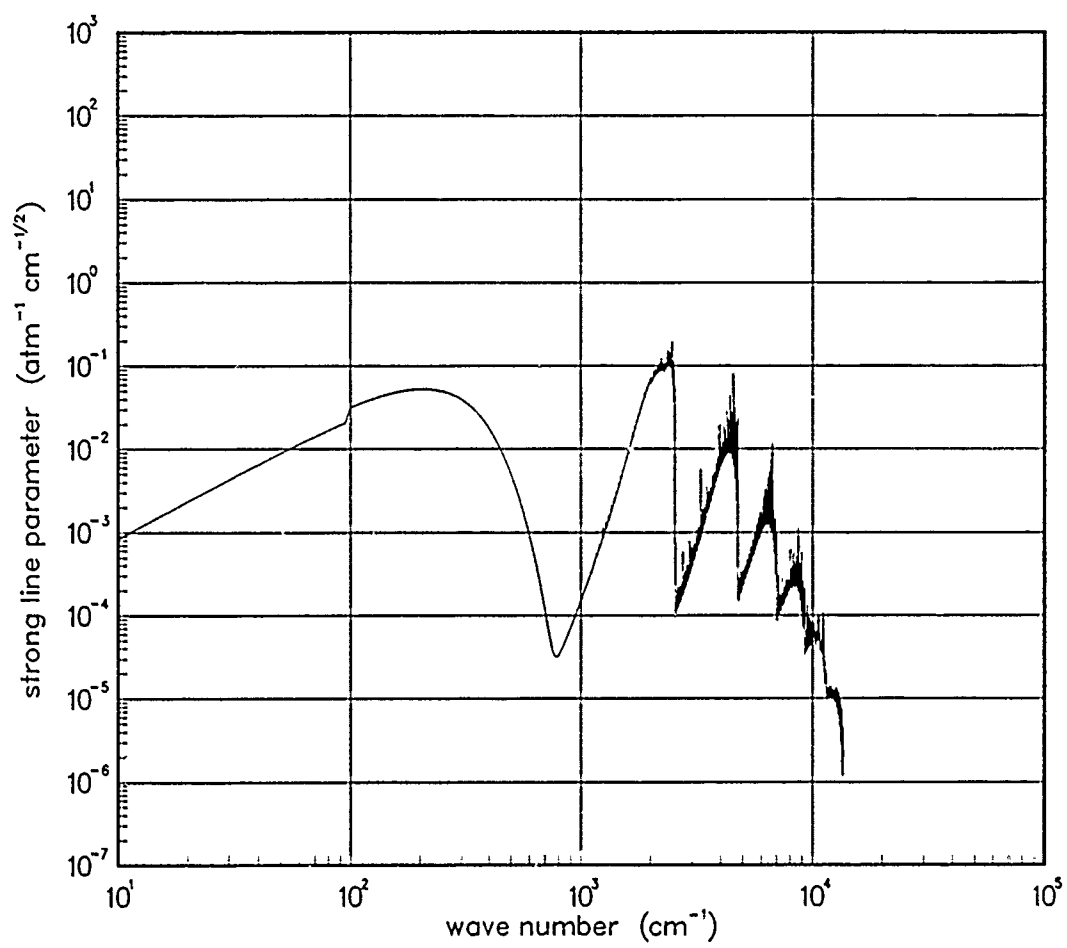


Figure 123. Strong-line parameter for NO⁺ at 5000°K.

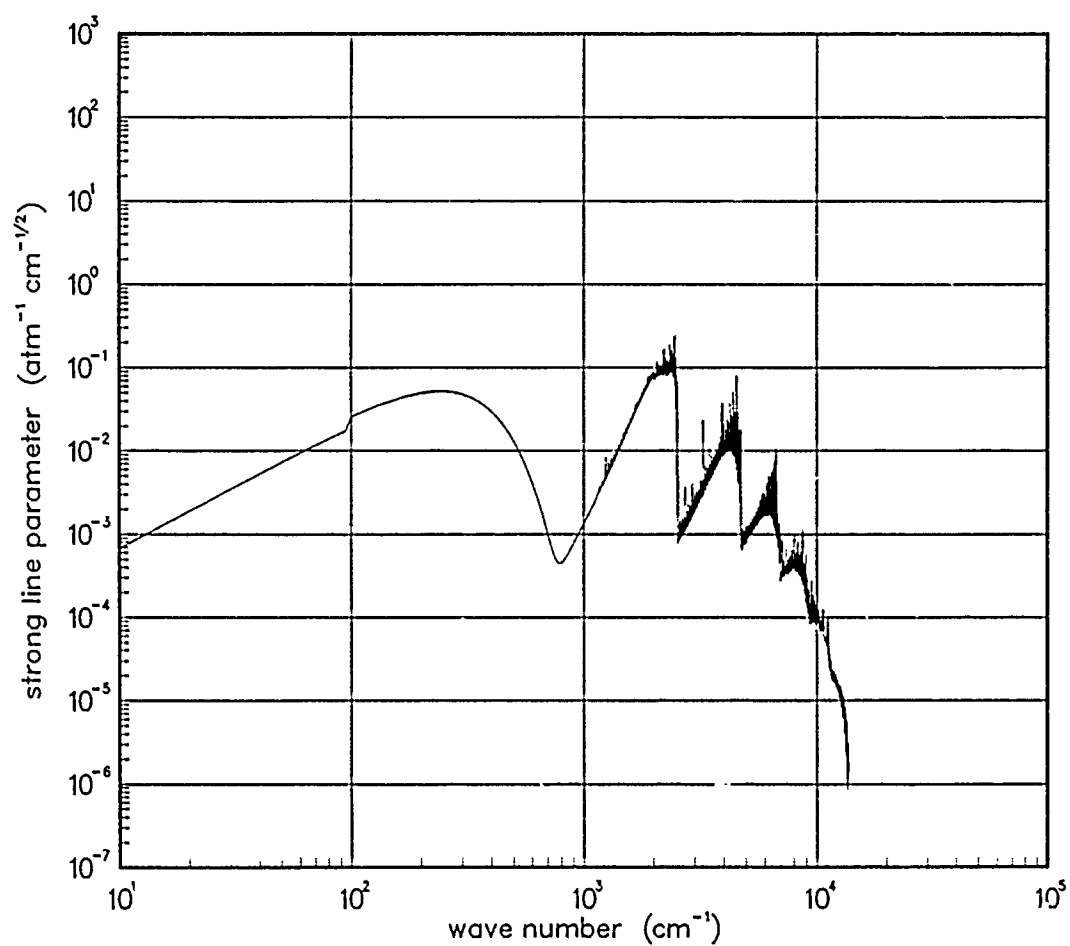


Figure 124. Strong-line parameter for NO⁺ at 7000°K.

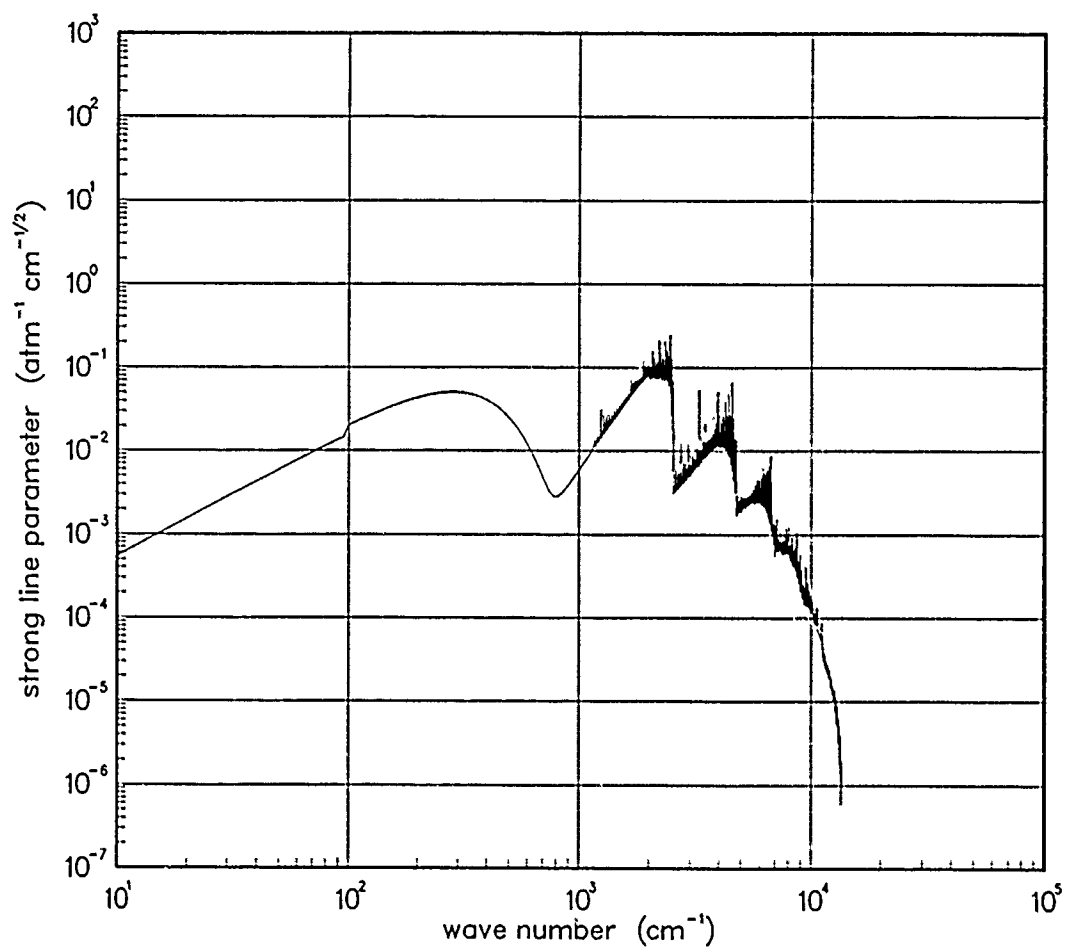


Figure 125. Strong-line parameter for NO⁺ at 10000°K.

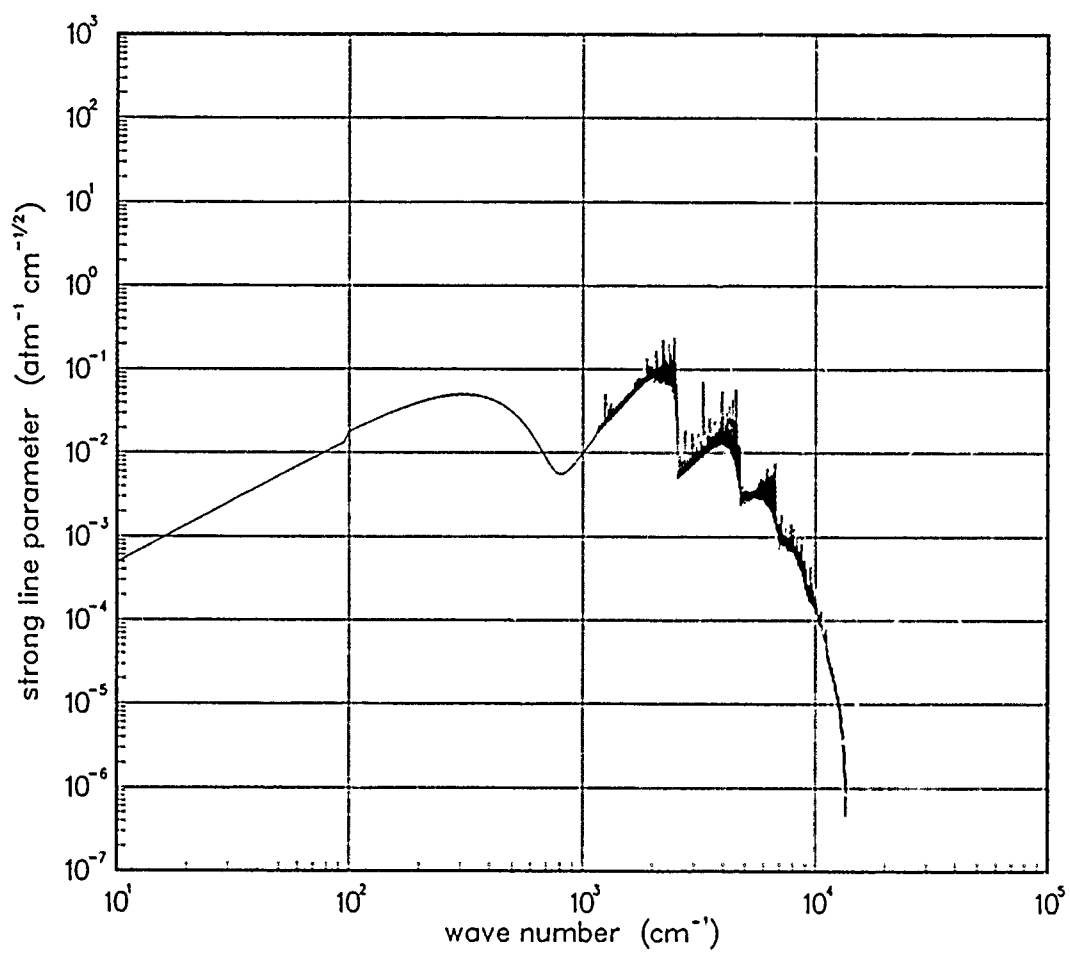


Figure 126. Strong-line parameter for NO^+ at 12000°K .

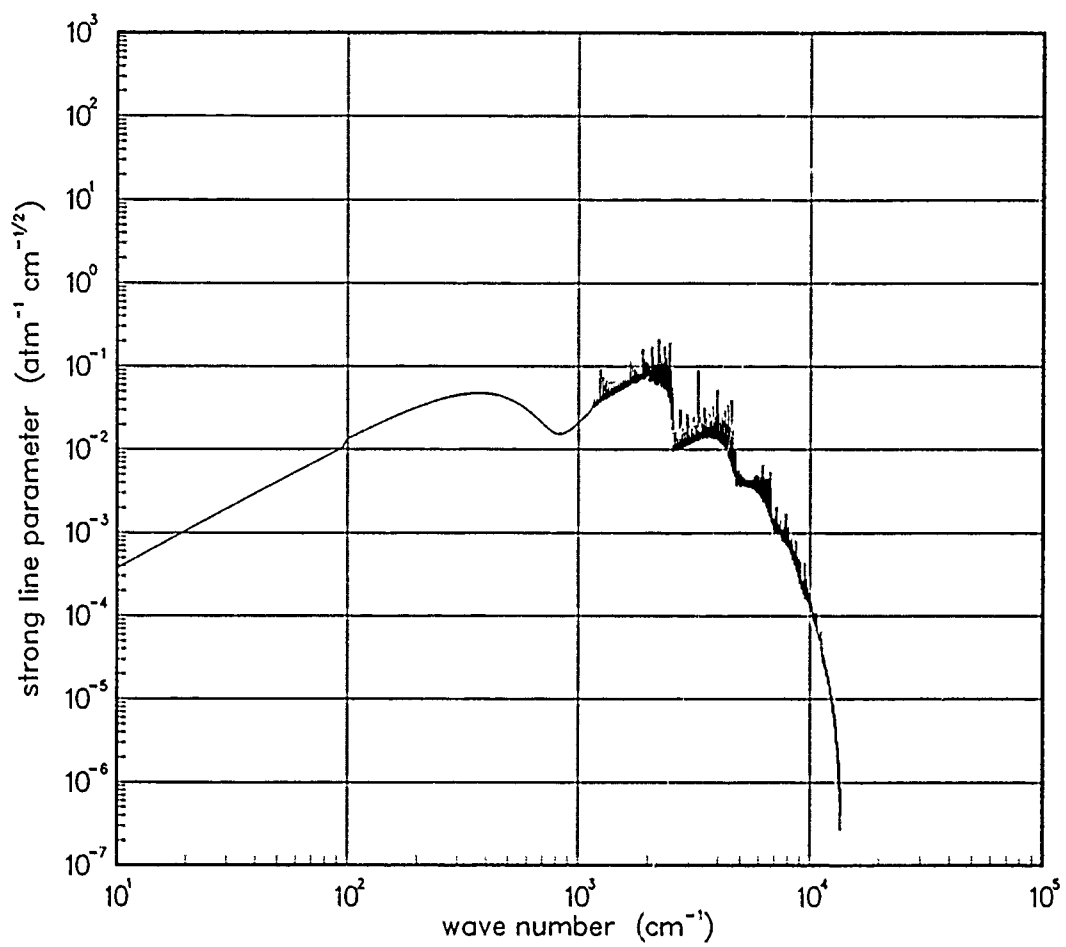


Figure 127. Strong-line parameter for NO⁺ at 18000°K.

4.5 OXYGEN (O₂).

The local thermal equilibrium emission spectra for the Oxygen molecule was calculated by VisiDyne Corporation* using an Air Force Weapons Laboratory opacity data base developed in the late sixties. Data for the weak-line parameter for O₂ in the visible region (5,000 cm⁻¹ - 100,000 cm⁻¹) is available. There is no inverse line spacing information available for this molecule.

Data Source:

*H. Smith, T. Keneshea, VisiDyne Corporation, private communication (1986).

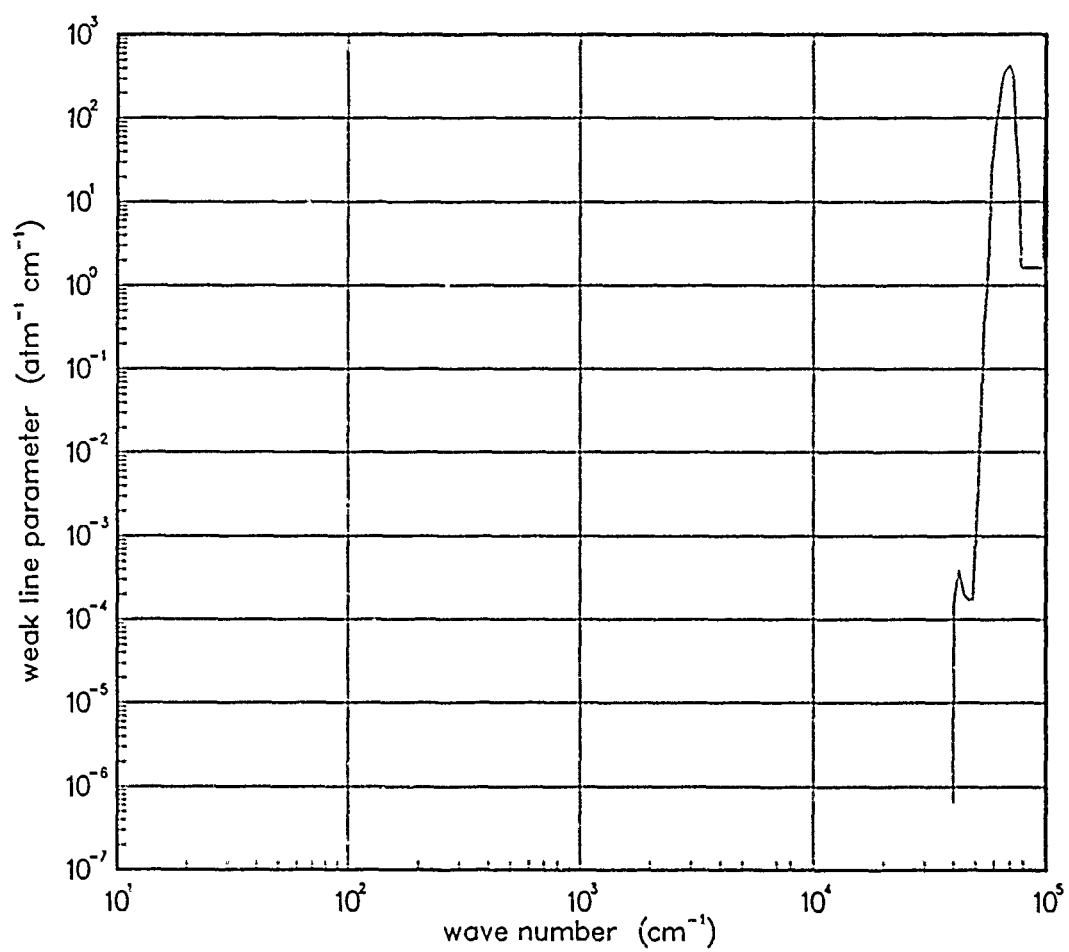


Figure 128. Weak-line parameter for O₂ at 200°K.

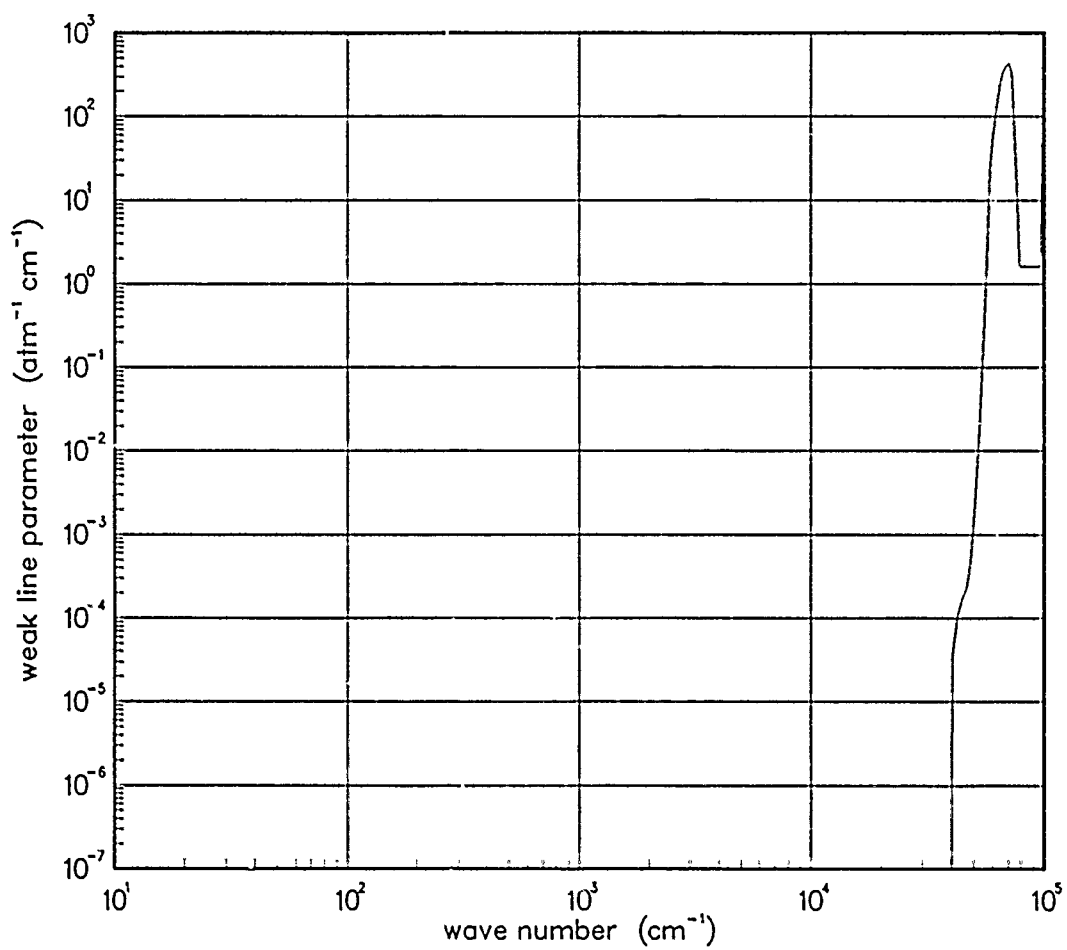


Figure 129. Weak-line parameter for O₂ at 300°K.

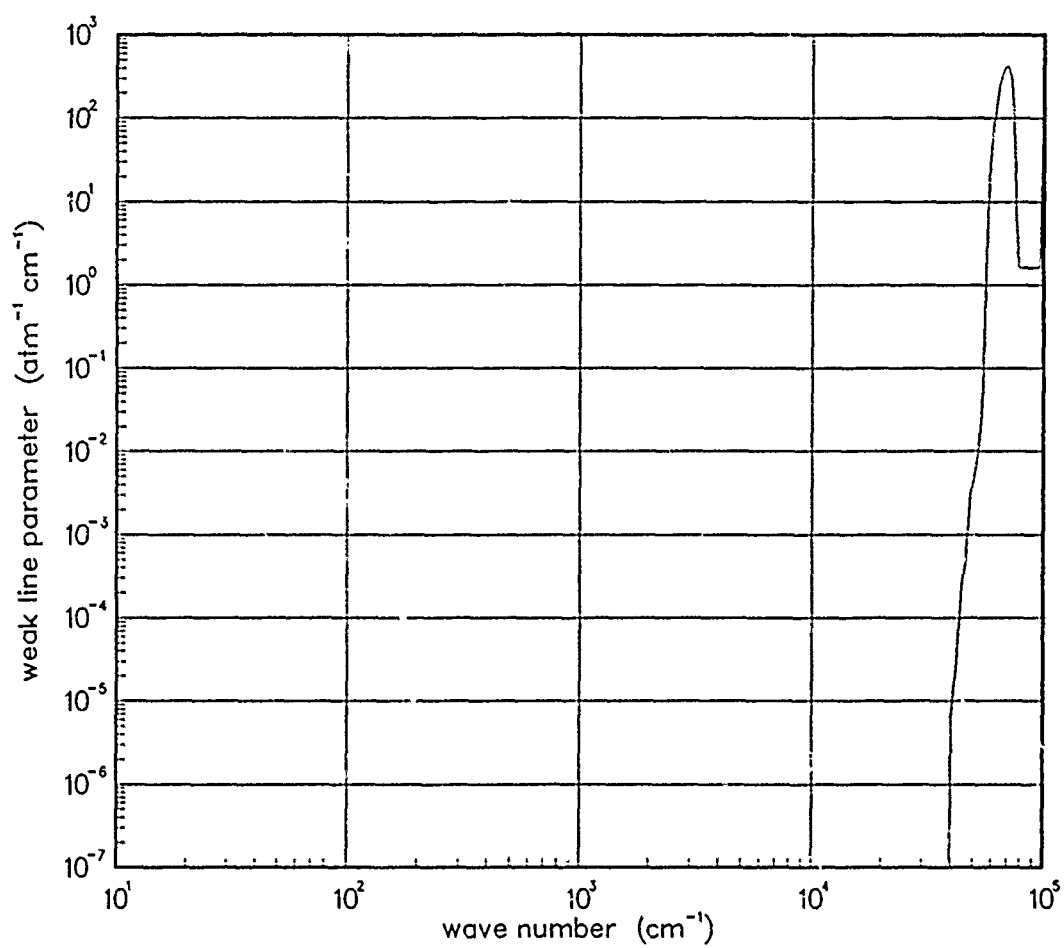


Figure 130. Weak-line parameter for O₂ at 500°K.

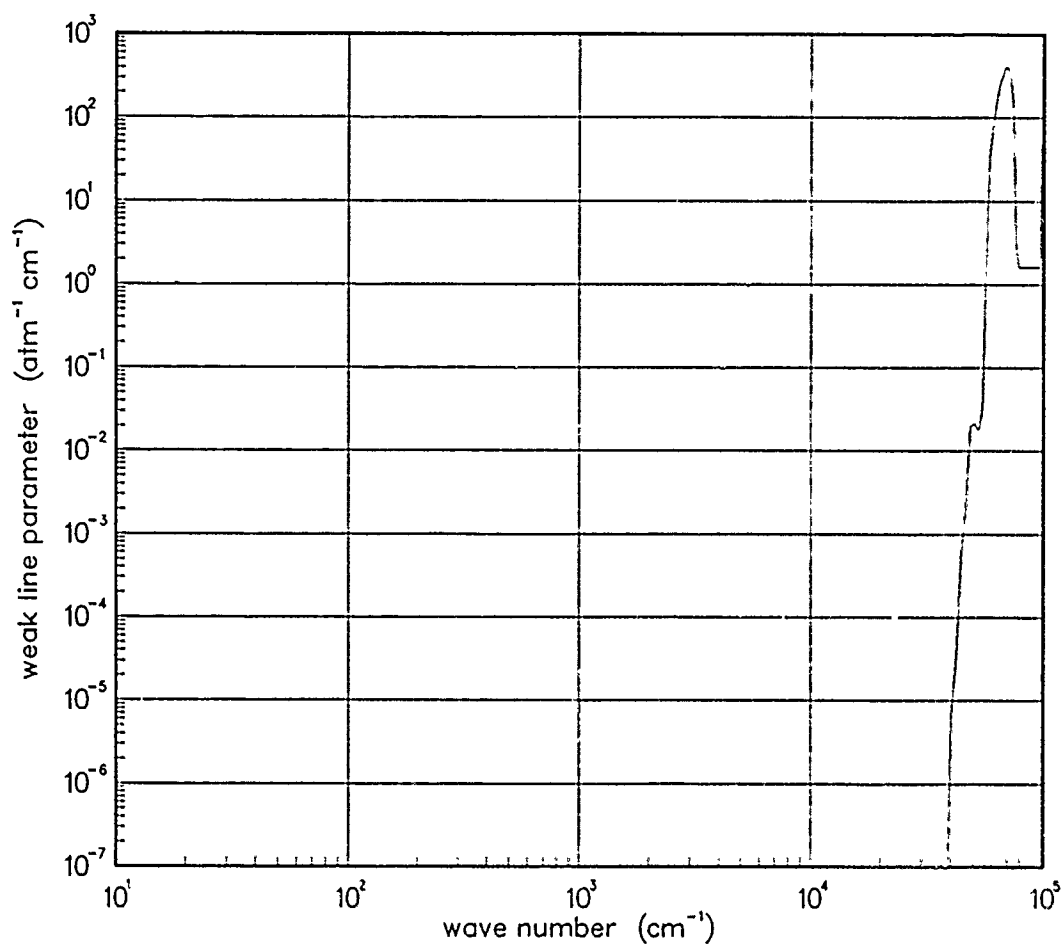


Figure 131. Weak-line parameter for O₂ at 750°K.

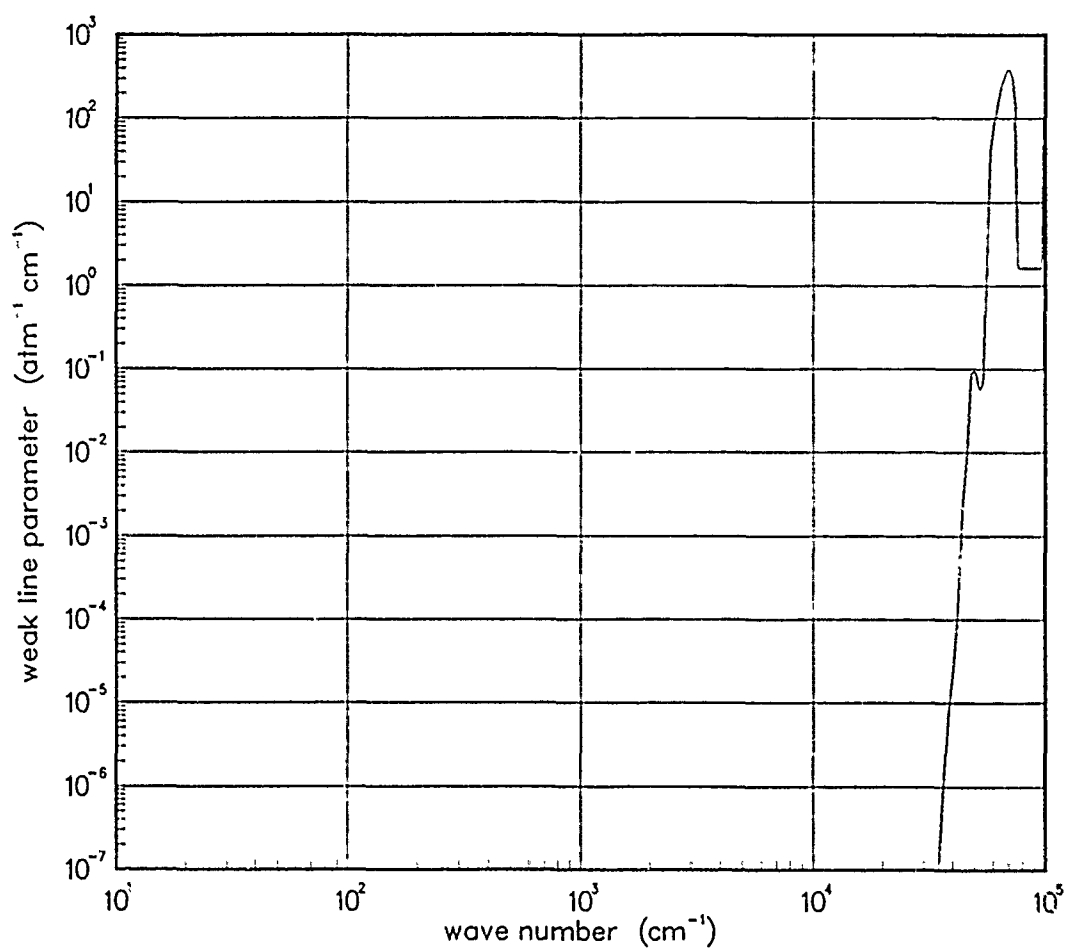


Figure 132. Weak-line parameter for O₂ at 1000°K.

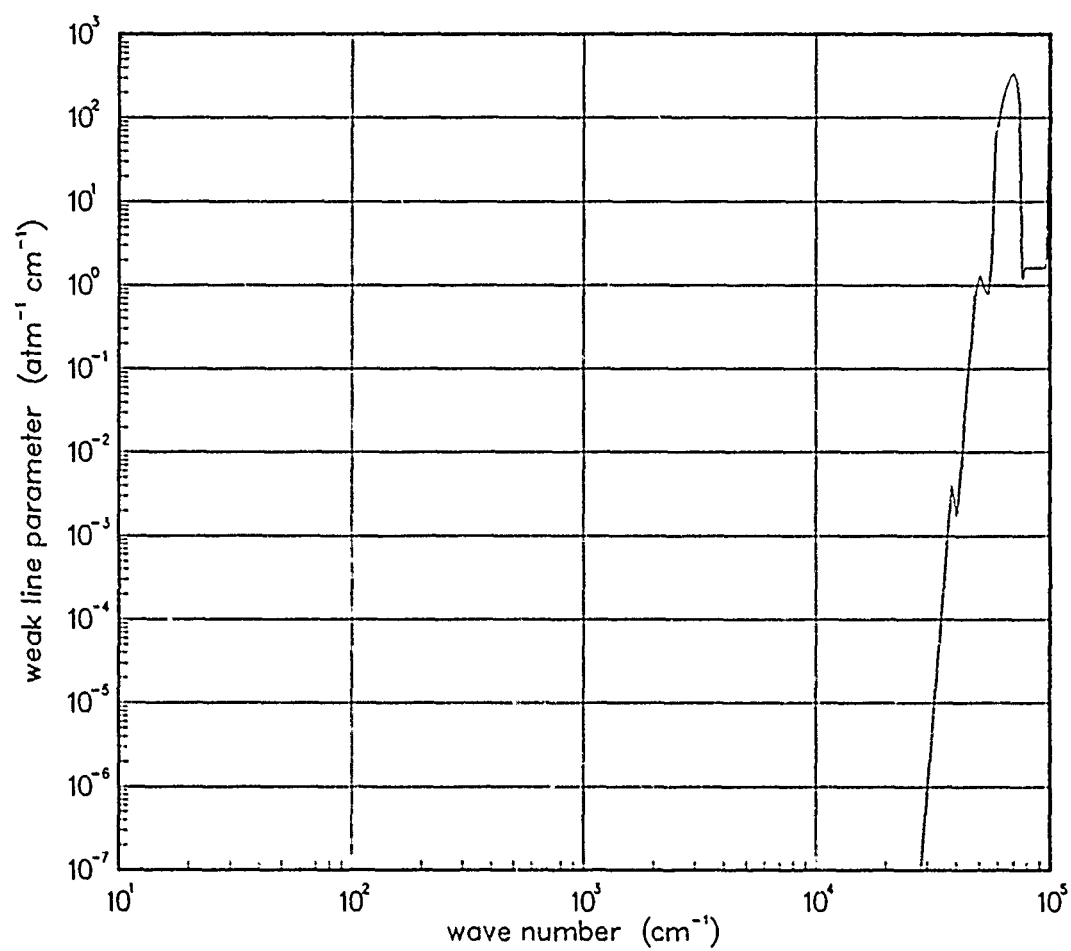


Figure 133. Weak-line parameter for O_2 at $1500^\circ K$.

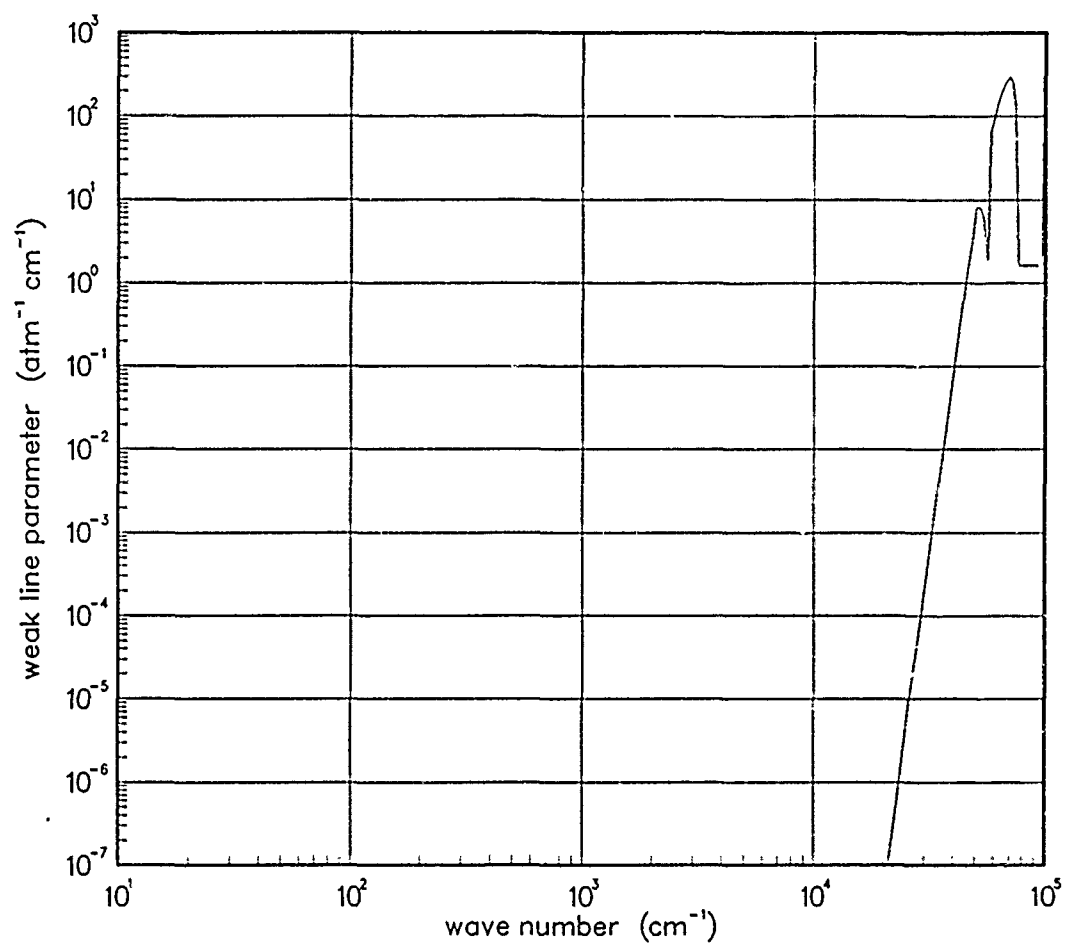


Figure 134. Weak-line parameter for O₂ at 2000°K.

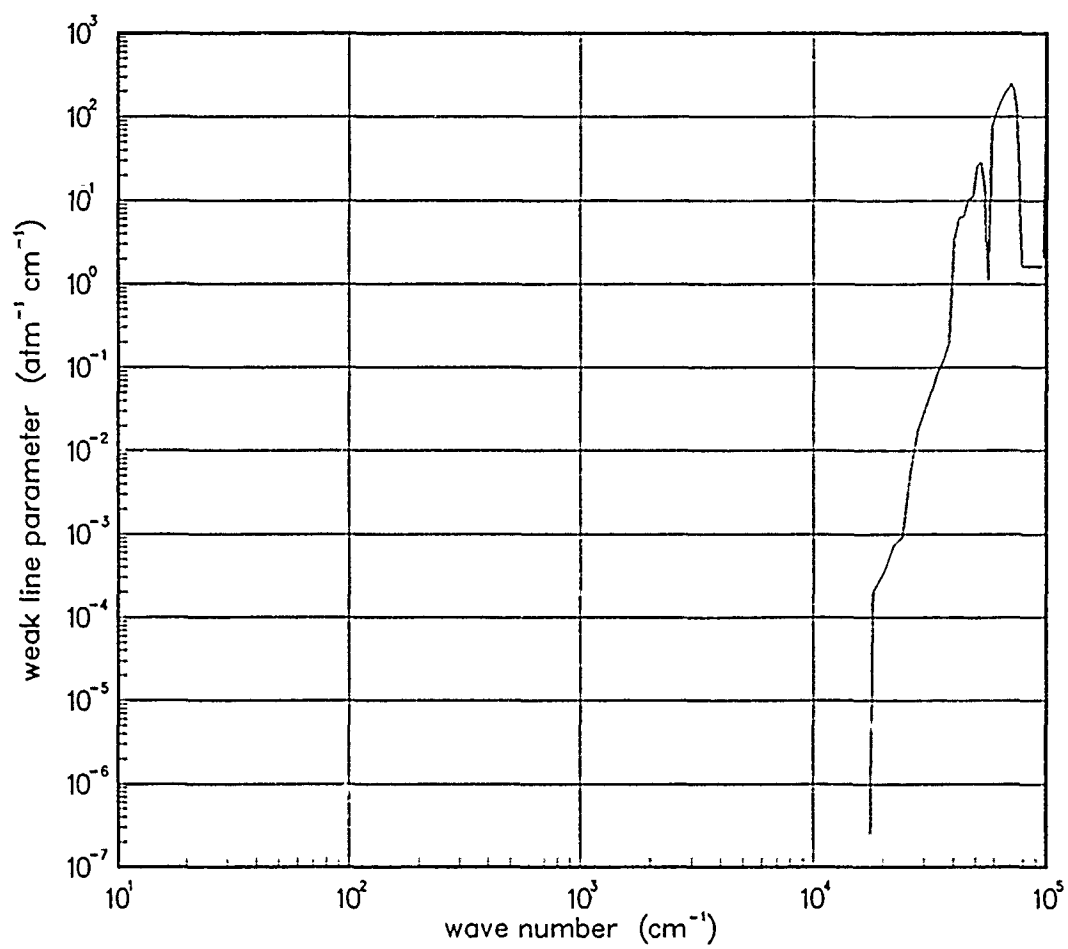


Figure 135. Weak-line parameter for O₂ at 3000°K.

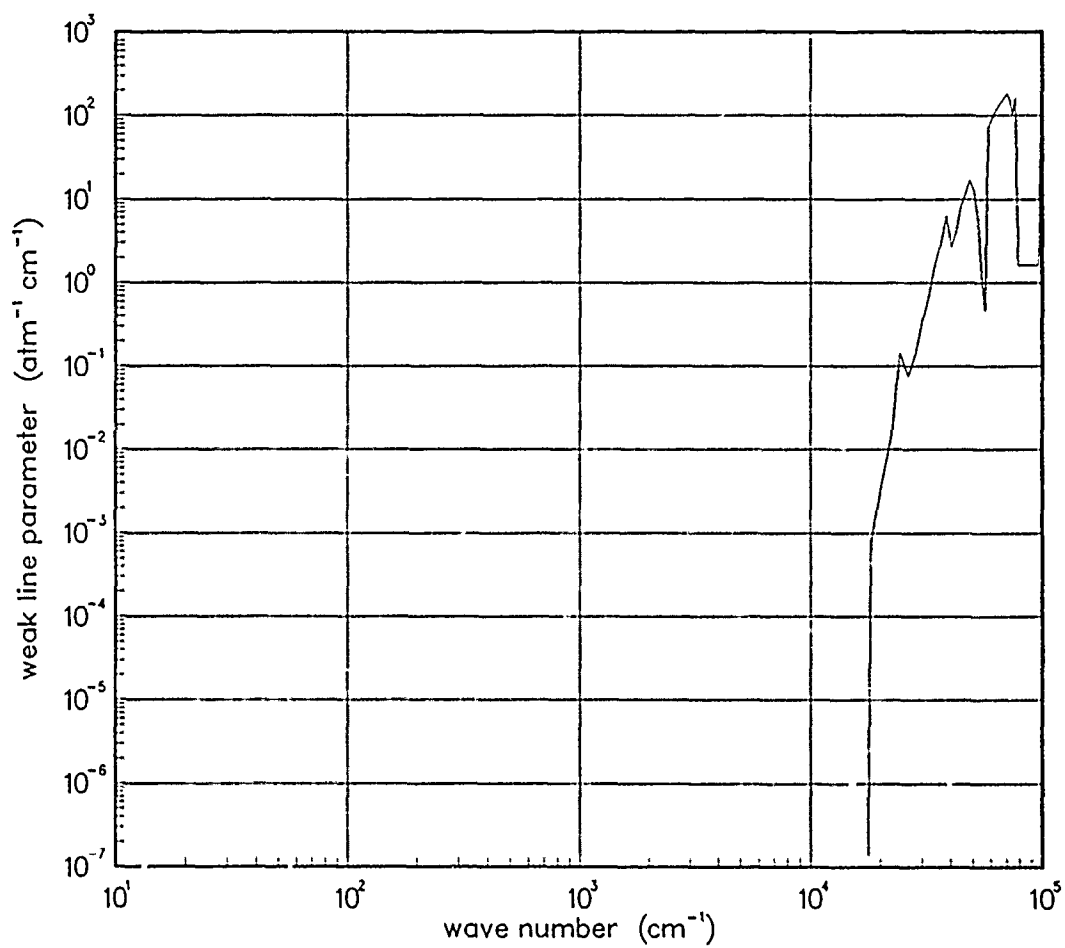


Figure 136. Weak-line parameter for O₂ at 5000°K.

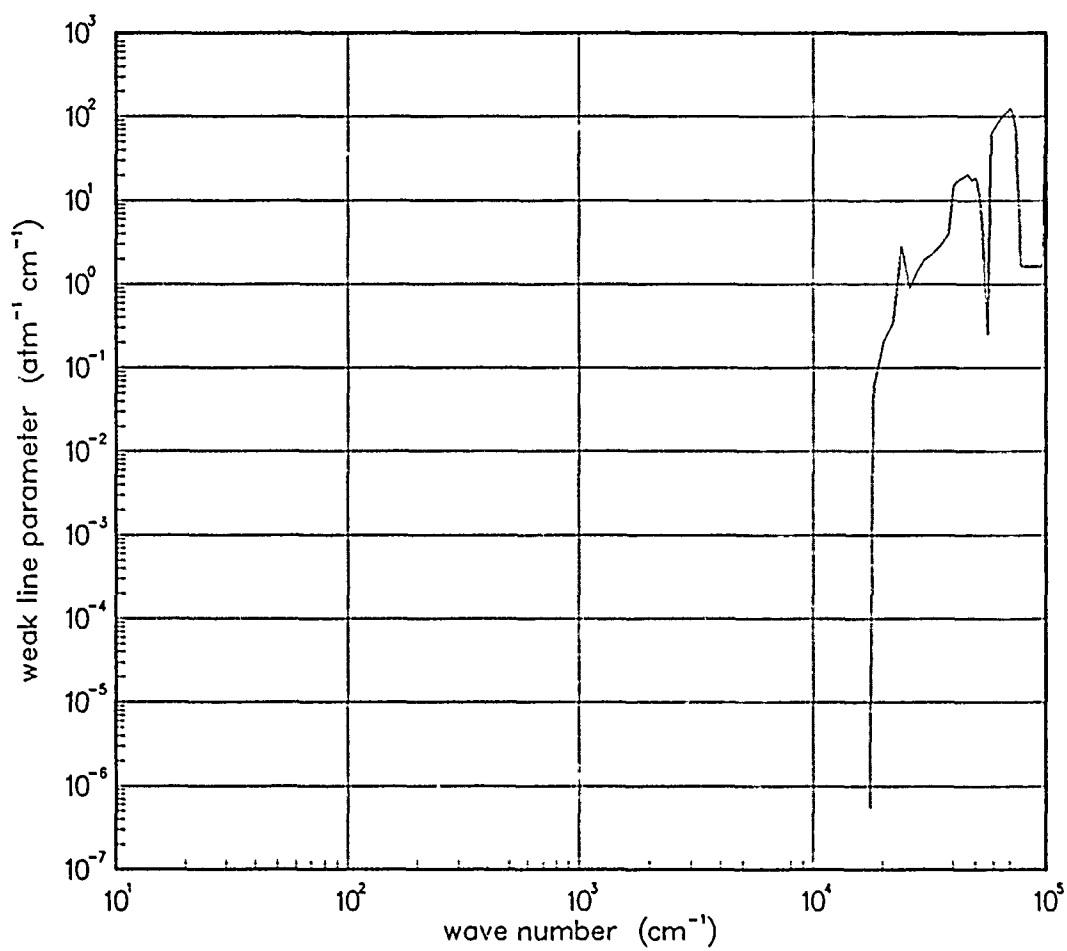


Figure 137. Weak-line parameter for O₂ at 7000°K.

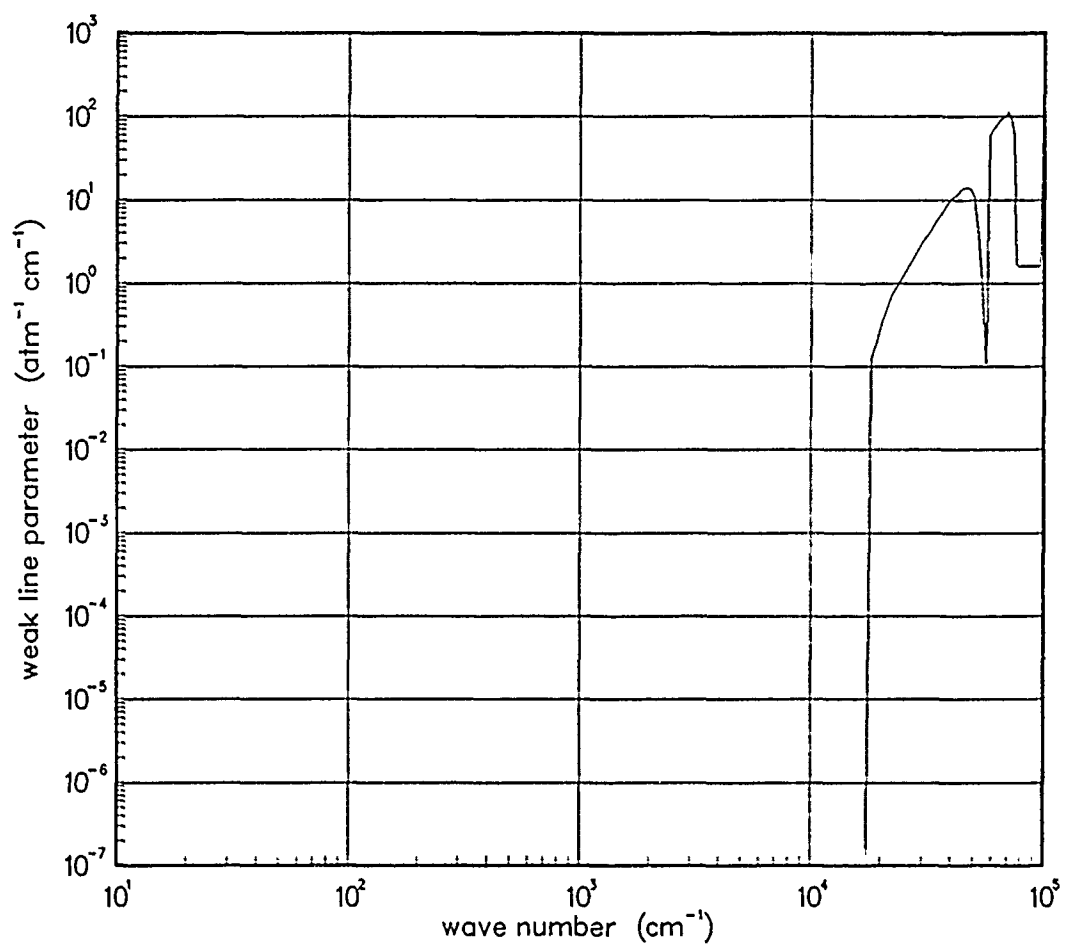


Figure 138. Weak-line parameter for O₂ at 10000°K.

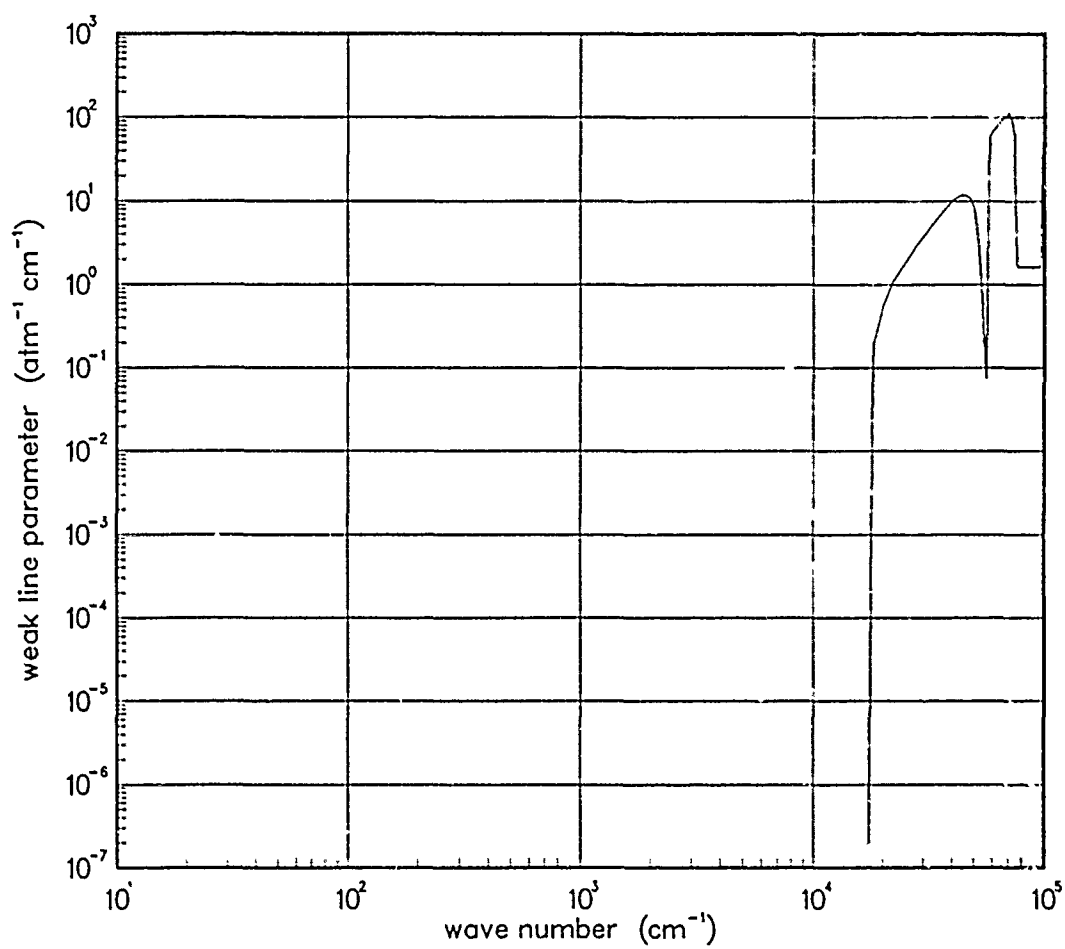


Figure 139. Weak-line parameter for O₂ at 12000°K.

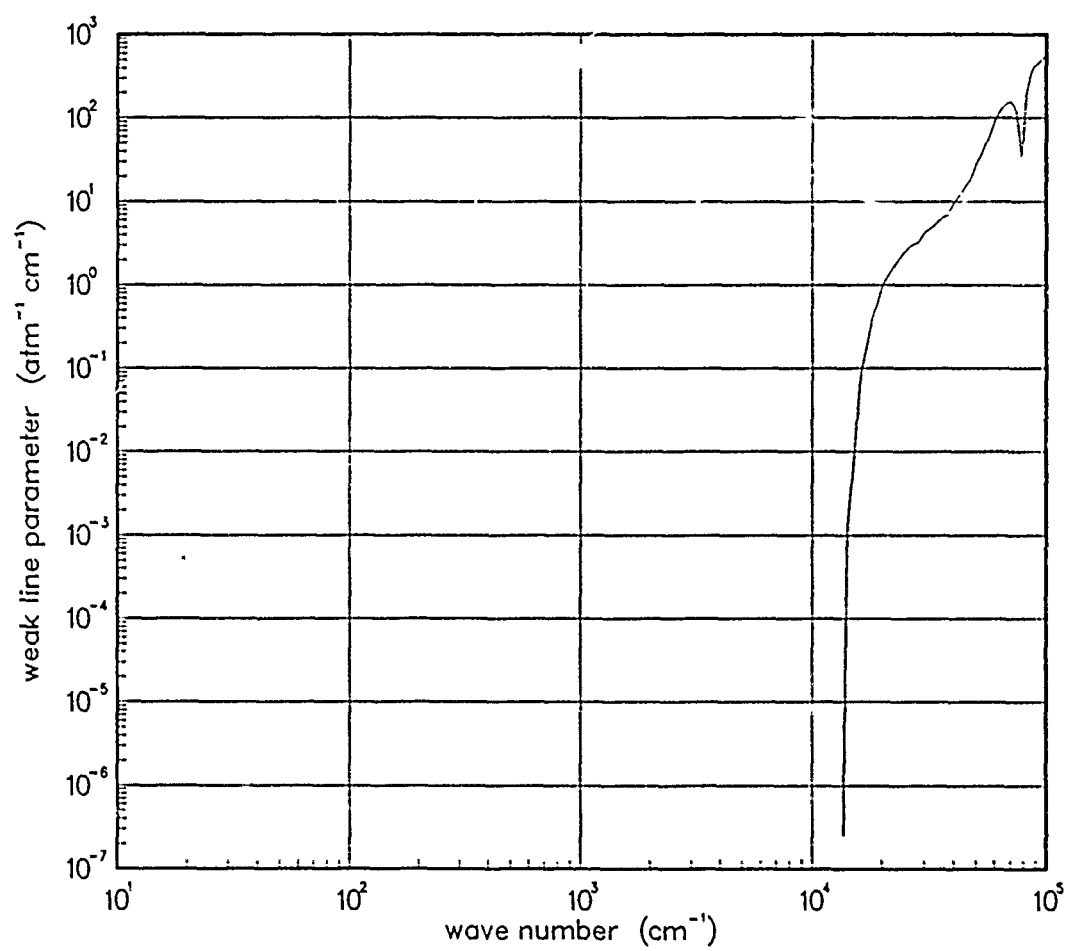


Figure 140. Weak-line parameter for O₂ at 18000°K.

SECTION 5

POLYATOMIC MOLECULES

The local thermal equilibrium emission spectra for polyatomics have been computed from a variety of sources including Triatomic Thermal Emission code (TATE), Air Force Geophysical Laboratory Line Atlas and the Air Force Weapons Laboratory Opacity Database.

5.1 AMMONIA (NH_3).

The local thermal equilibrium emission spectra for Ammonia has been developed from the Air Force Geophysical Laboratory line atlas for 200, 300, 500, 750, 1000 °K.

The NH_3 molecule has been included within the NORSE LTE data base because of its contribution to ambient atmospheric absorption. The inclusion of accurate parameters for this species above 1000 °K is felt to be of low priority.

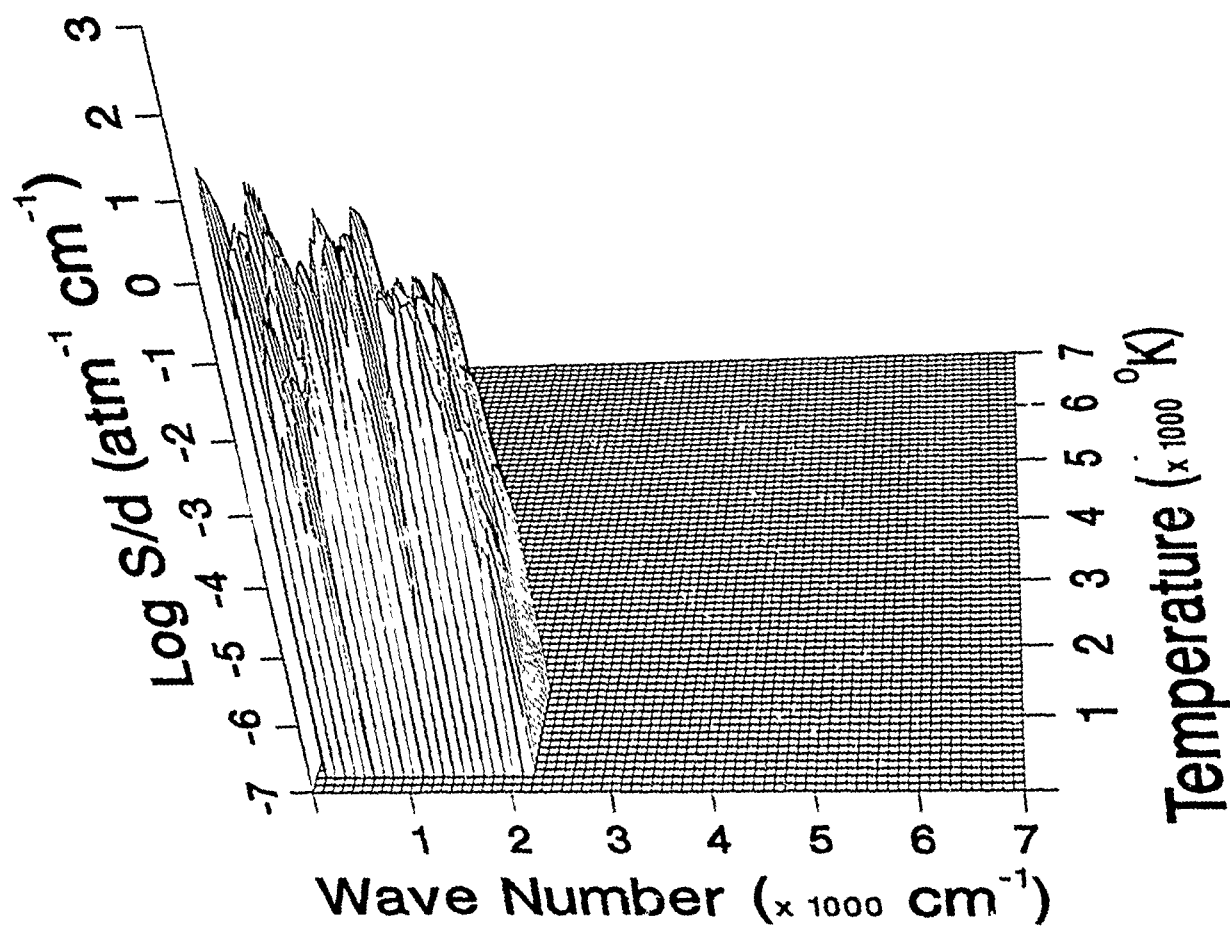


Figure 141. Weak-line parameter for NH_3 .

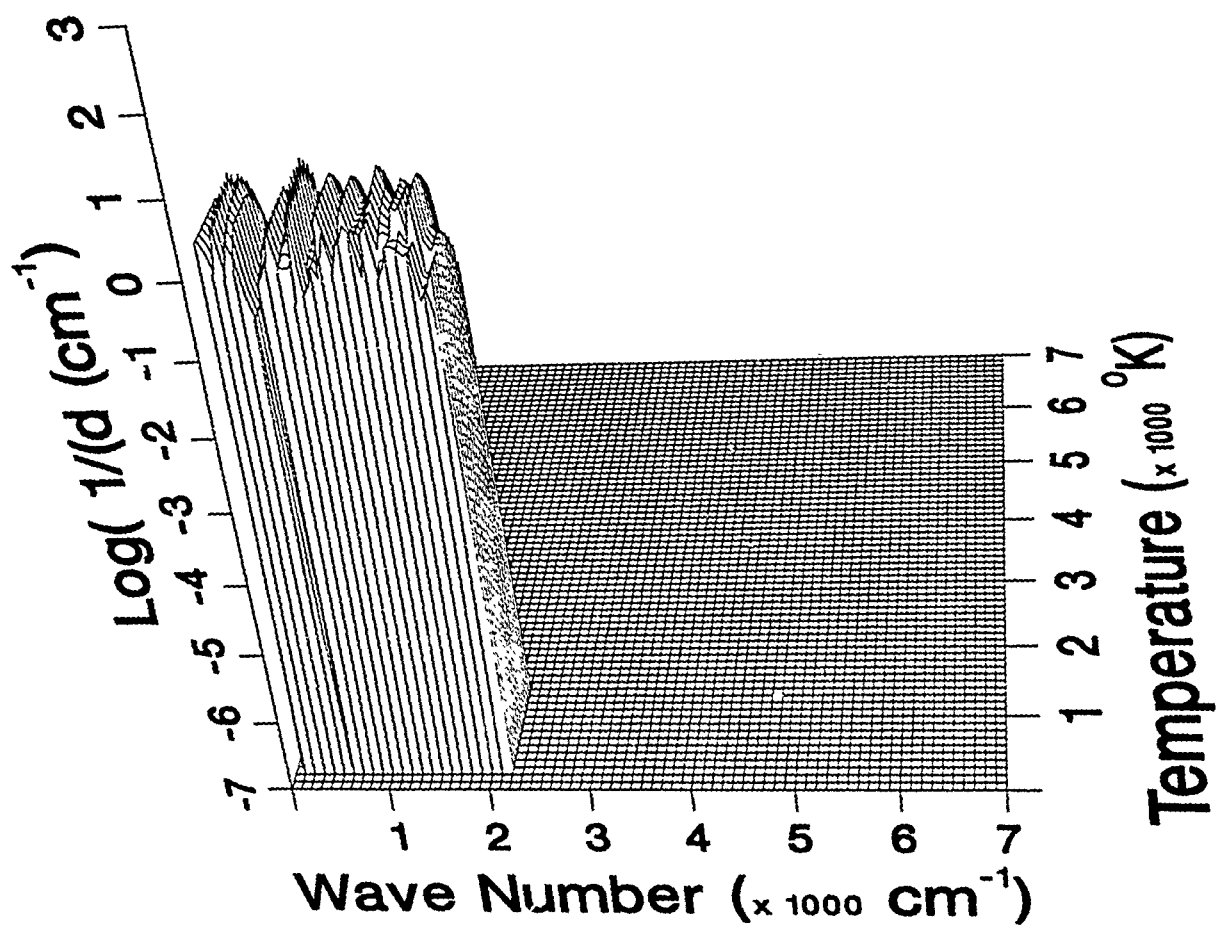


Figure 142. Inverse line spacing for NH_3 .

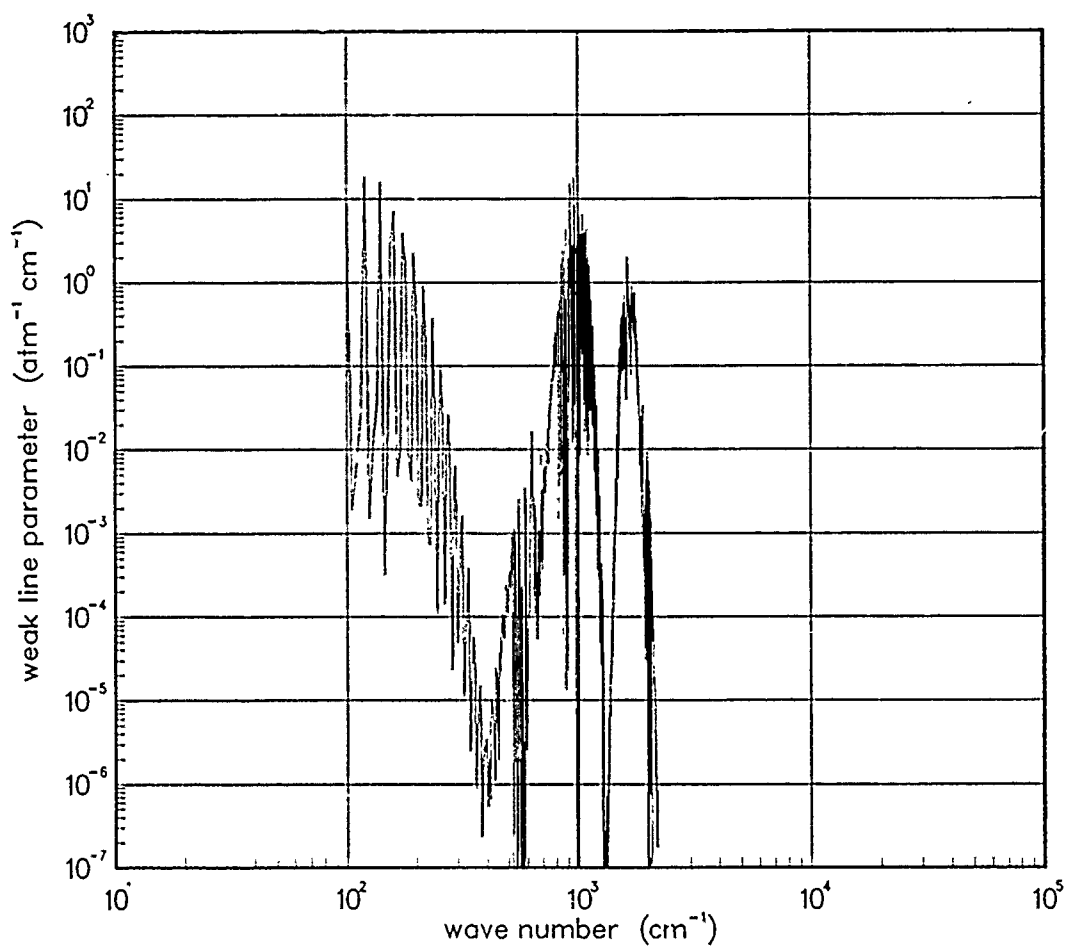


Figure 143. Weak-line parameter for NH_3 at 200°K .

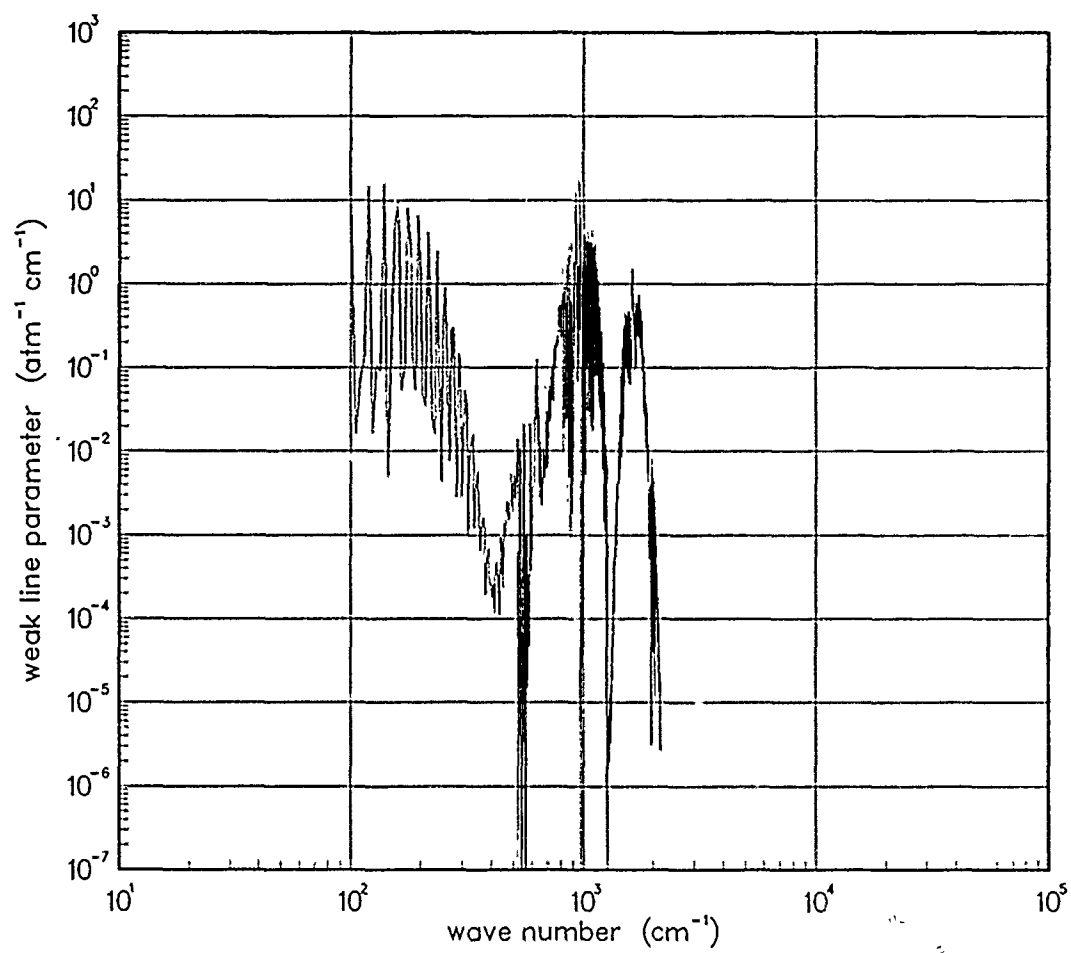


Figure 144. Weak-line parameter for NH_3 at 300°K .

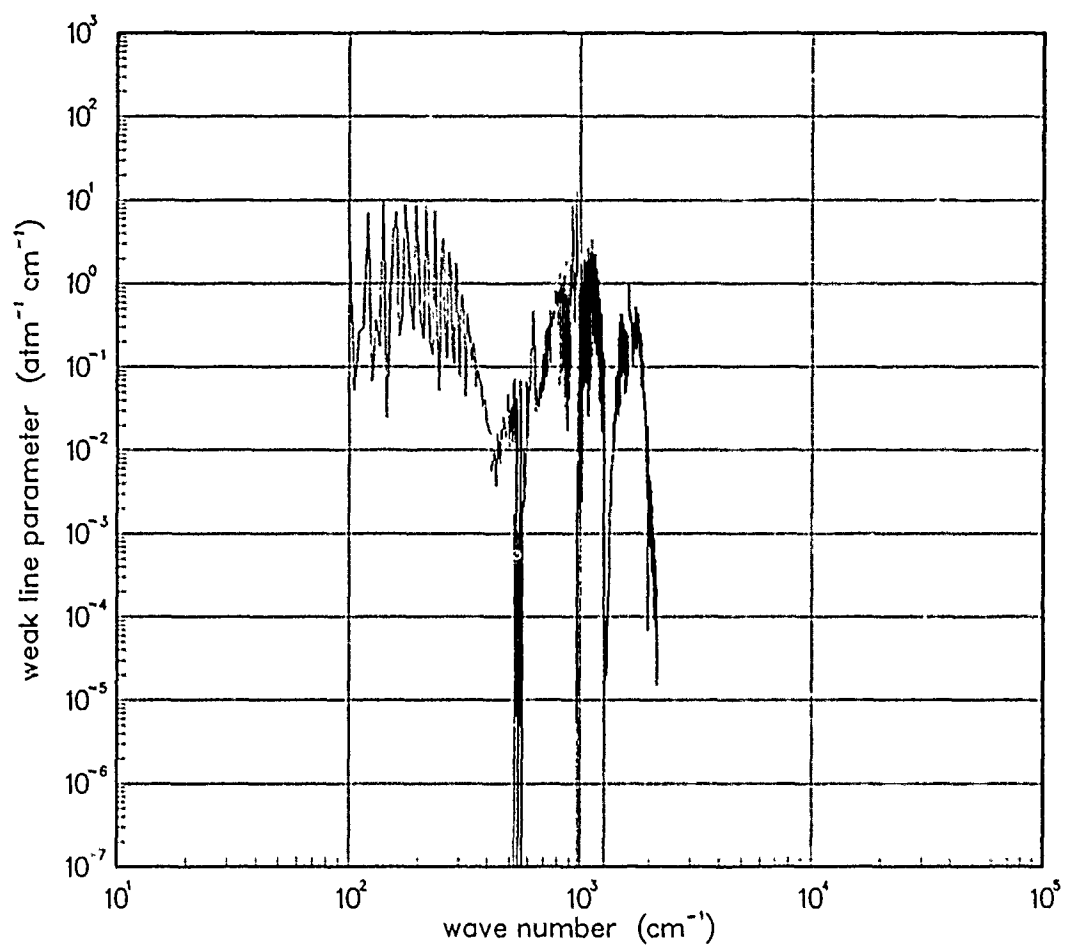


Figure 145. Weak-line parameter for NH_3 at 500°K .

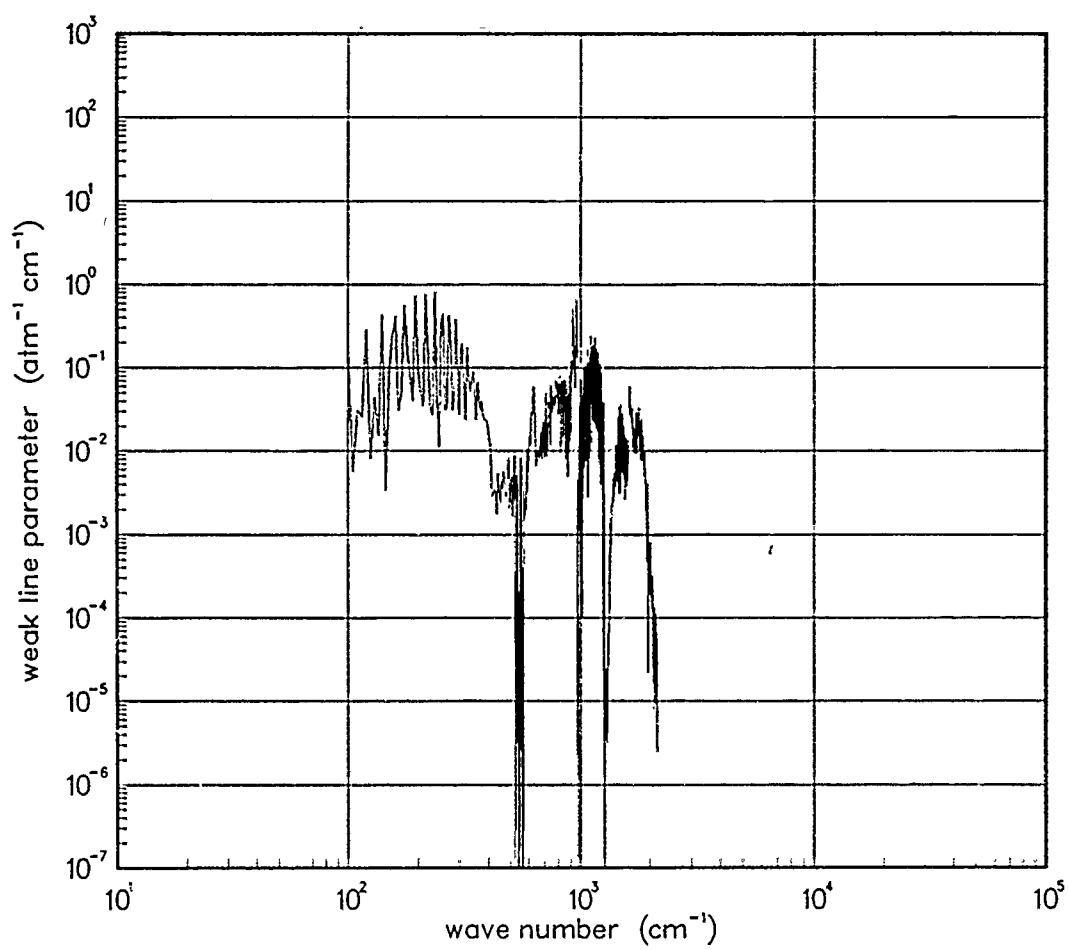


Figure 146. Weak-line parameter for NH_3 at 750°K .

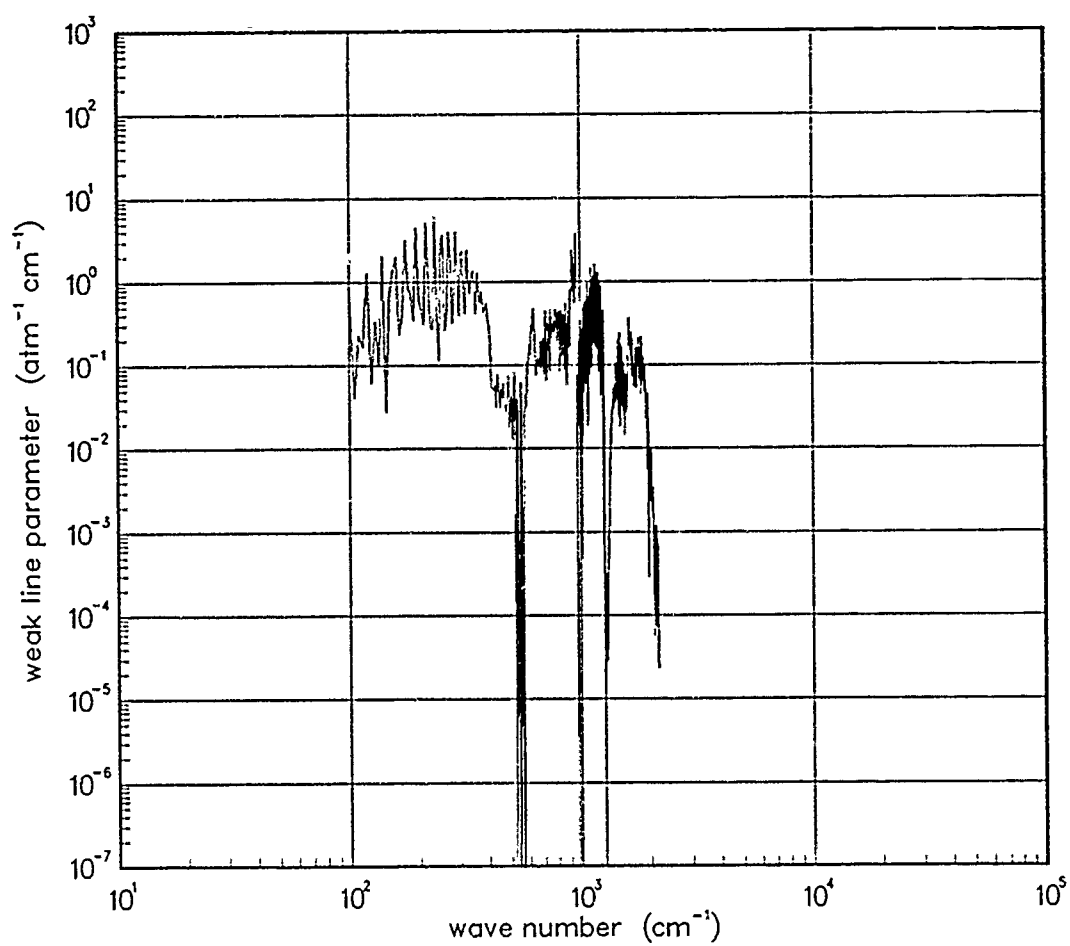


Figure 147. Weak-line parameter for NH_3 at 1000°K .

5.2 CARBON DIOXIDE (CO₂).

The weak-line and inverse line-spacing parameters for the eight most abundant isotopic species of CO₂ were calculated using the LTE smeared-band model code LINTRA^{*}. The model requires band strengths and molecular constants for the contributing transitions; these constants were obtained from the Air Force Geophysical Laboratory[†]. Theoretical calculations for excited bands of the 626 isotopic species of CO₂ were obtained from VisiDyne[‡]. The smeared band model correctly accounts for the increased population of the rotational states with increasing temperature.

These band model parameters were calculated for each wavenumber between 100 cm⁻¹ and 10,000 cm⁻¹ and then averaged to obtain the required resolution for the NORSE optics database. The temperatures at which these calculations were performed were 200, 300, 500, 750, 1000, 1500, 2000, 3000, 5000, 7000, 10000, 12000, 18000 °K. The band model parameters calculated for temperatures much above 1500 °K are deficient due to the lack of essential experimental and theoretical data.

Data Source:

^{*}LINTRA, (LINEar TRiAtomic) smeared-line band model Fortran code developed by R. Parker, Physical Research Inc., 1987.

[†]L.S. Rothman, Appl. Opt., 25, 1975 (1986).

[‡]R.B. Wattson, L.S.Rothman, J. Mol. Spectrosc., 119, 83 (1986).

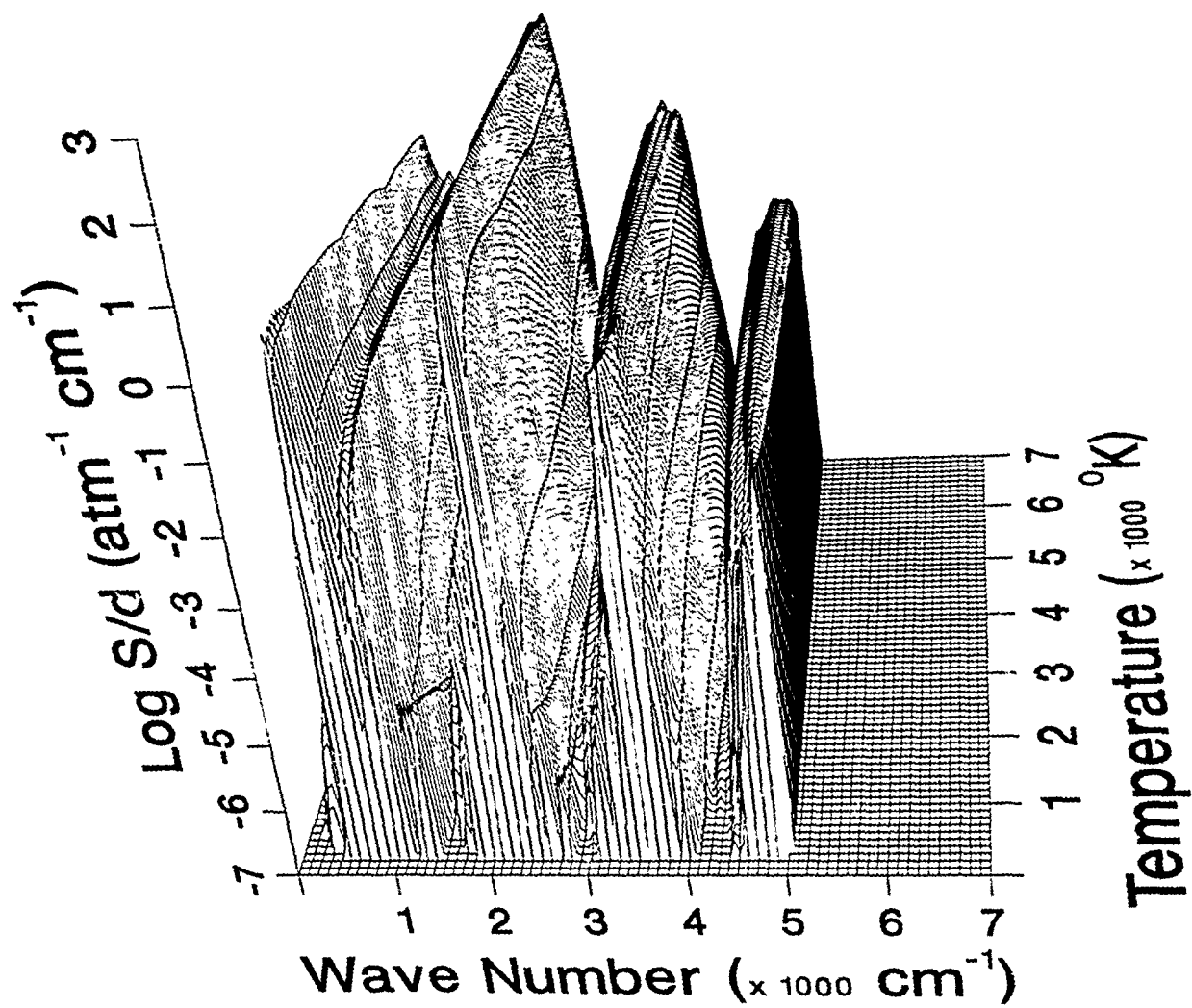


Figure 148. Weak-line parameter for CO₂.

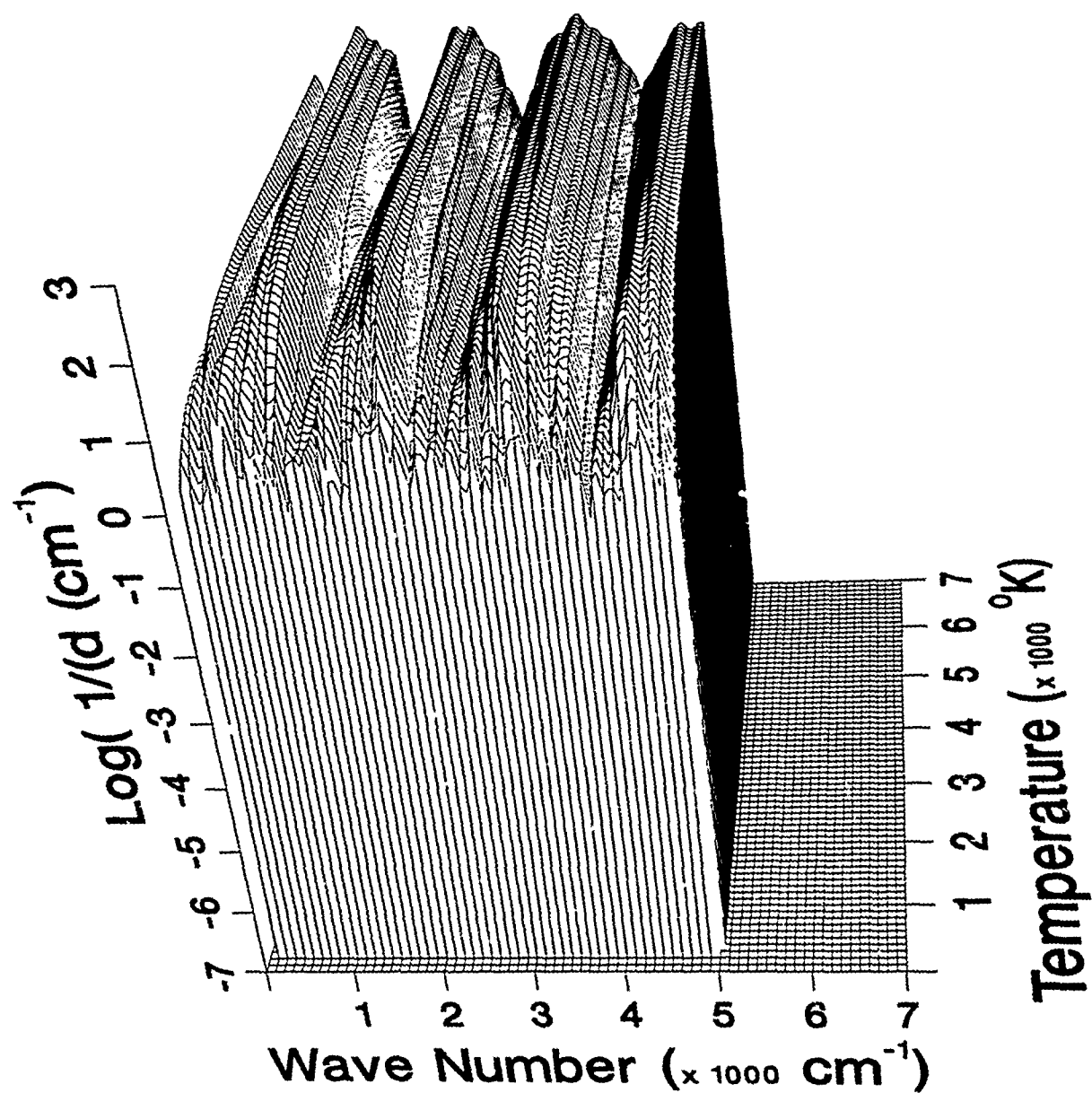


Figure 149. Inverse line spacing for CO₂.

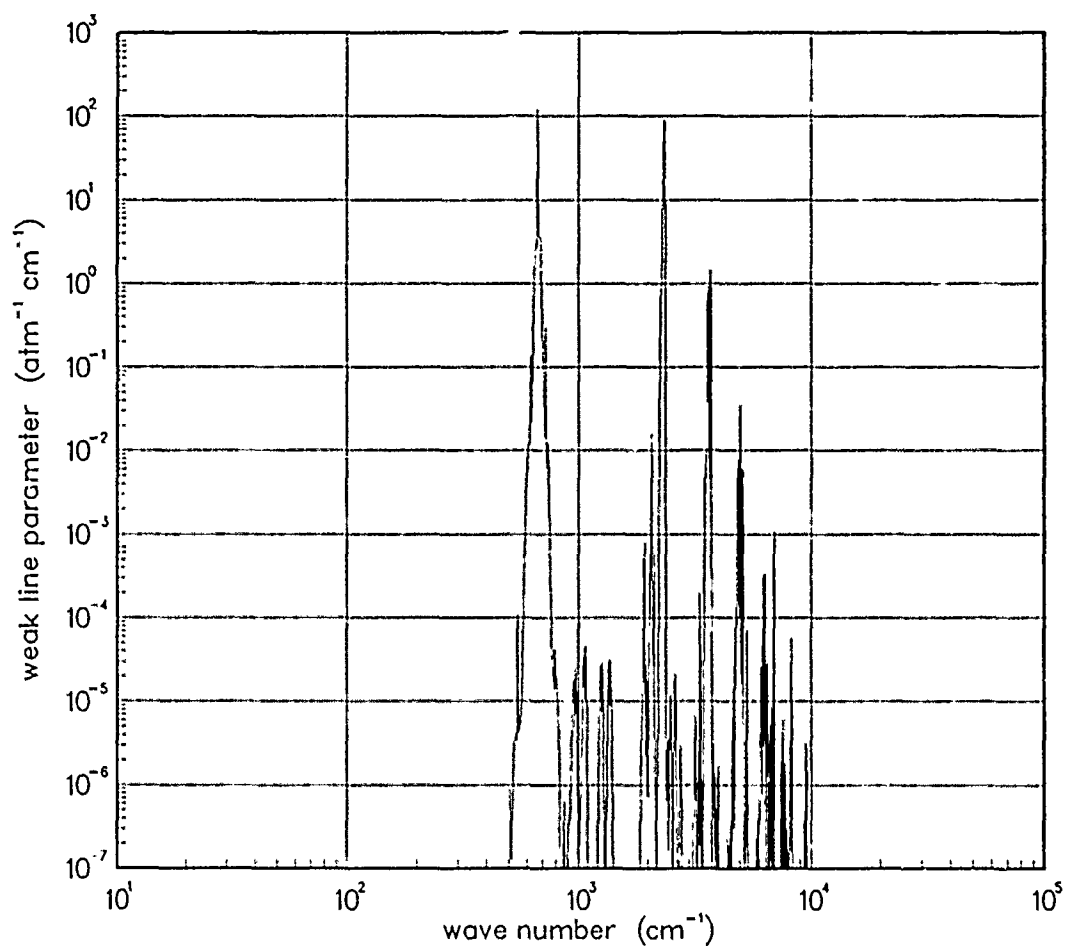


Figure 150. Weak-line parameter for CO₂ at 200°K.

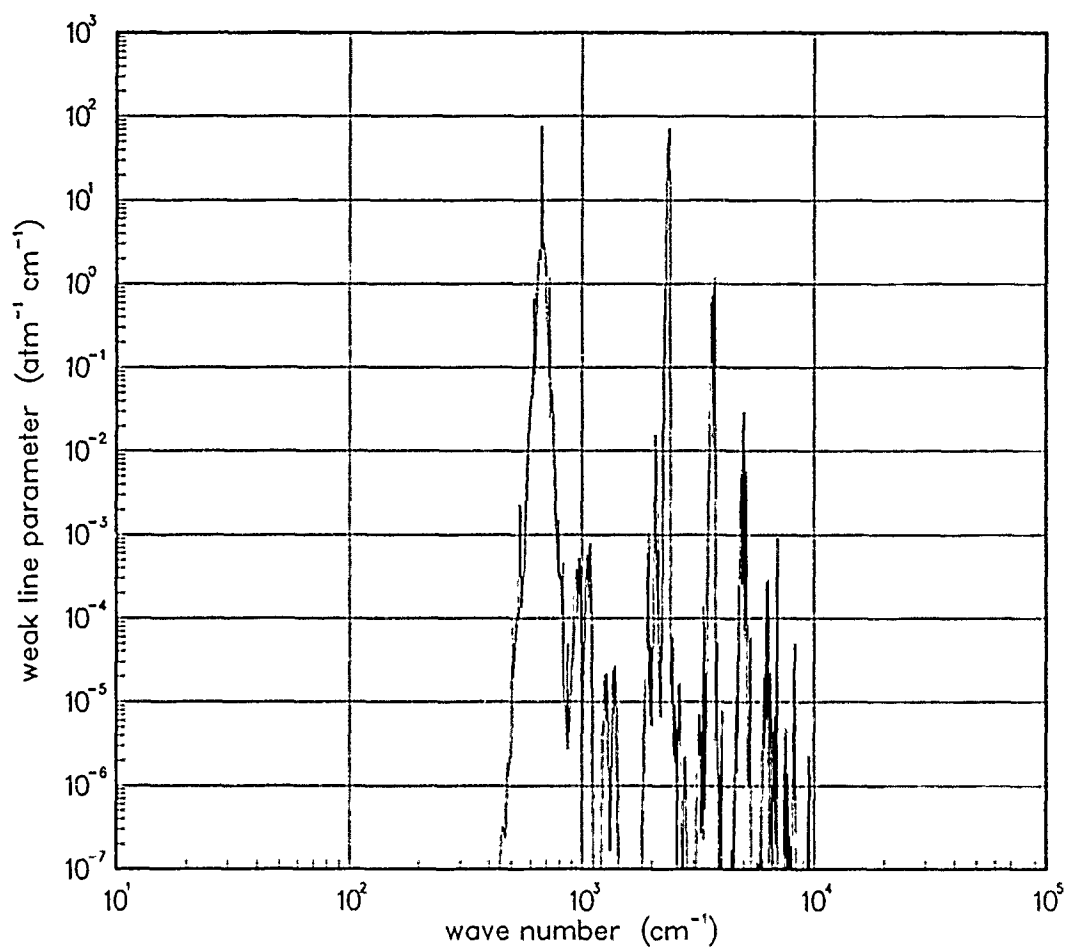


Figure 151. Weak-line parameter for CO₂ at 300°K.

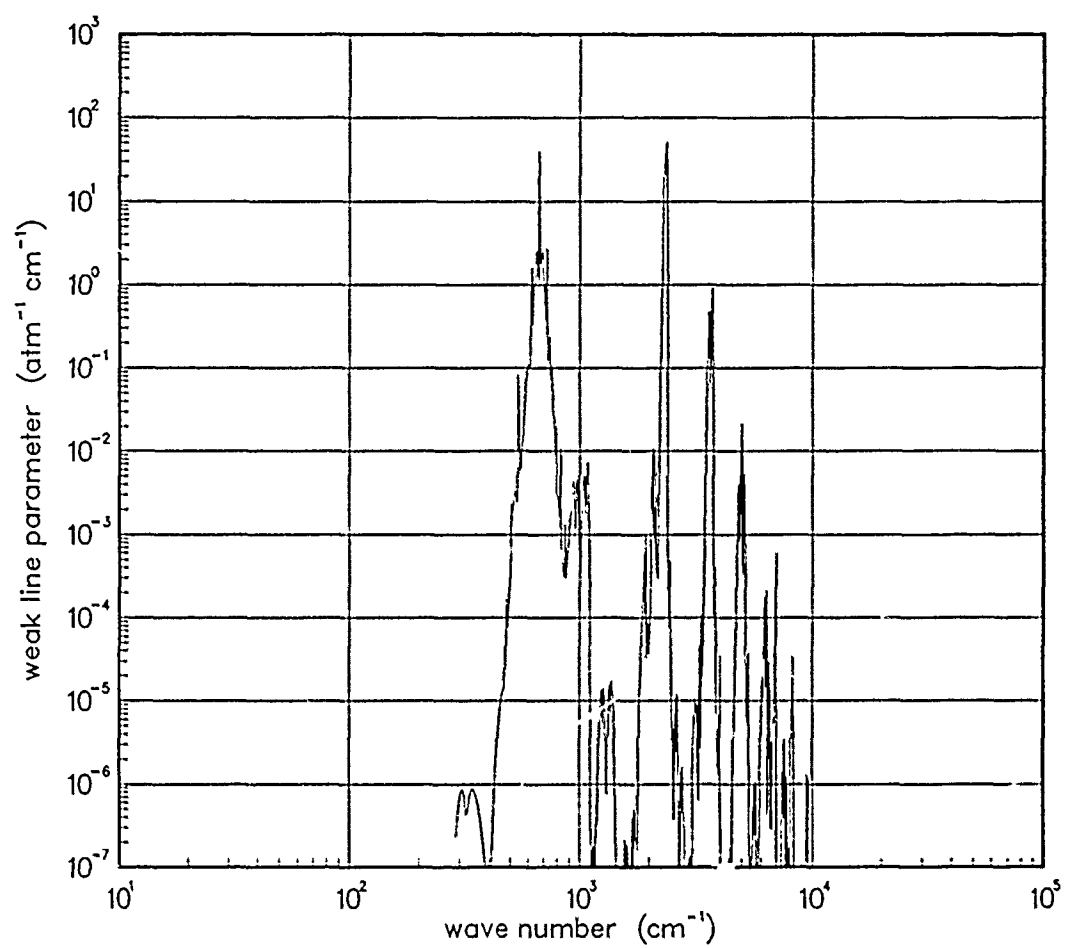


Figure 152. Weak-line parameter for CO₂ at 500°K.

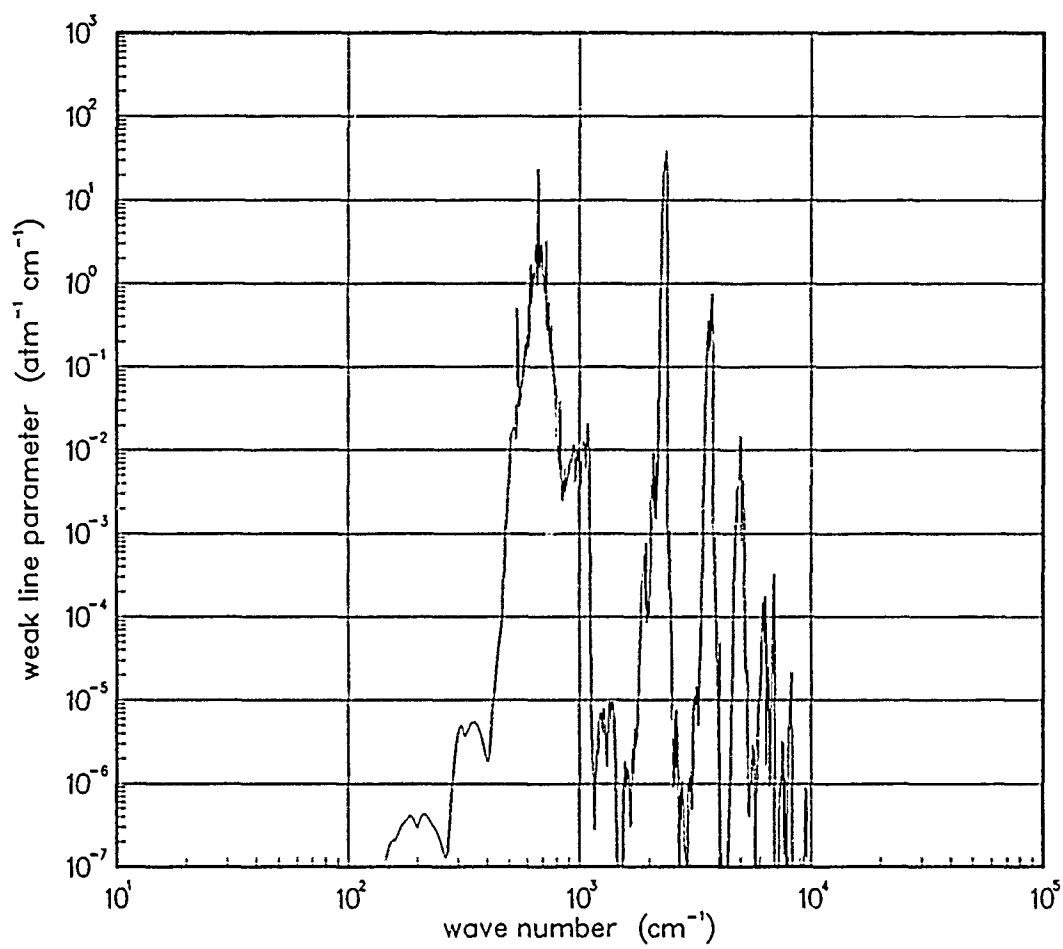


Figure 153. Weak-line parameter for CO₂ at 750°K.

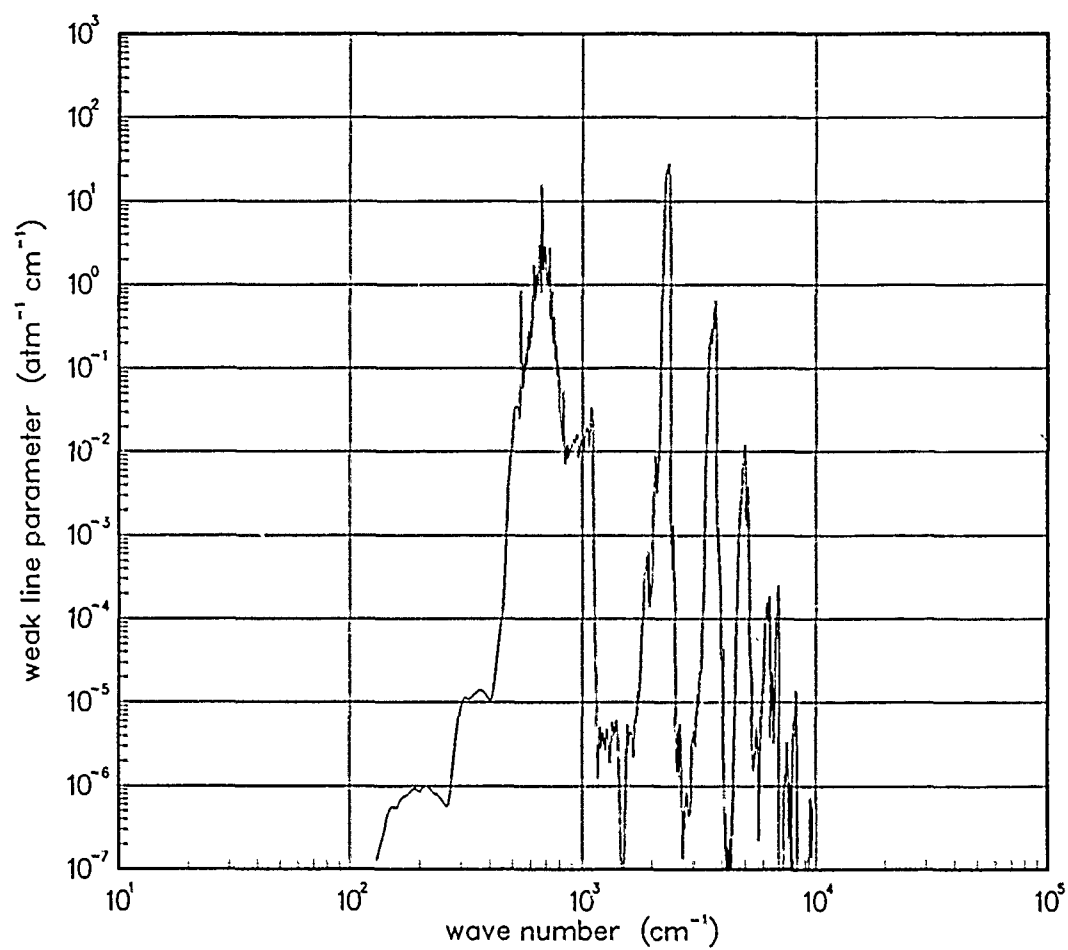


Figure 154. Weak-line parameter for CO₂ at 1000°K.

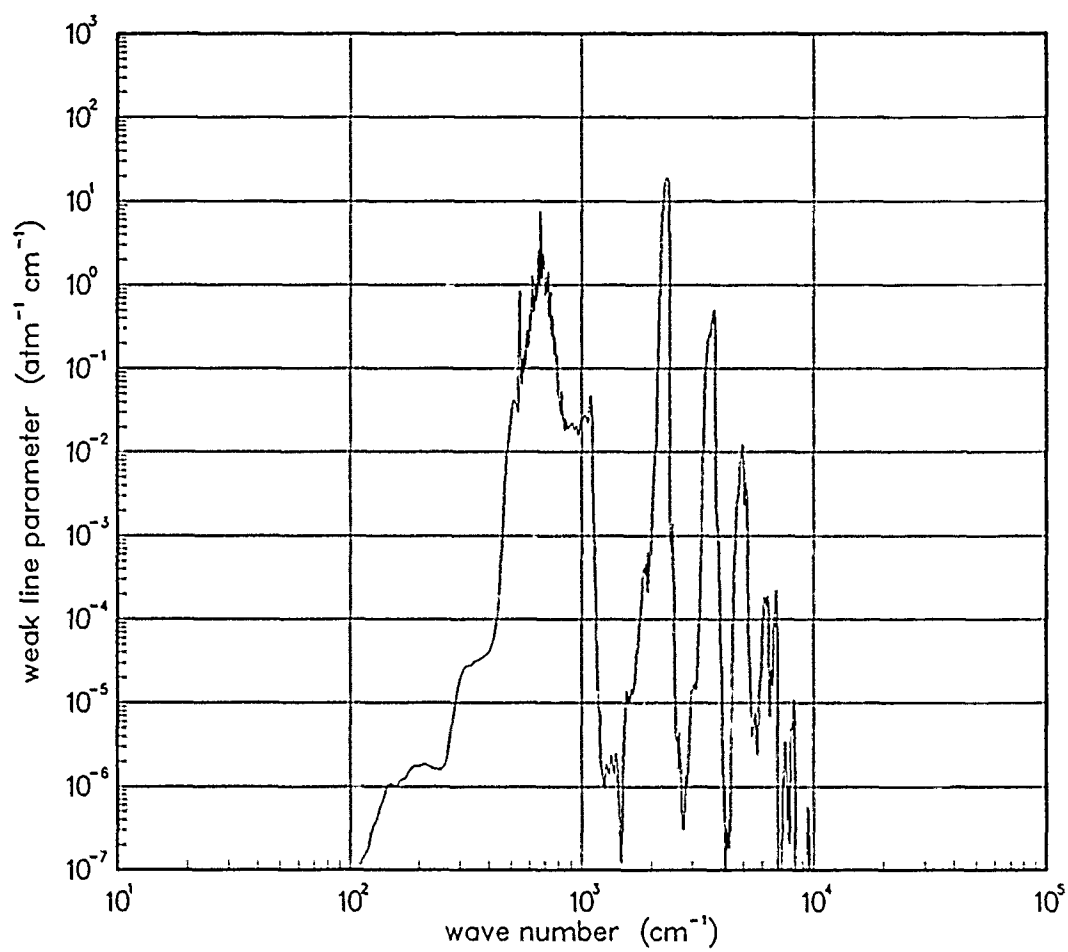


Figure 155. Weak-line parameter for CO₂ at 1500°K.

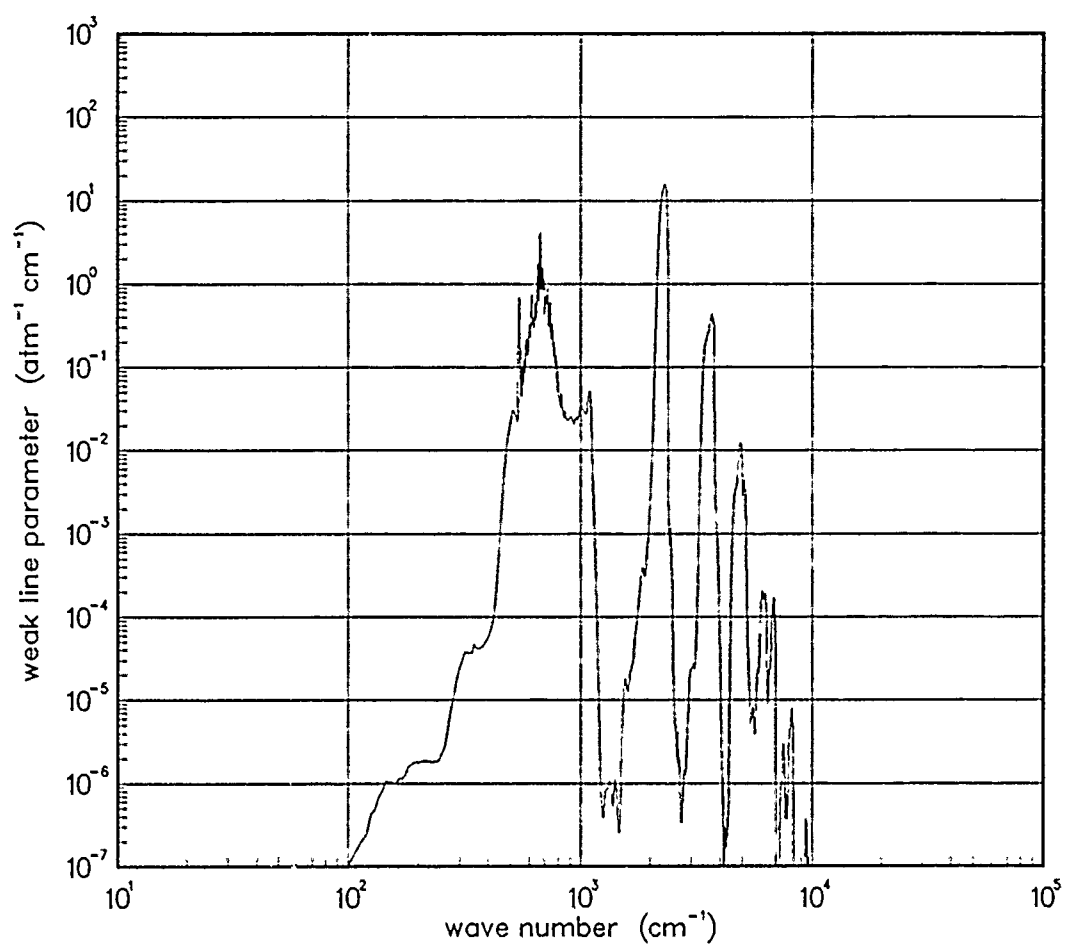


Figure 156. Weak-line parameter for CO₂ at 2000°K.

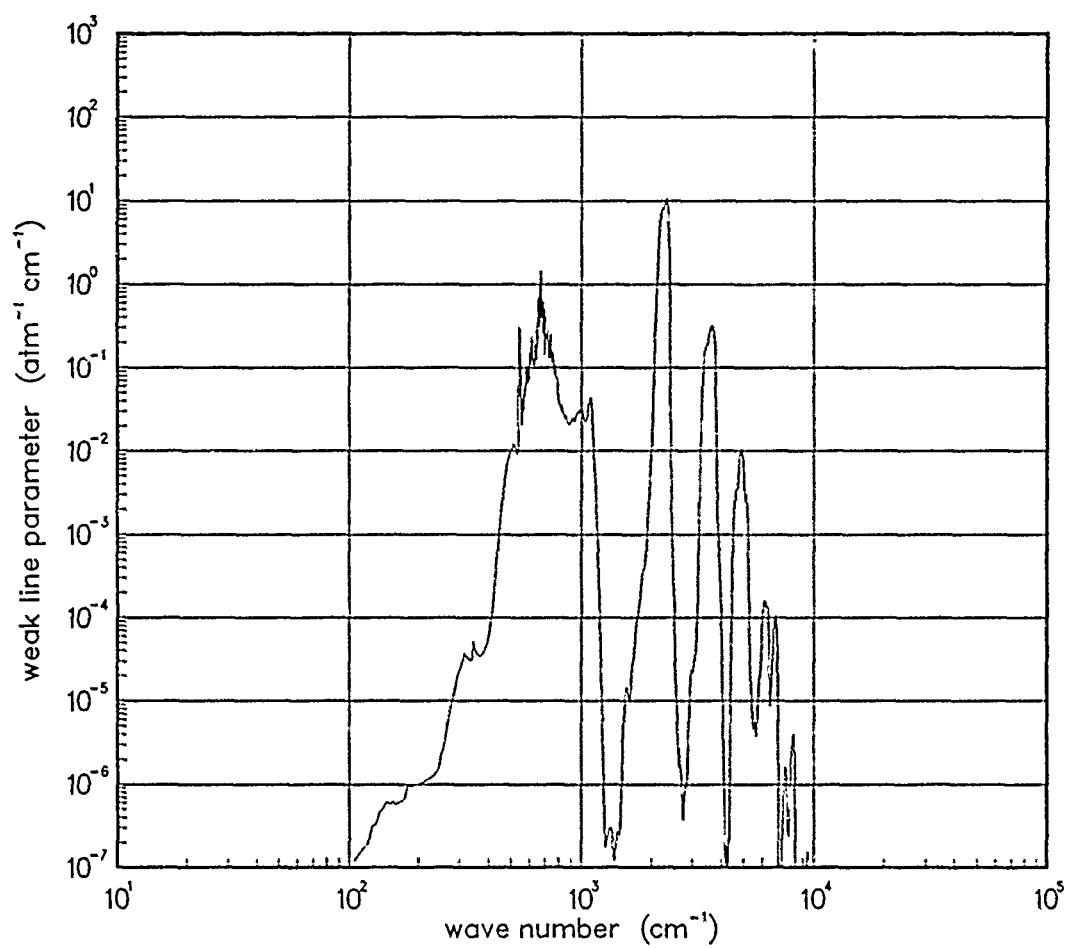


Figure 157. Weak-line parameter for CO₂ at 3000°K.

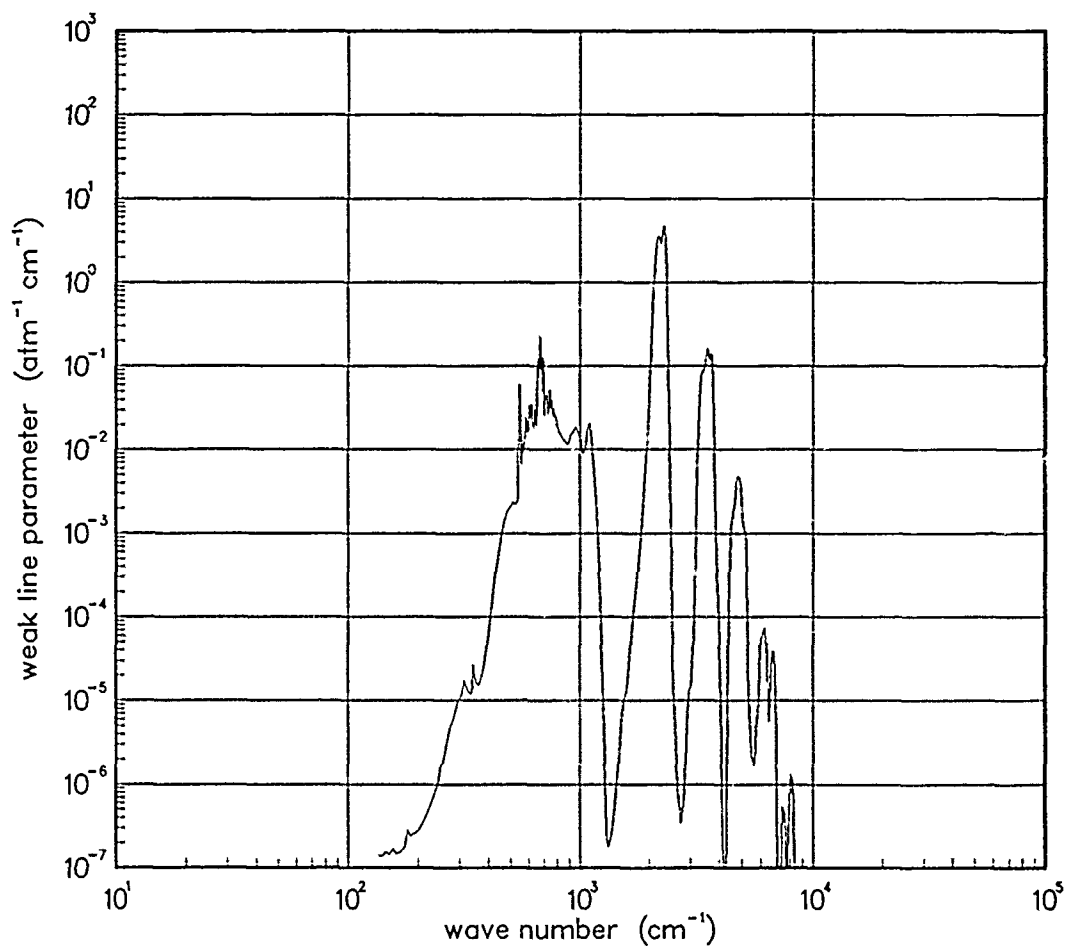


Figure 158. Weak-line parameter for CO₂ at 5000°K.

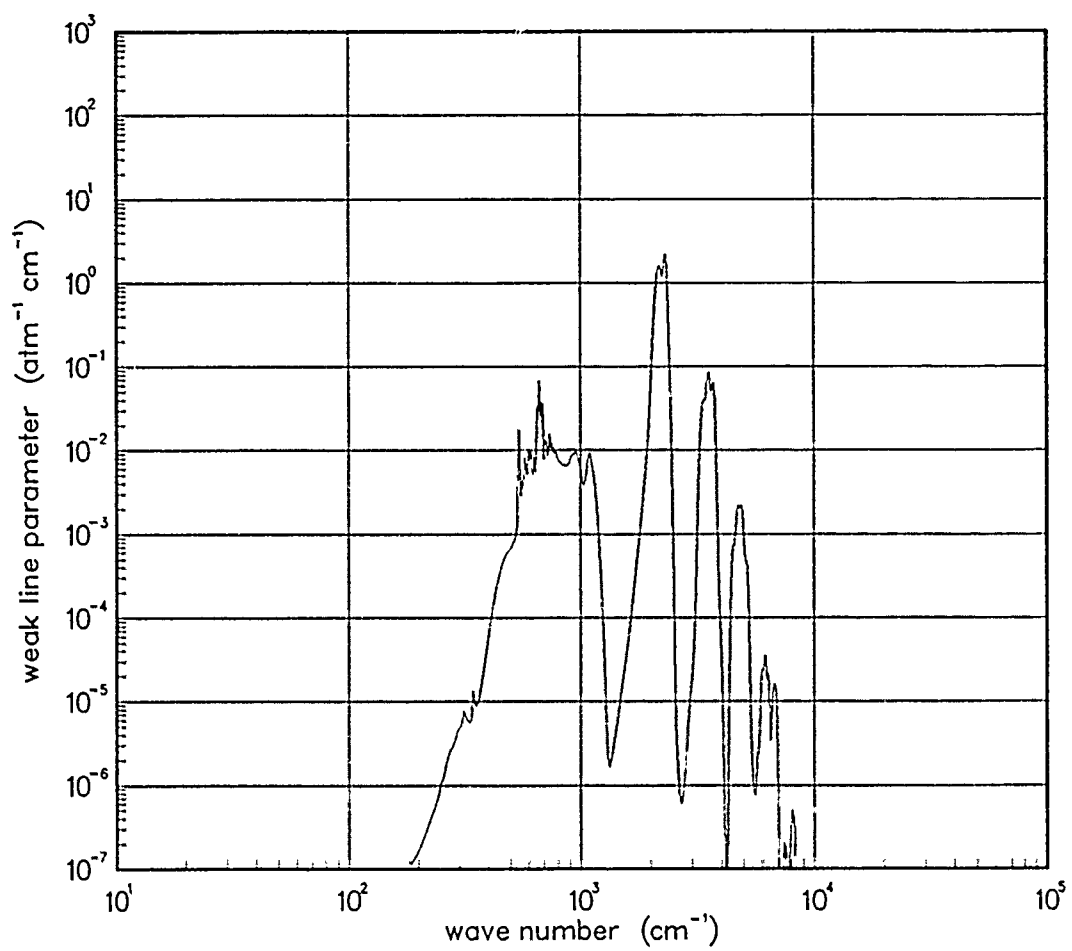


Figure 159. Weak-line parameter for CO₂ at 7000°K.

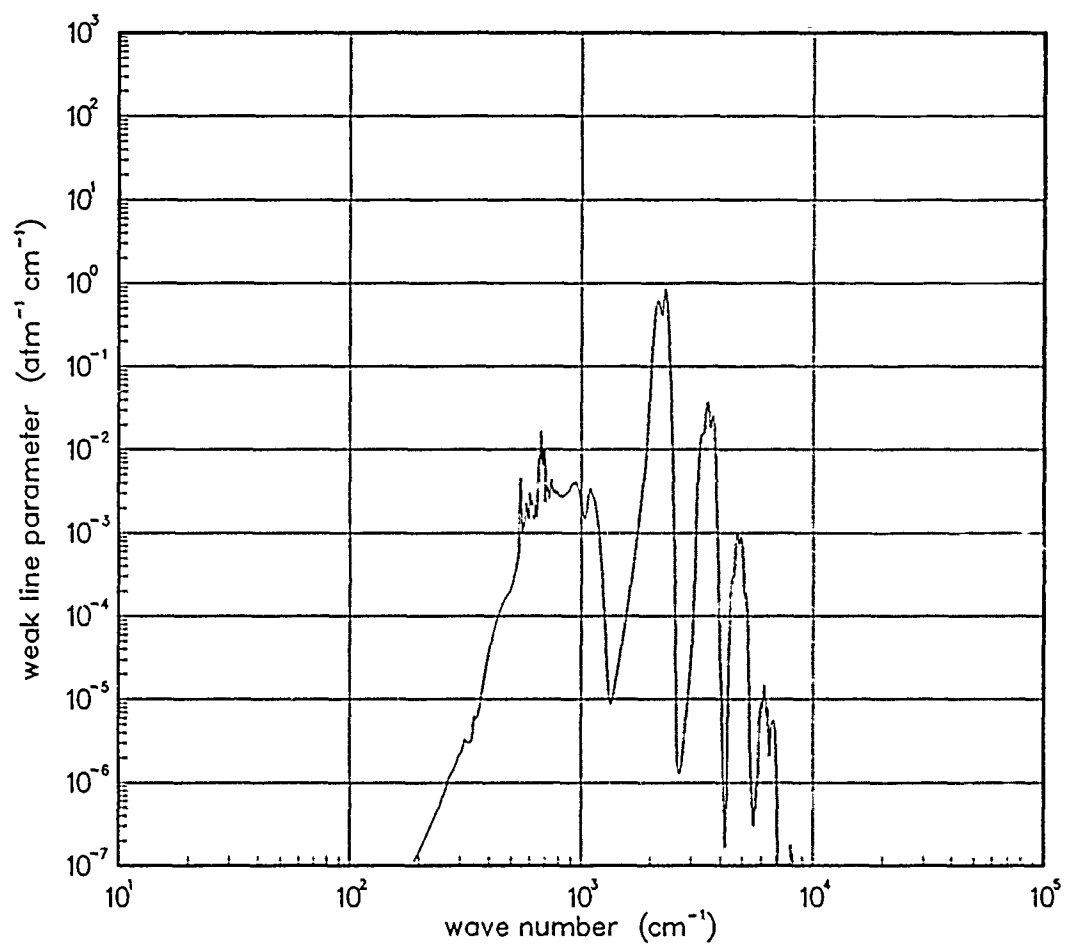


Figure 160. Weak-line parameter for CO₂ at 10000°K.

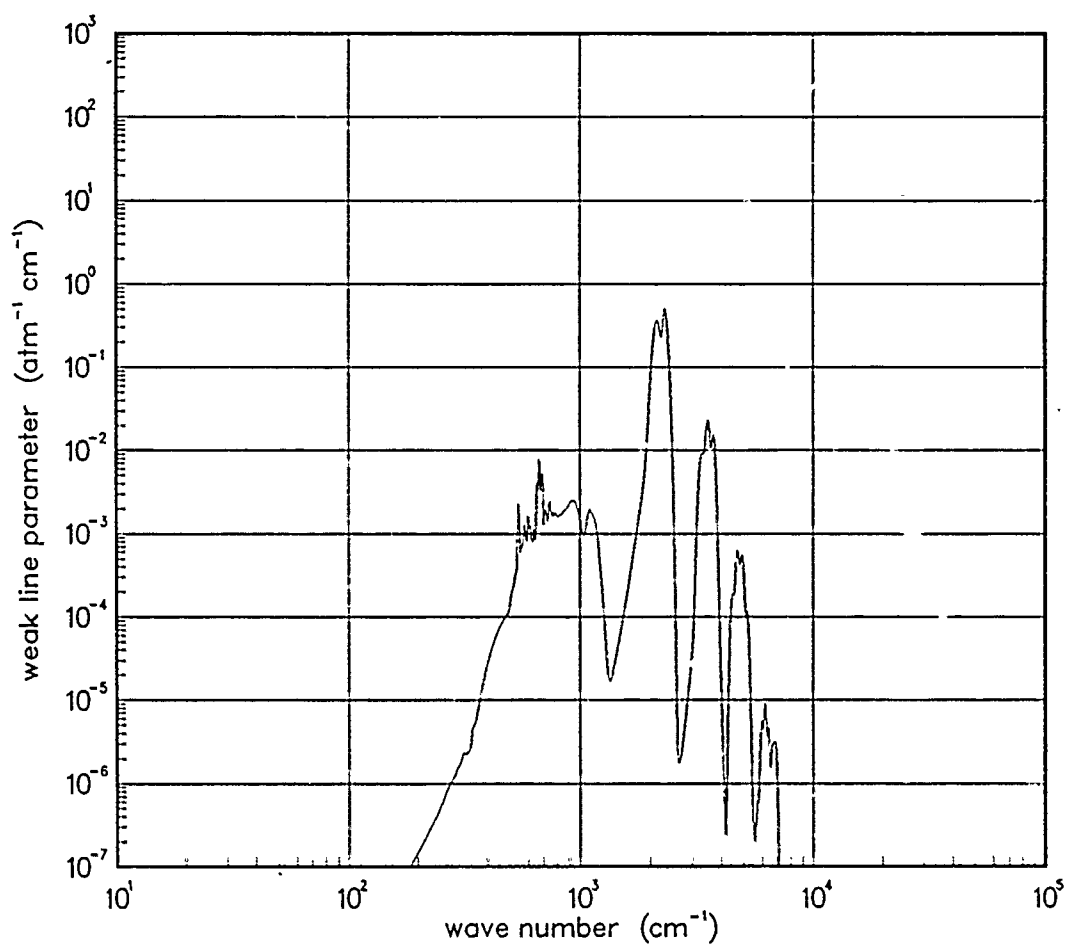


Figure 161. Weak-line parameter for CO₂ at 12000°K.

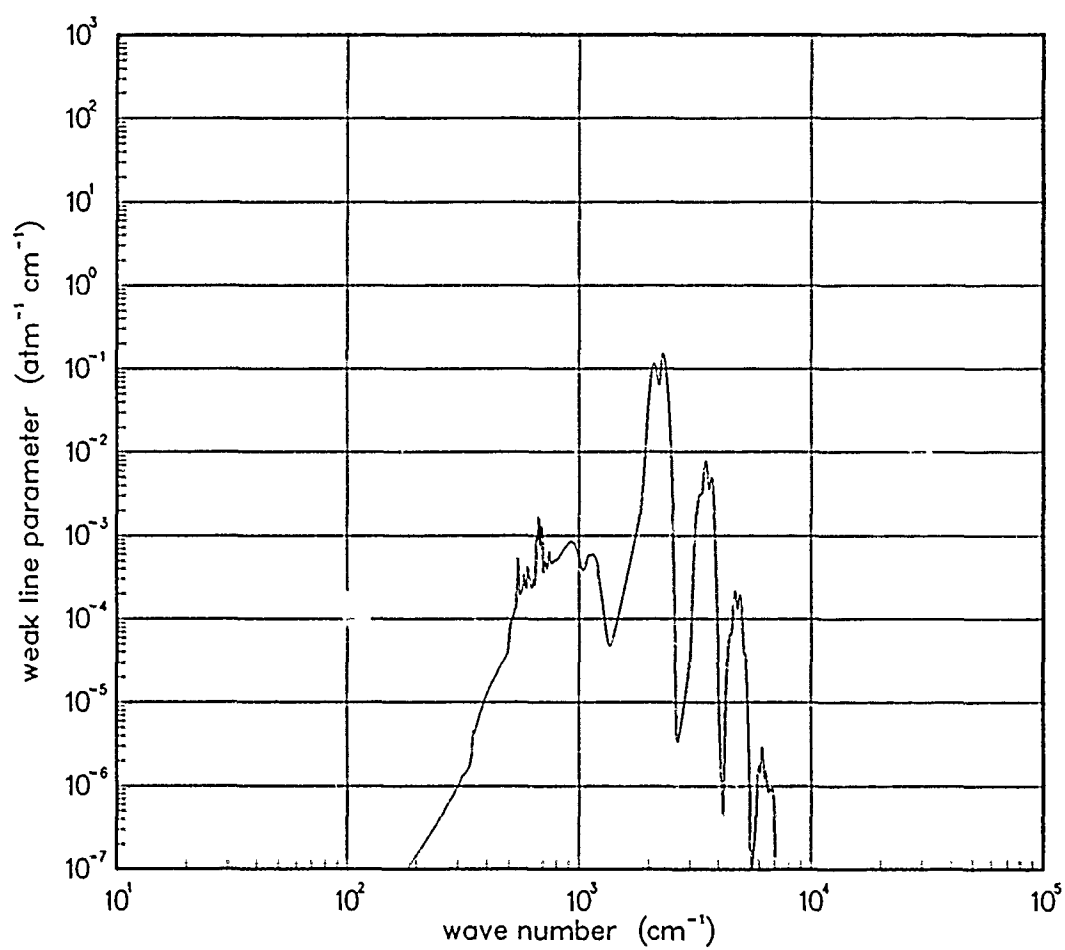


Figure 162. Weak-line parameter for CO₂ at 18000°K.

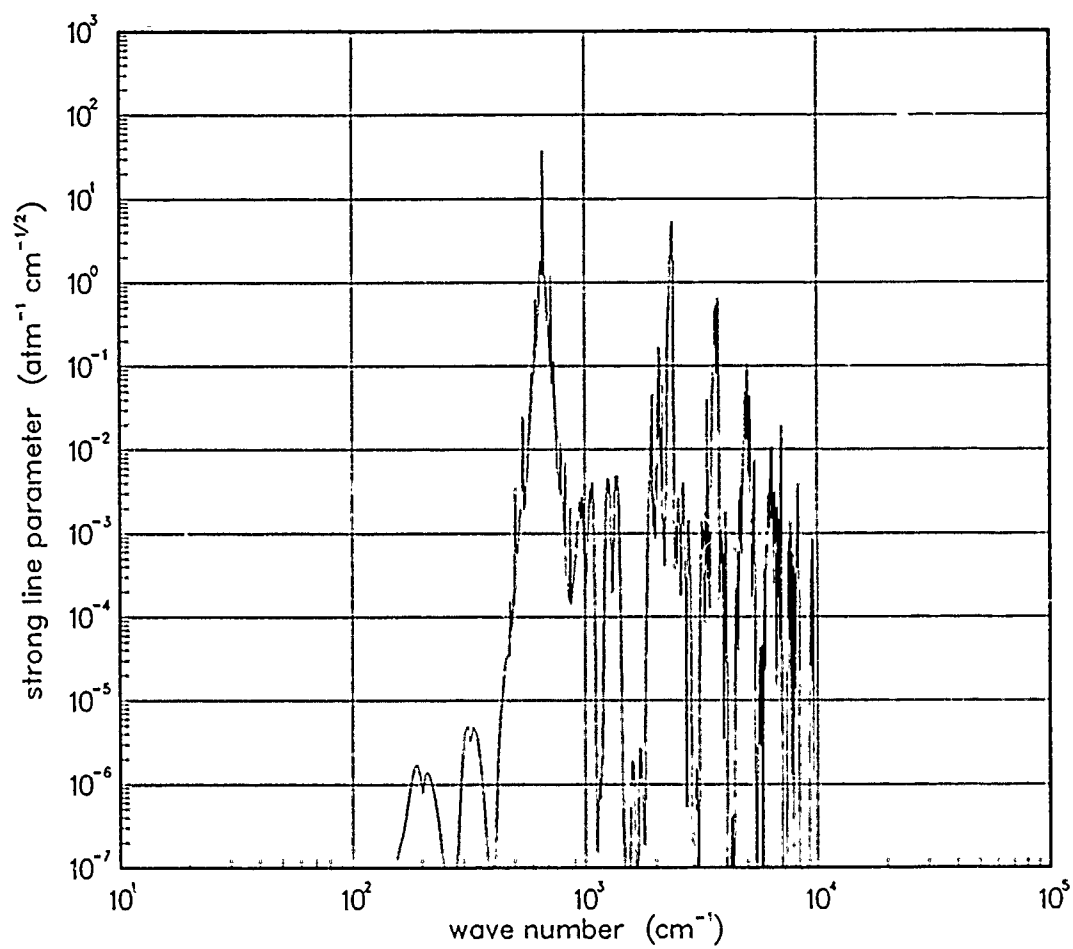


Figure 163. Strong-line parameter for CO₂ at 200°K.

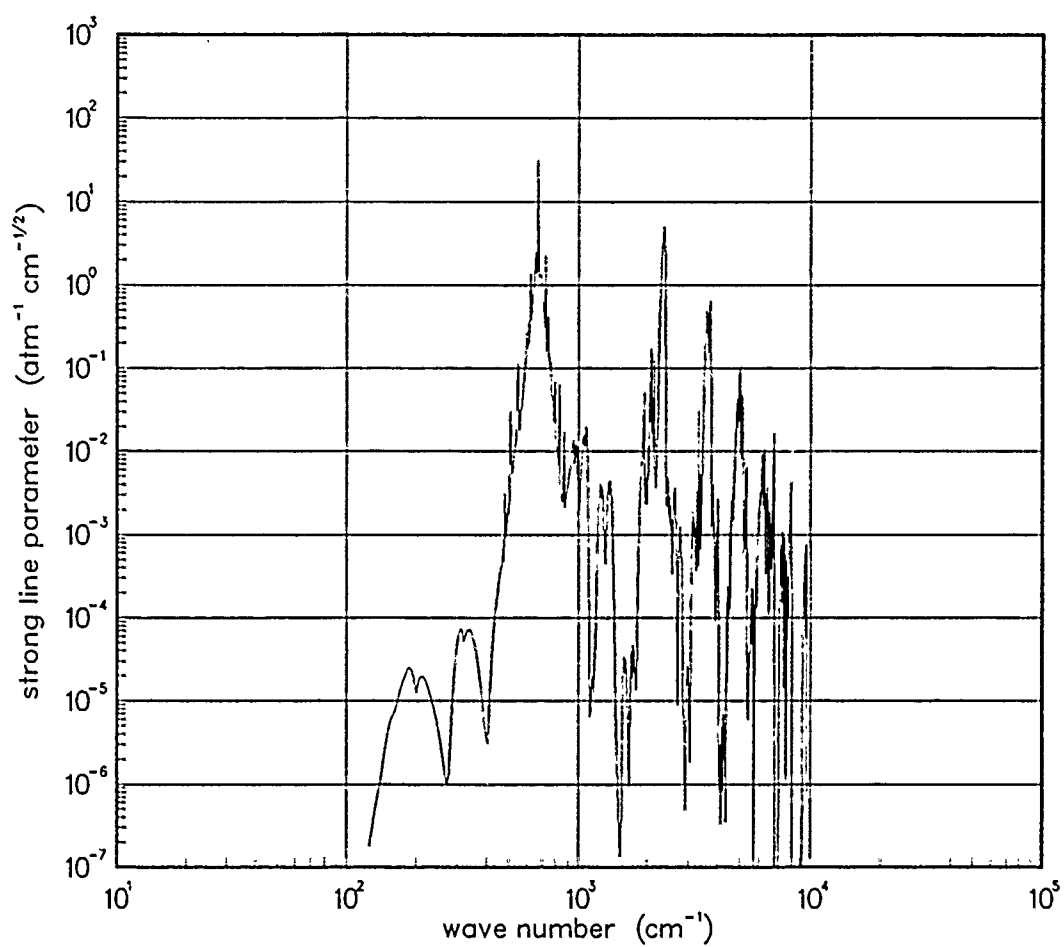


Figure 164. Strong-line parameter for CO₂ at 300°K.

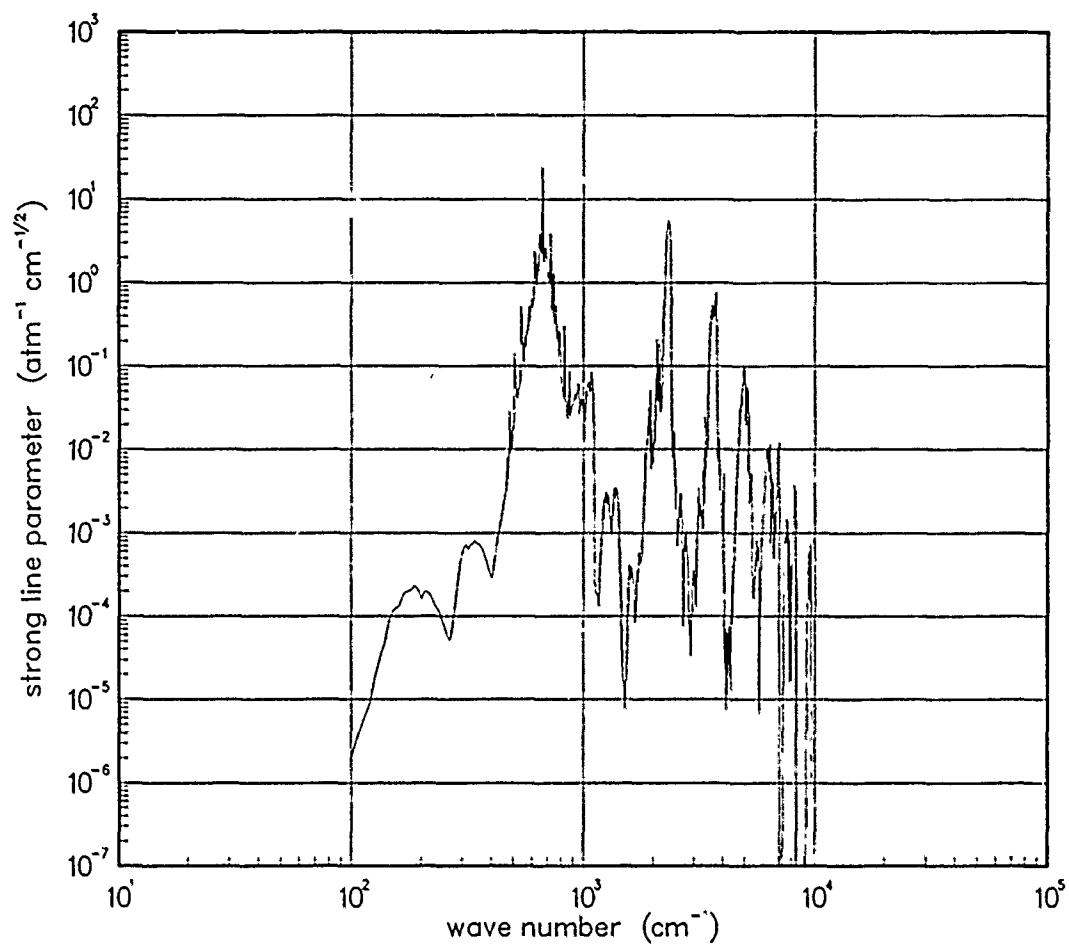


Figure 165. Strong-line parameter for CO₂ at 500°K.

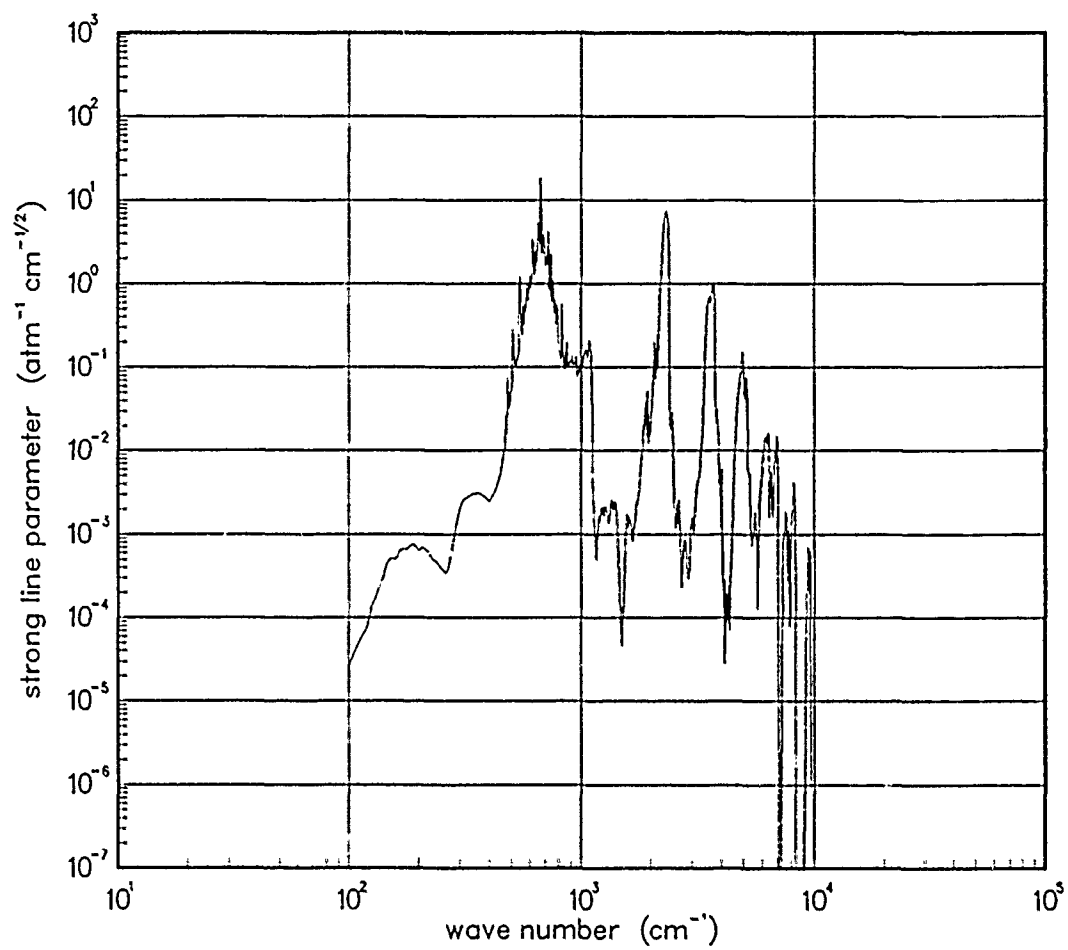


Figure 166. Strong-line parameter for CO₂ at 750°K.

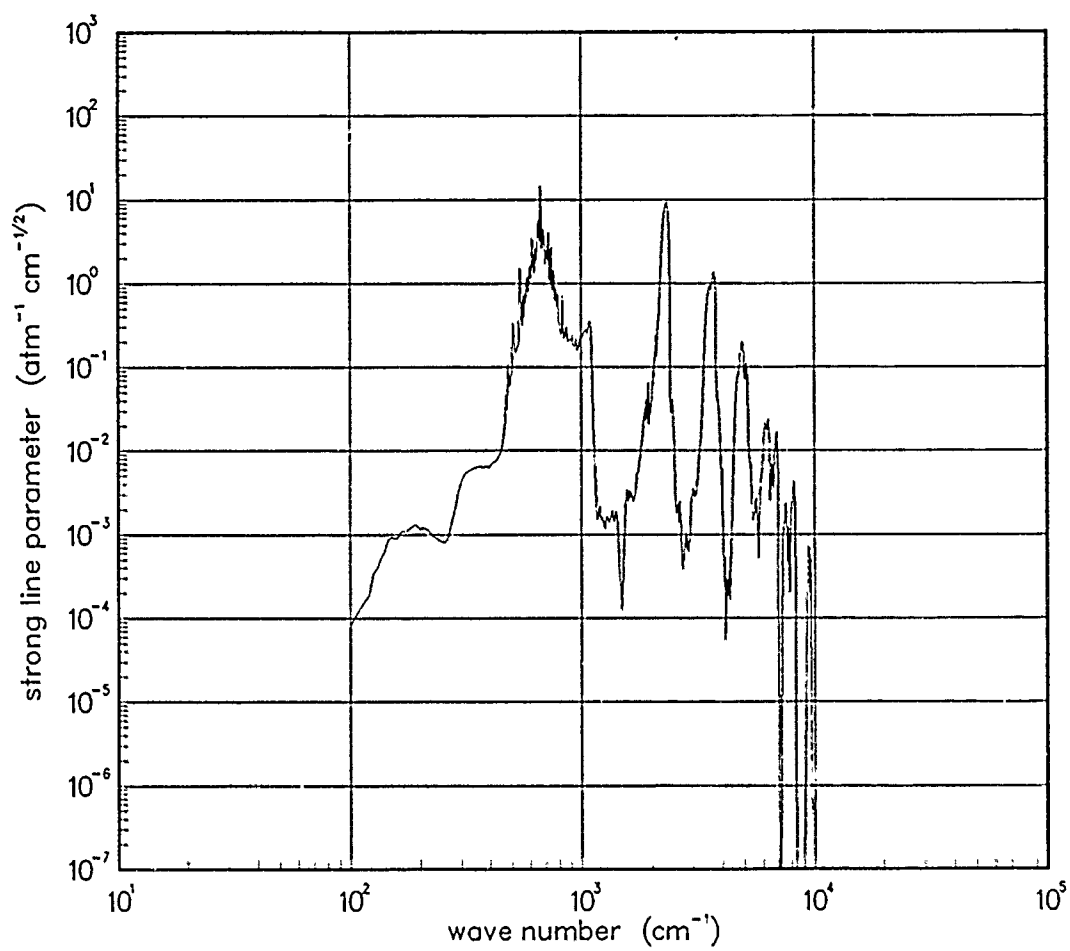


Figure 167. Strong-line parameter for CO₂ at 1000°K.

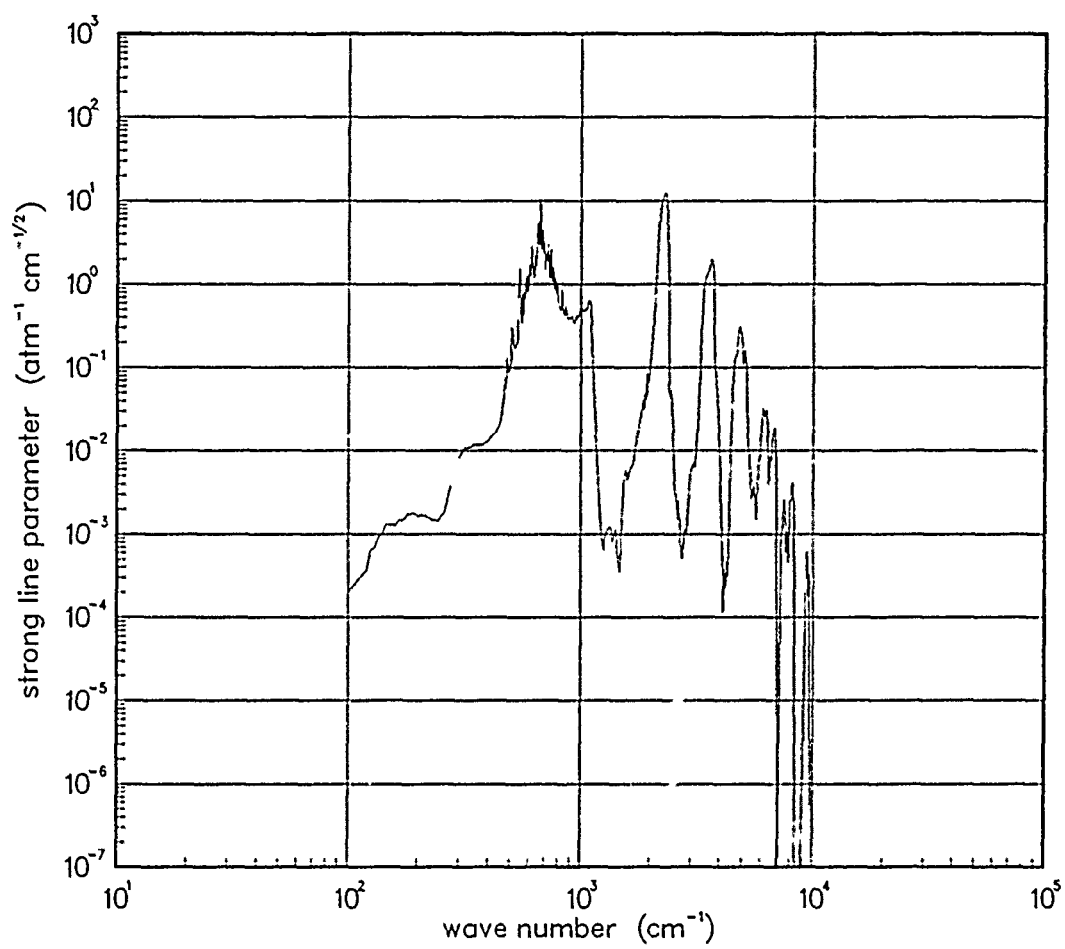


Figure 168. Strong-line parameter for CO₂ at 1500°K.

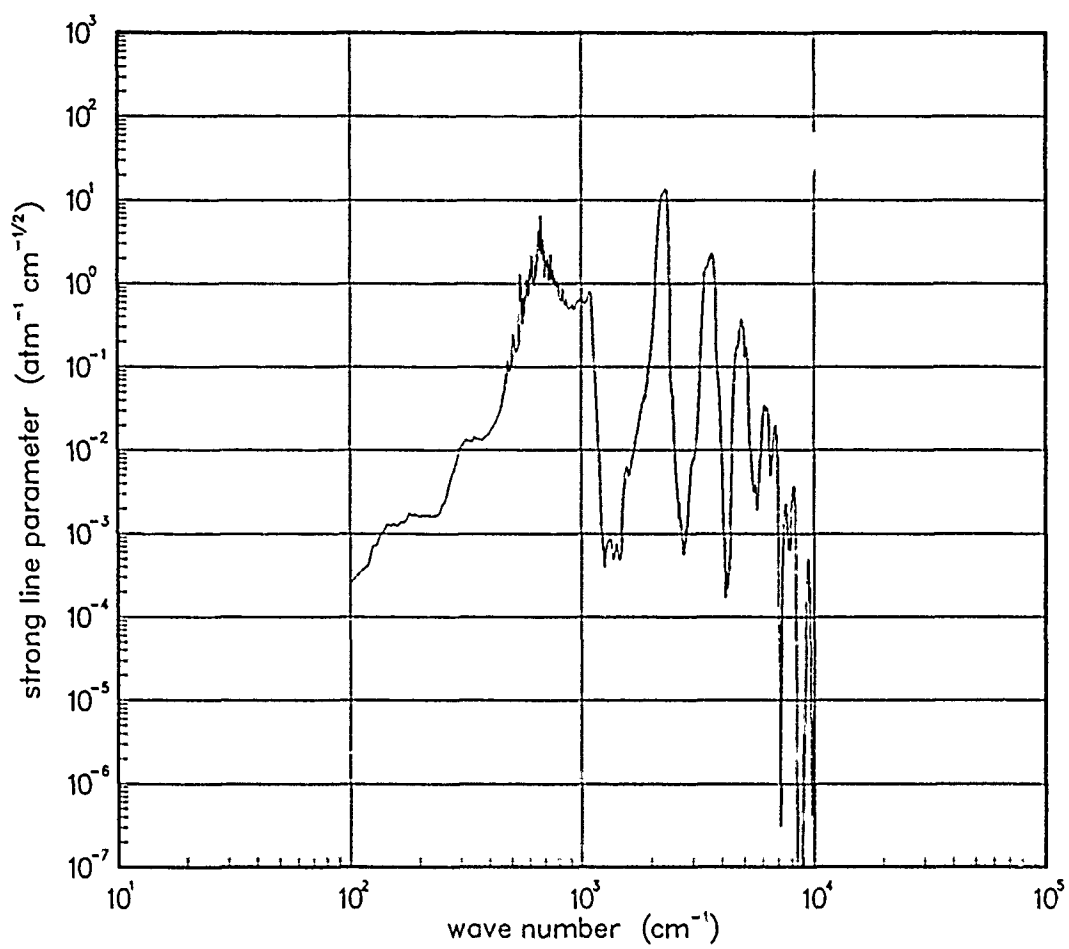


Figure 169. Strong-line parameter for CO₂ at 2000°K.

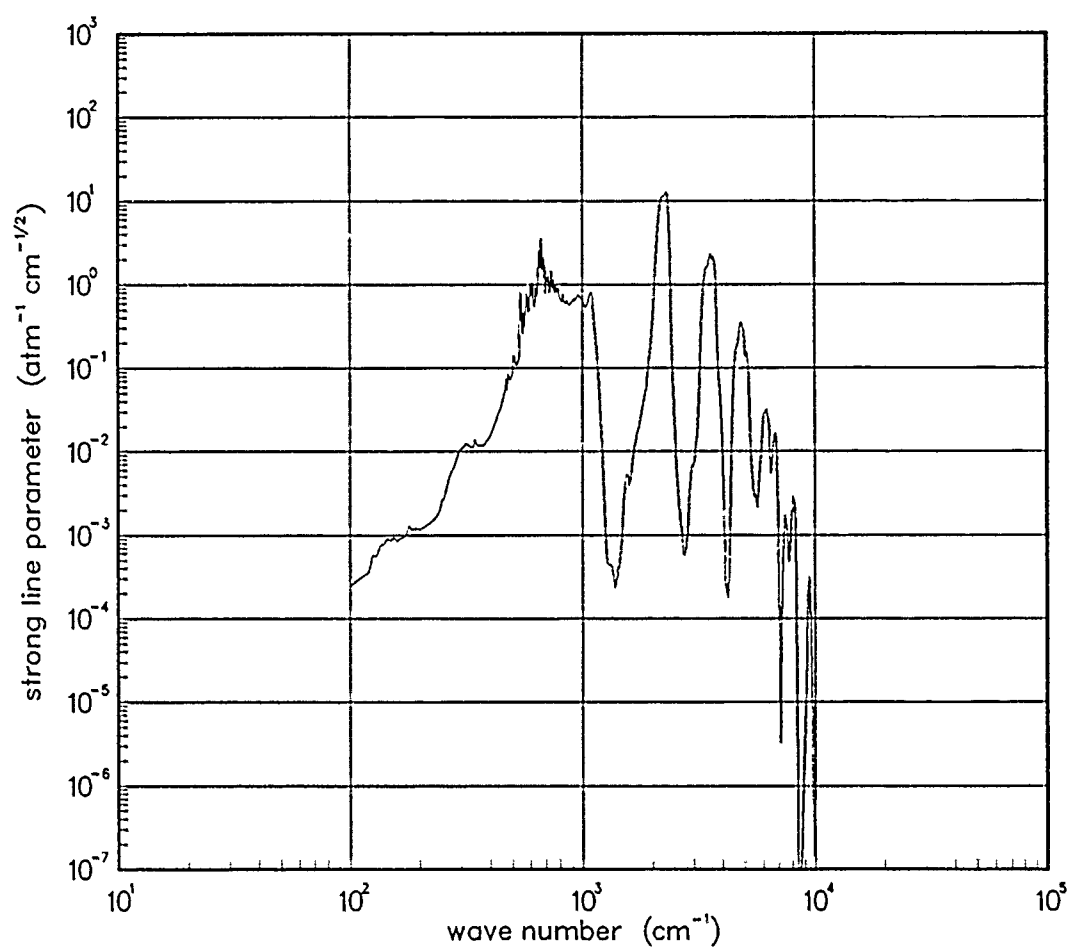


Figure 170. Strong-line parameter for CO₂ at 3000°K.

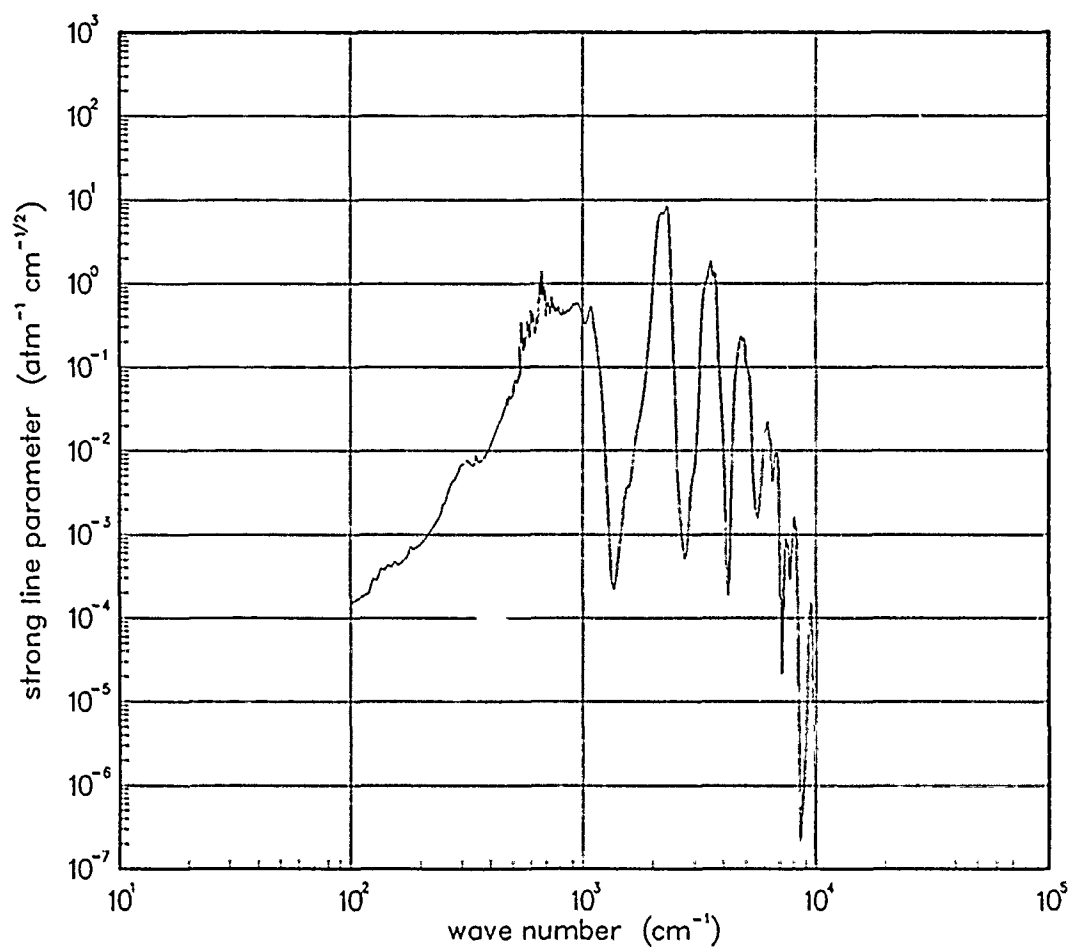


Figure 171. Strong-line parameter for CO₂ at 5000°K.

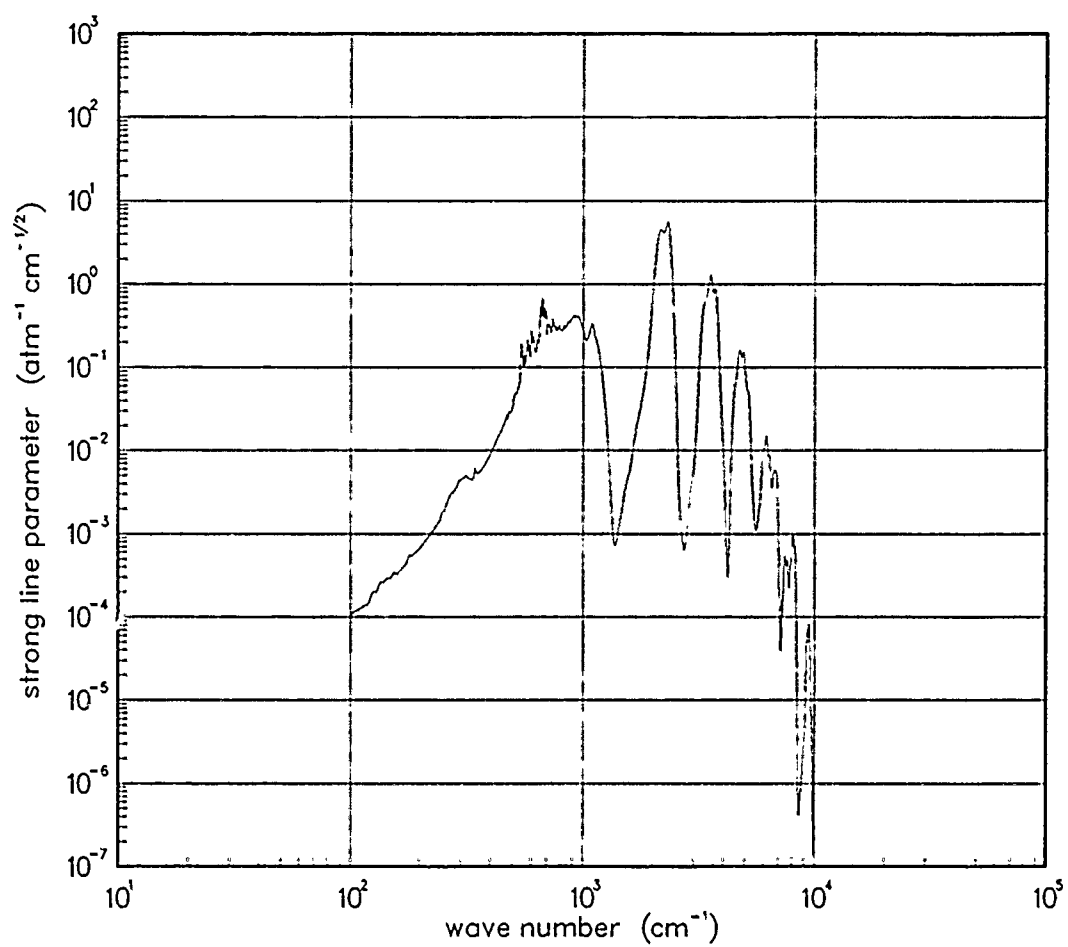


Figure 172. Strong-line parameter for CO₂ at 7000°K.

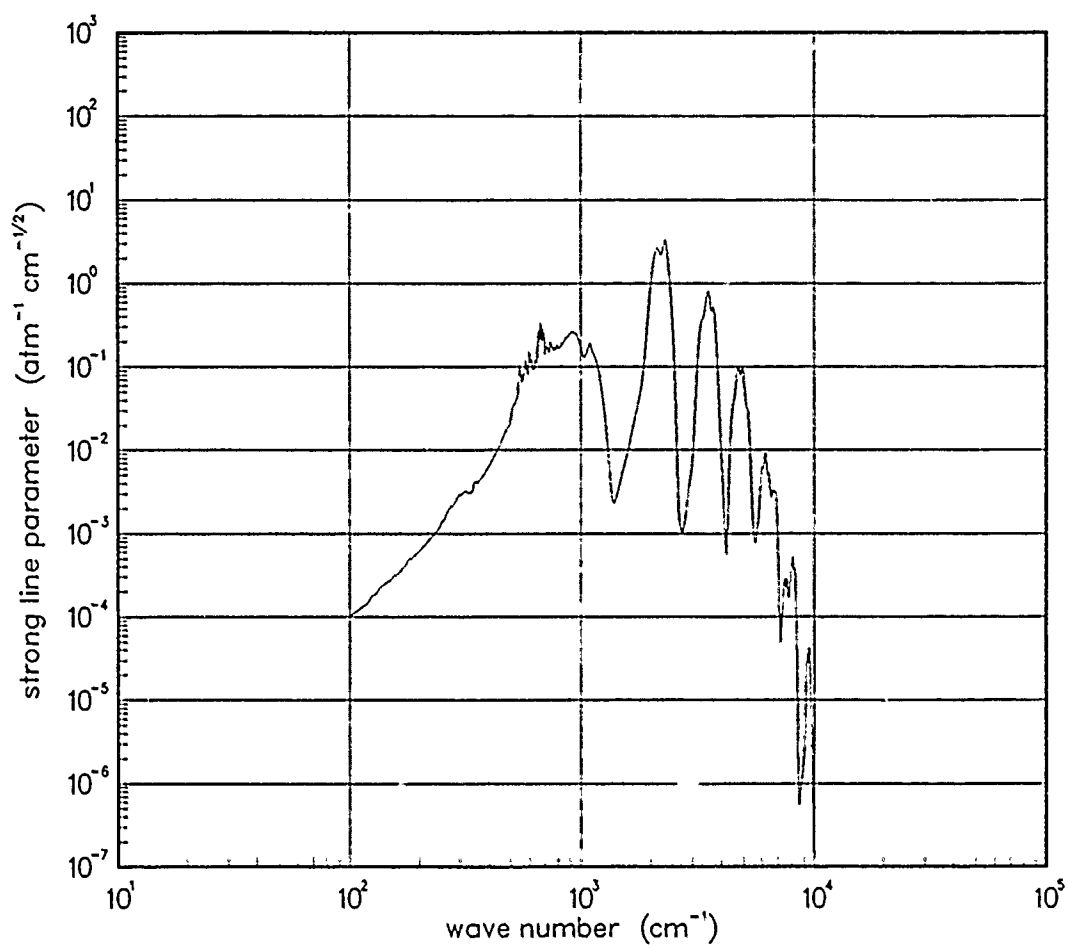


Figure 173. Strong-line parameter for CO₂ at 10000°K.

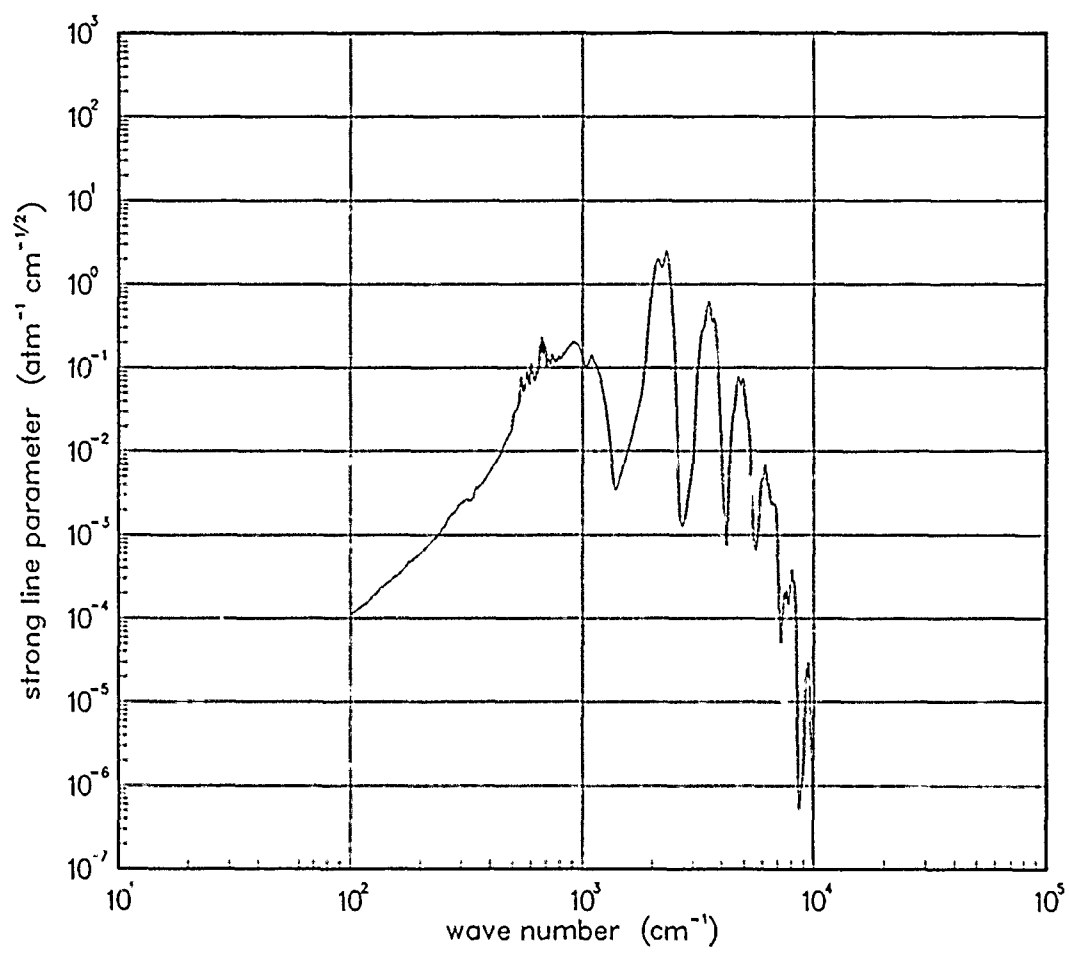


Figure 174. Strong-line parameter for CO₂ at 12000°K.

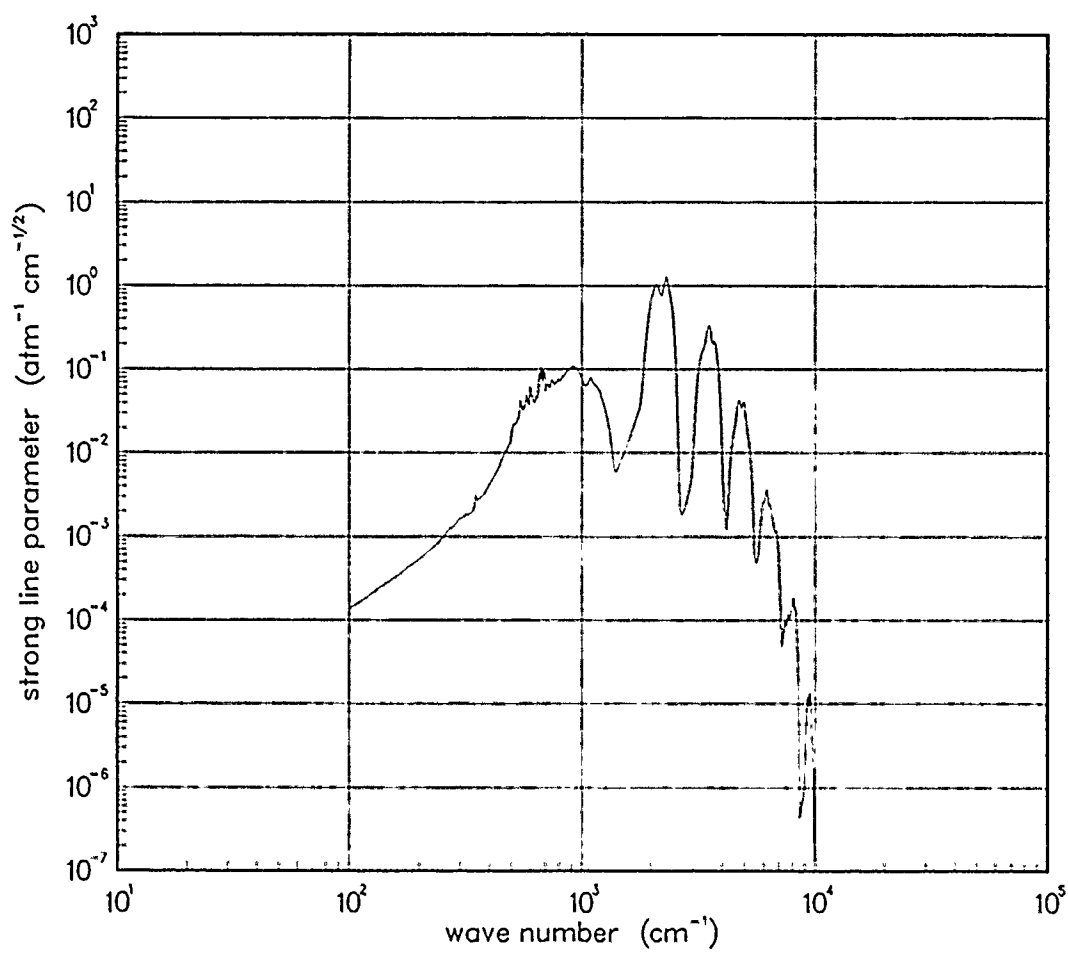


Figure 175. Strong-line parameter for CO₂ at 18000°K.

5.3 DINITROGEN OXIDE (N₂O).

The Data Curves for N₂O at temperatures < 1000 °K have been generated from the Air Force Geophysical Laboratory Line Atlas*. At temperatures above 1000 °K the curves were generated by combining the Air Force Geophysical Laboratory spectra at high temperatures with the "Boxcar" shapes†.

Data Source:

*R.A. McClatchey, et al, AFCRL Atmospheric Line Parameters Compilation , AFCRL-TR-73-0096, Air Force Cambridge Research Laboratories, (January 1973) 1982 version of the data tape.

†L.E. Ewing, Modeling Detail in the Weapon Optical Effects Code (U) , 69TMP-77, General Electric -- TEMPO, (October 1969) (Secret-Restricted Data).

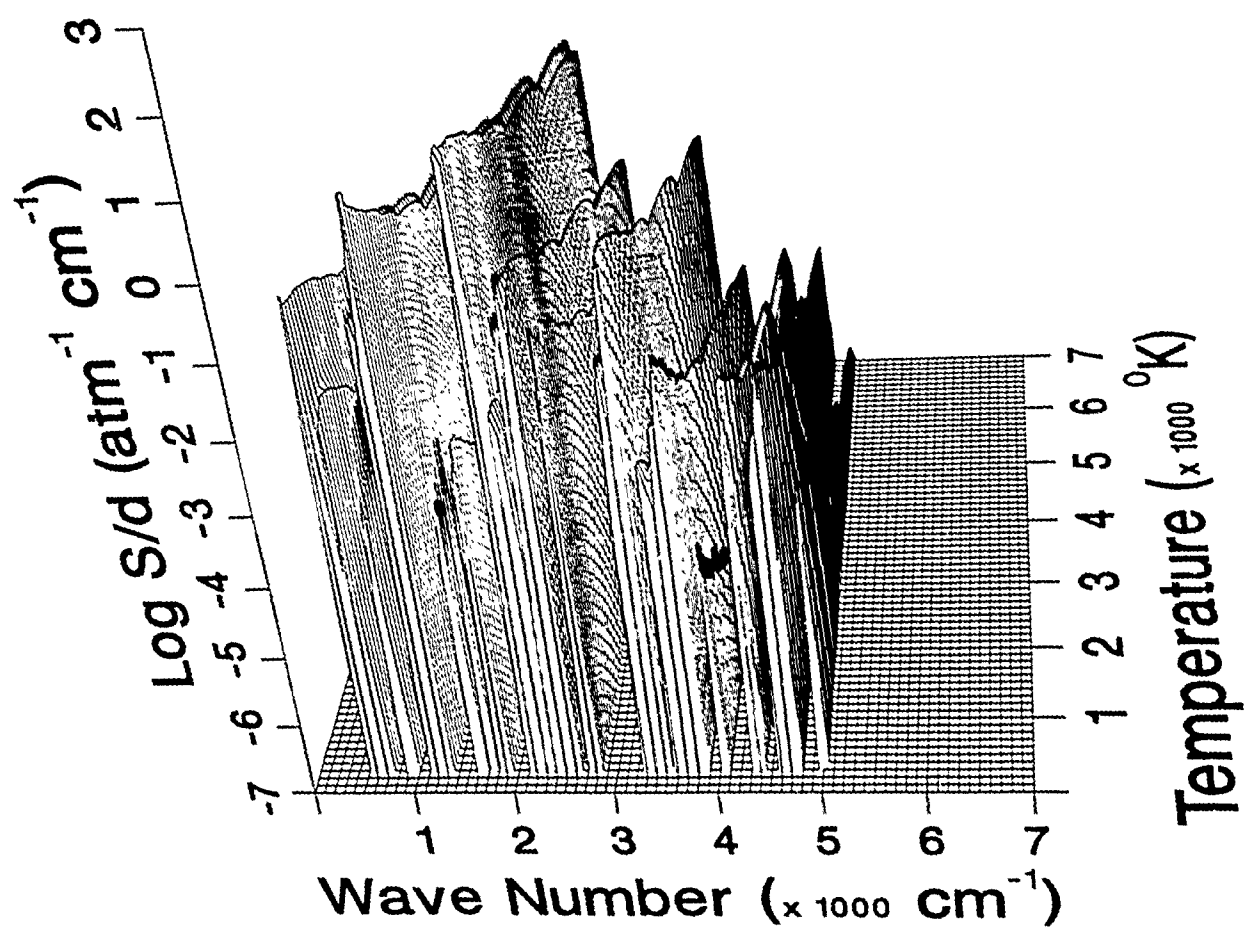


Figure 176. Weak-line parameter for N_2O .

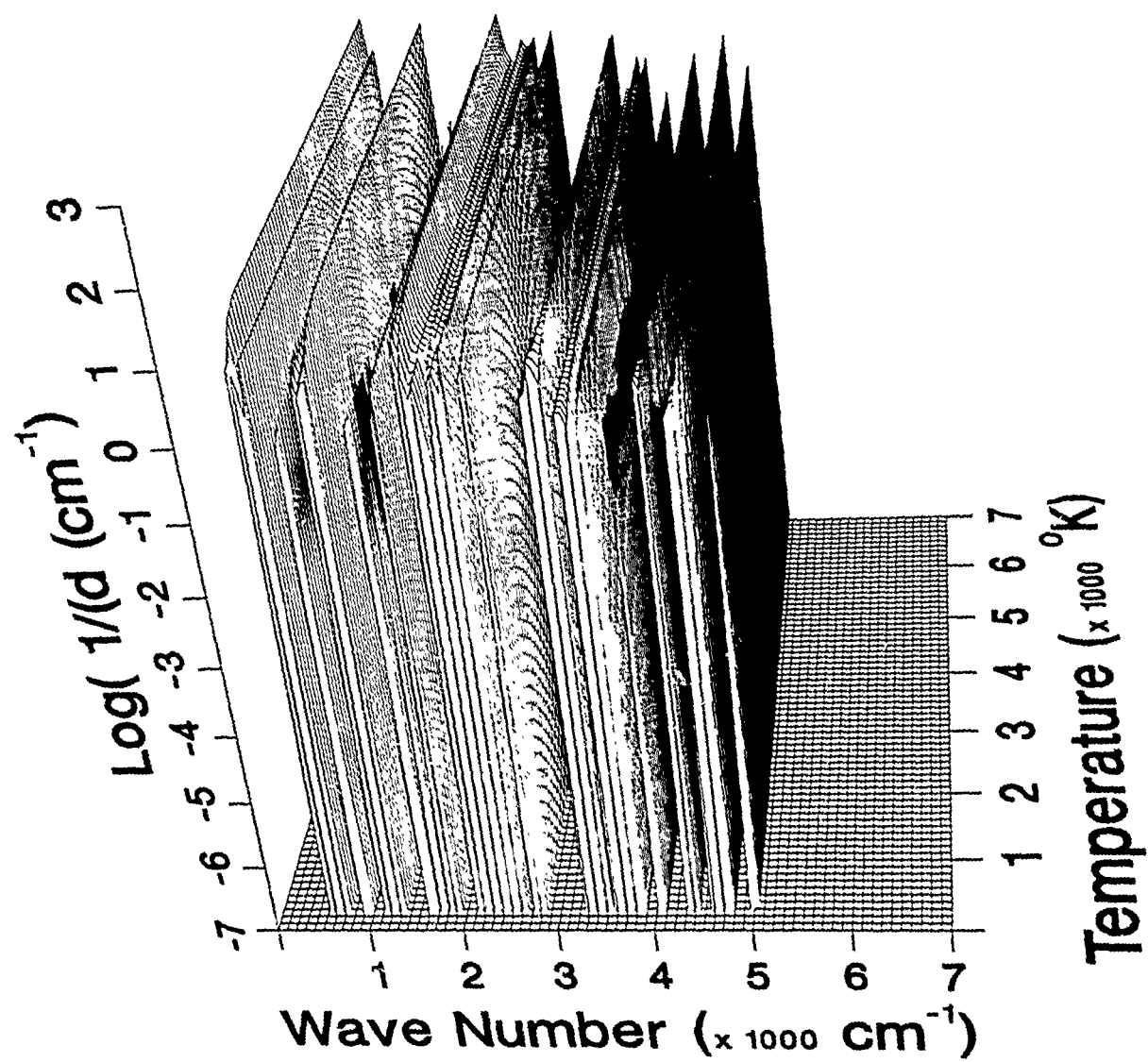


Figure 177. Inverse line spacing for N_2O .

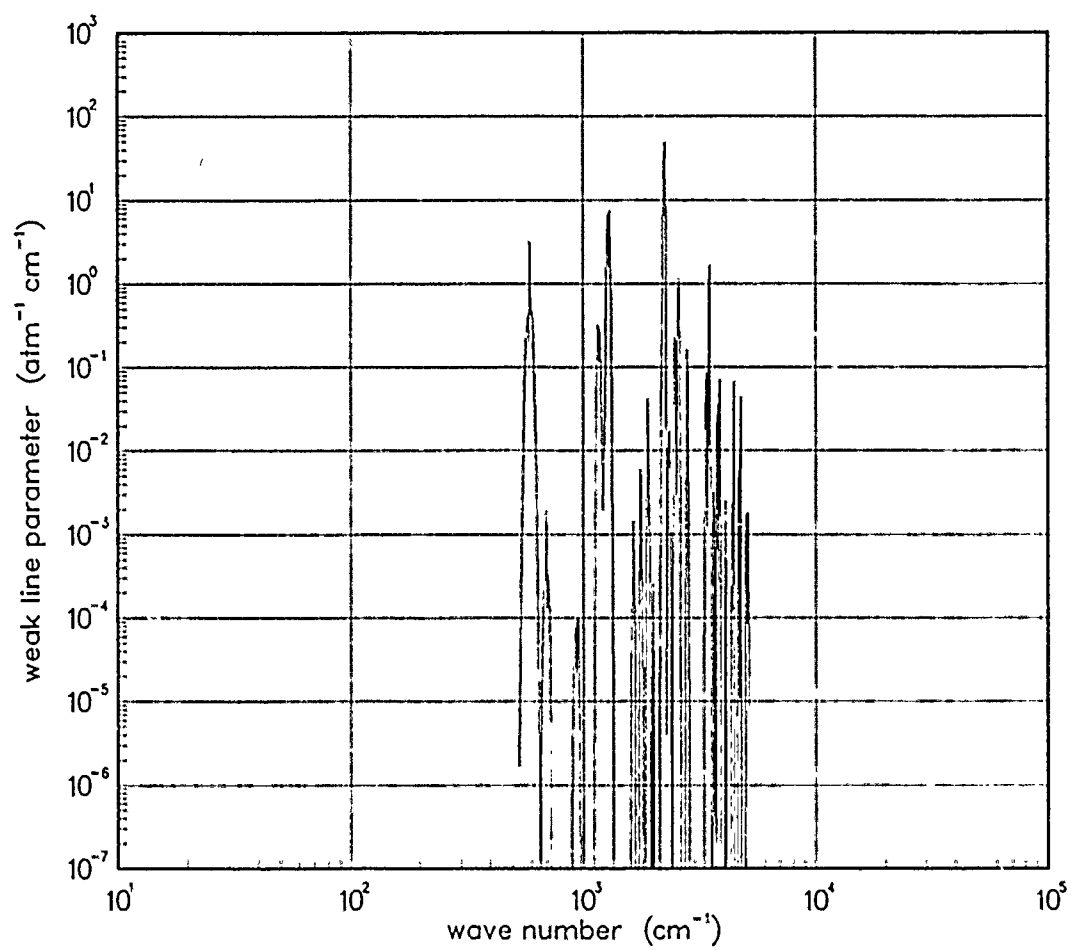


Figure 178. Weak-line parameter for N₂O at 200°K.

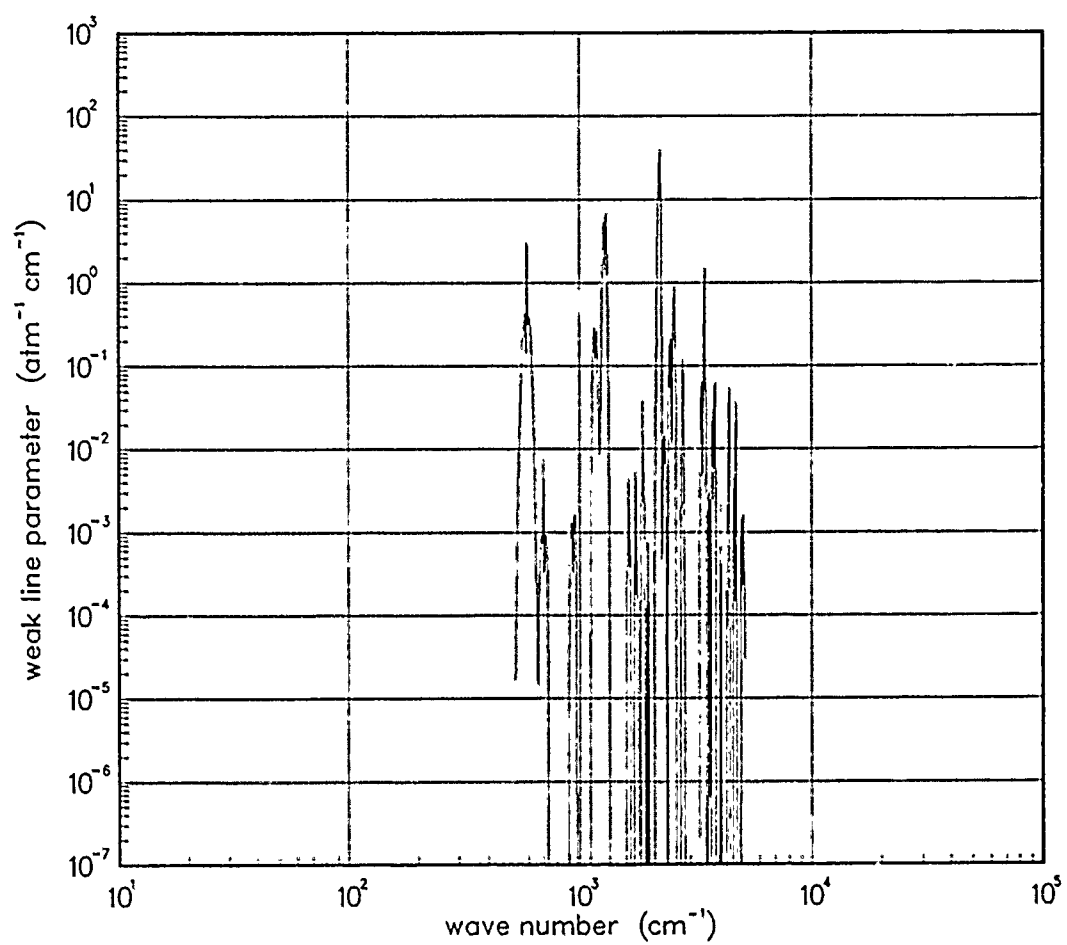


Figure 179. Weak-line parameter for N₂O at 300°K.

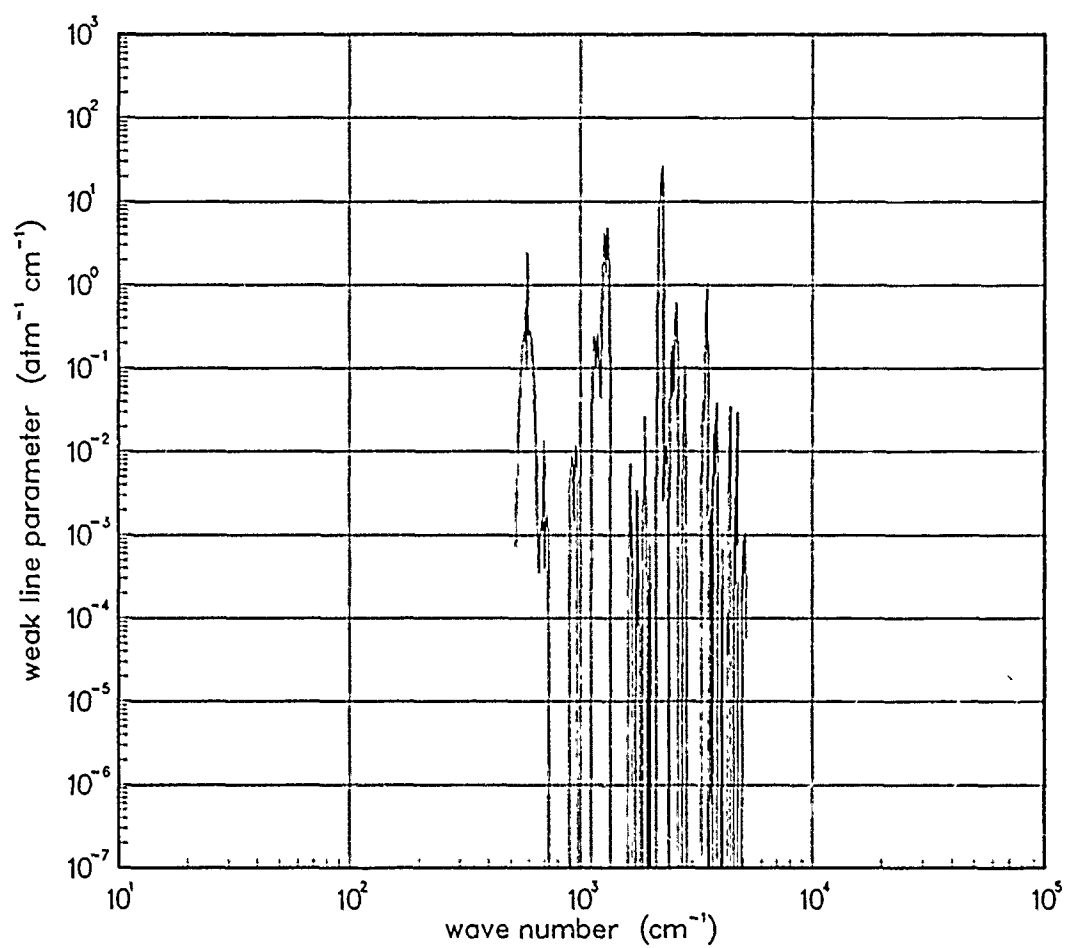


Figure 180. Weak-line parameter for N₂O at 500°K.

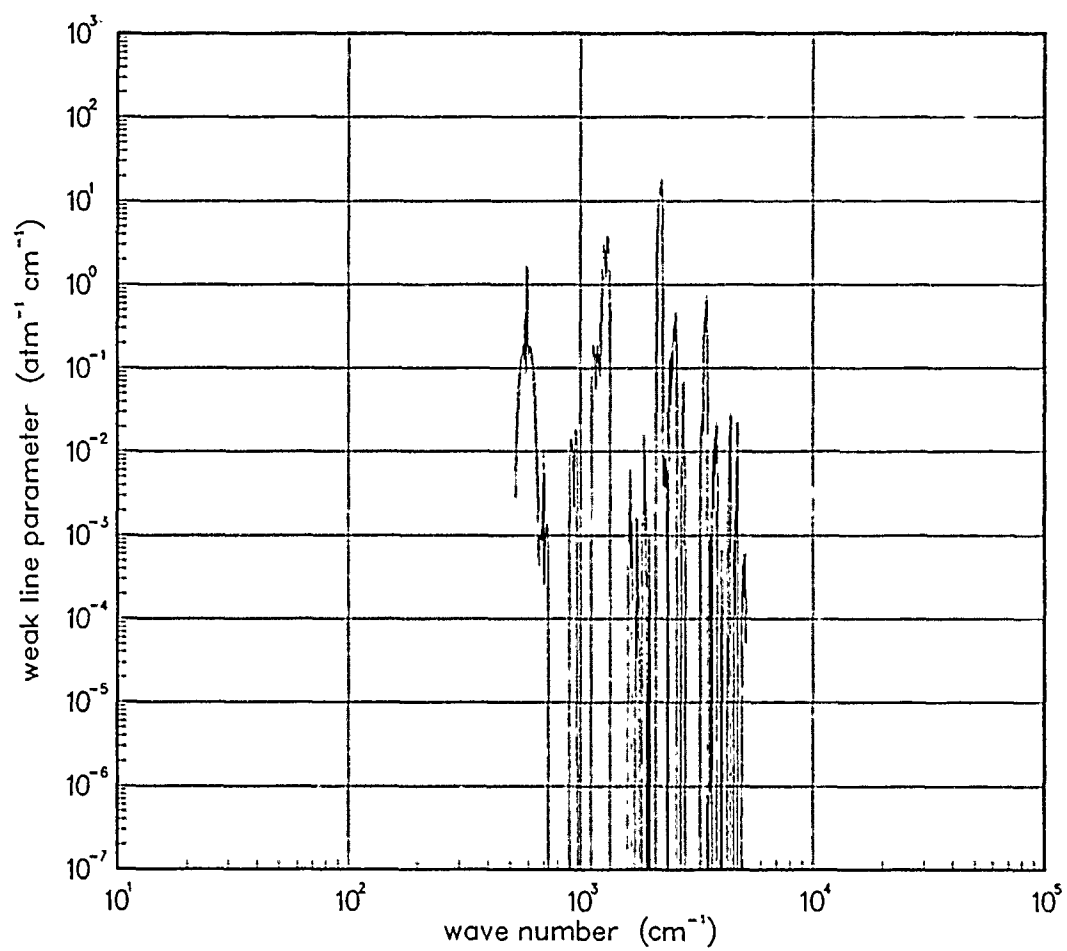


Figure 181. Weak-line parameter for N₂O at 750°K.

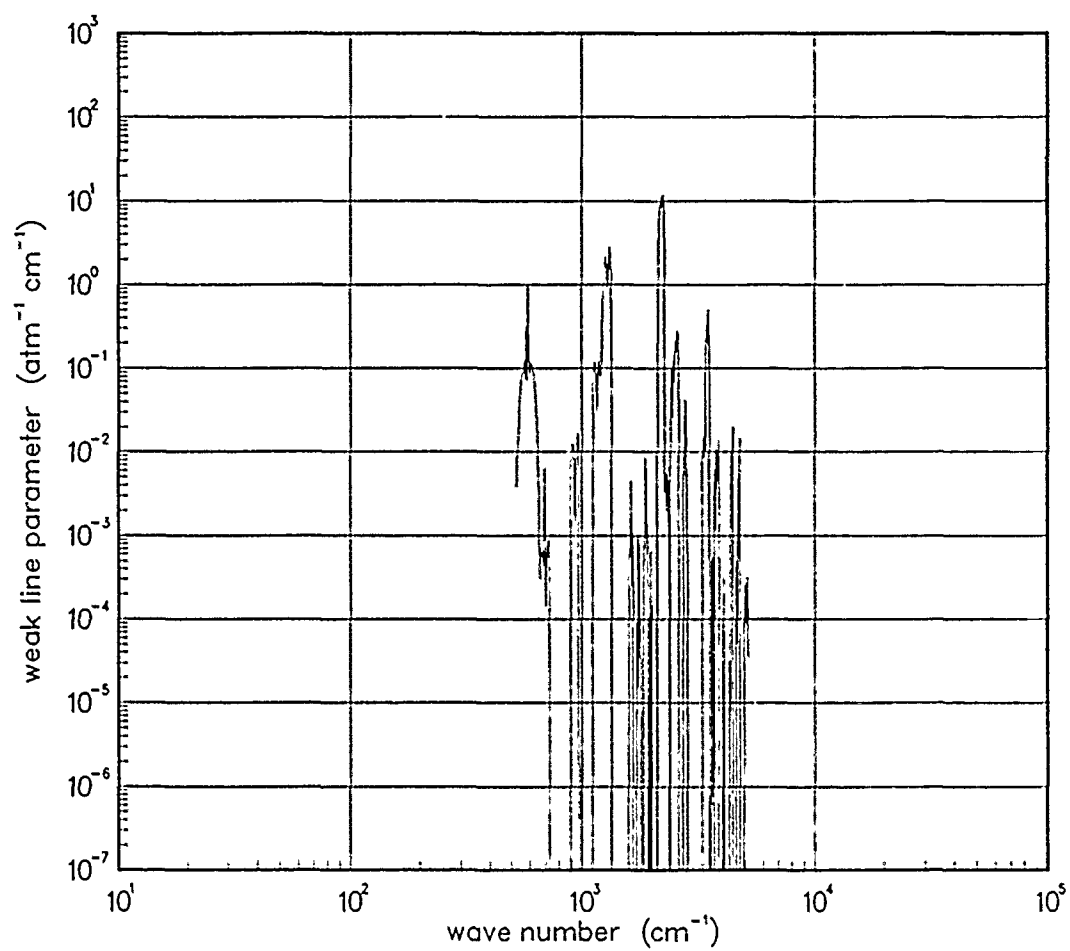


Figure 182. Weak-line parameter for N₂O at 1000°K.

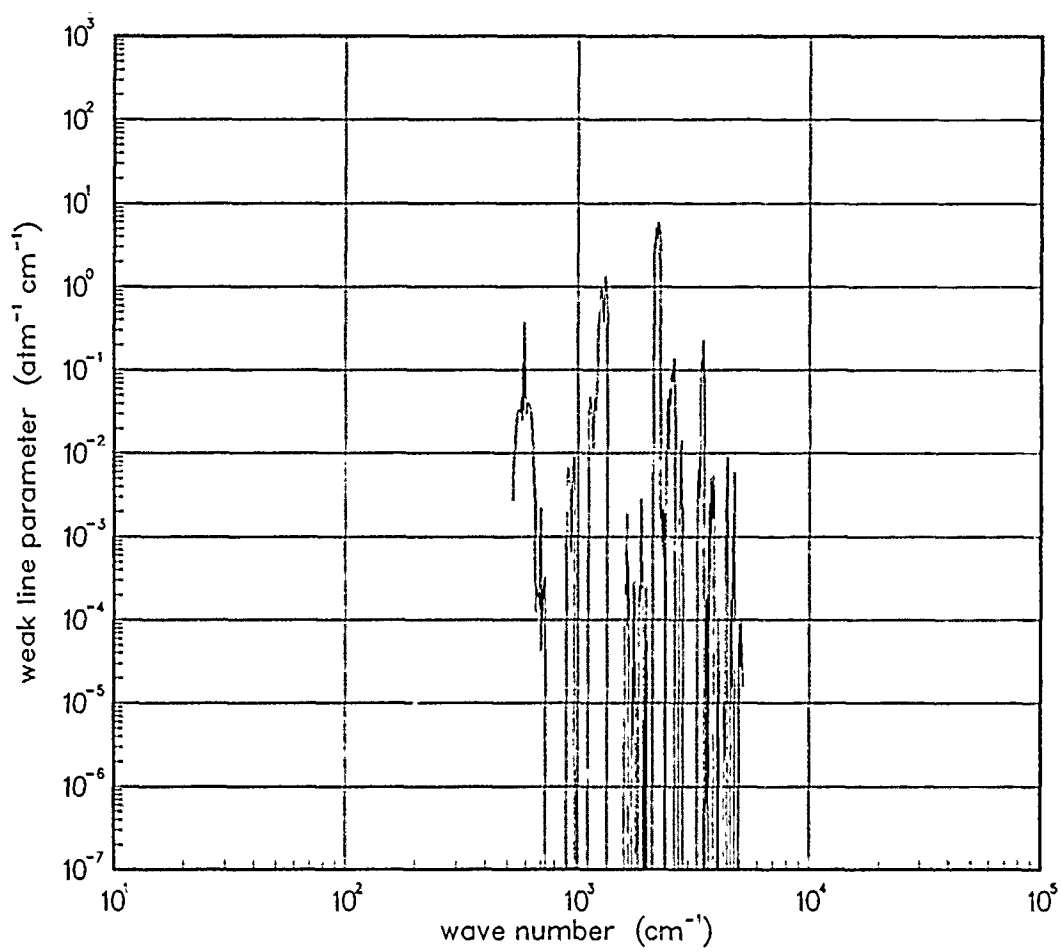


Figure 183. Weak-line parameter for N₂O at 1500°K.

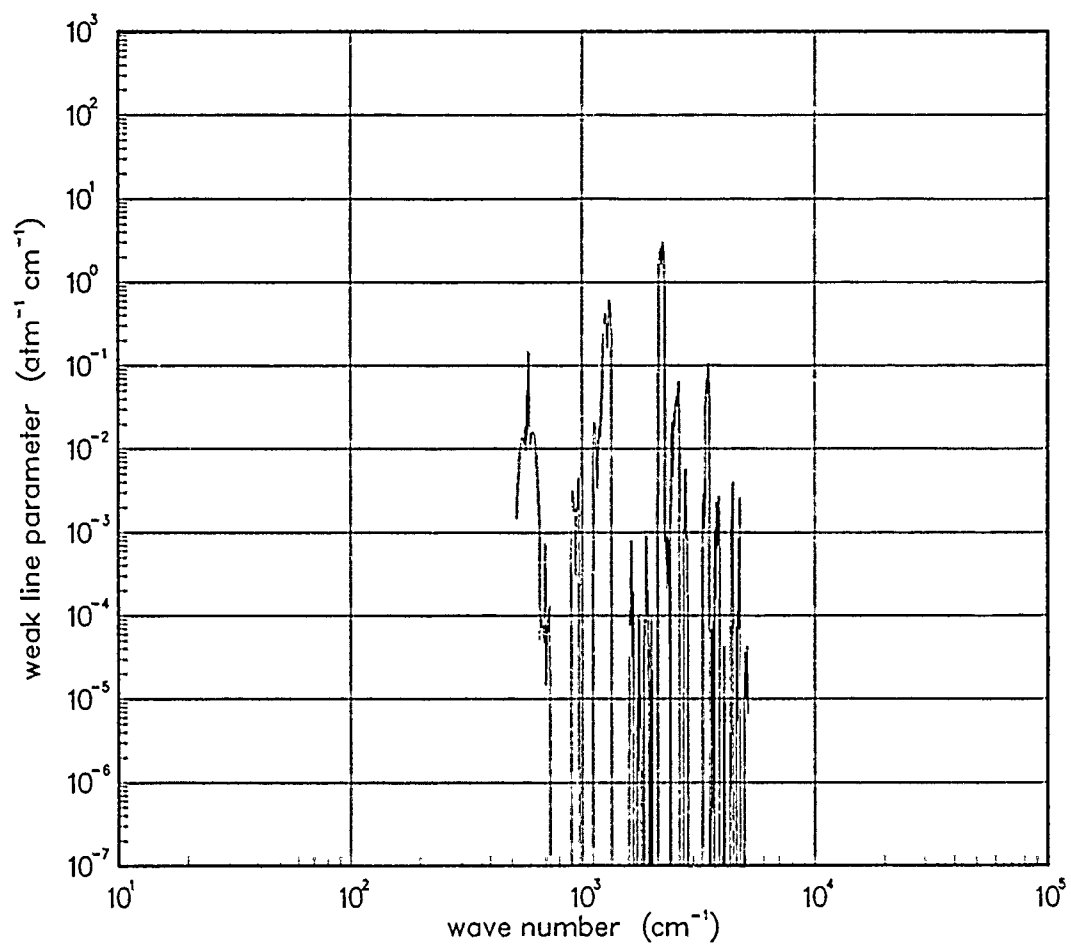


Figure 184. Weak-line parameter for N₂O at 2000°K.

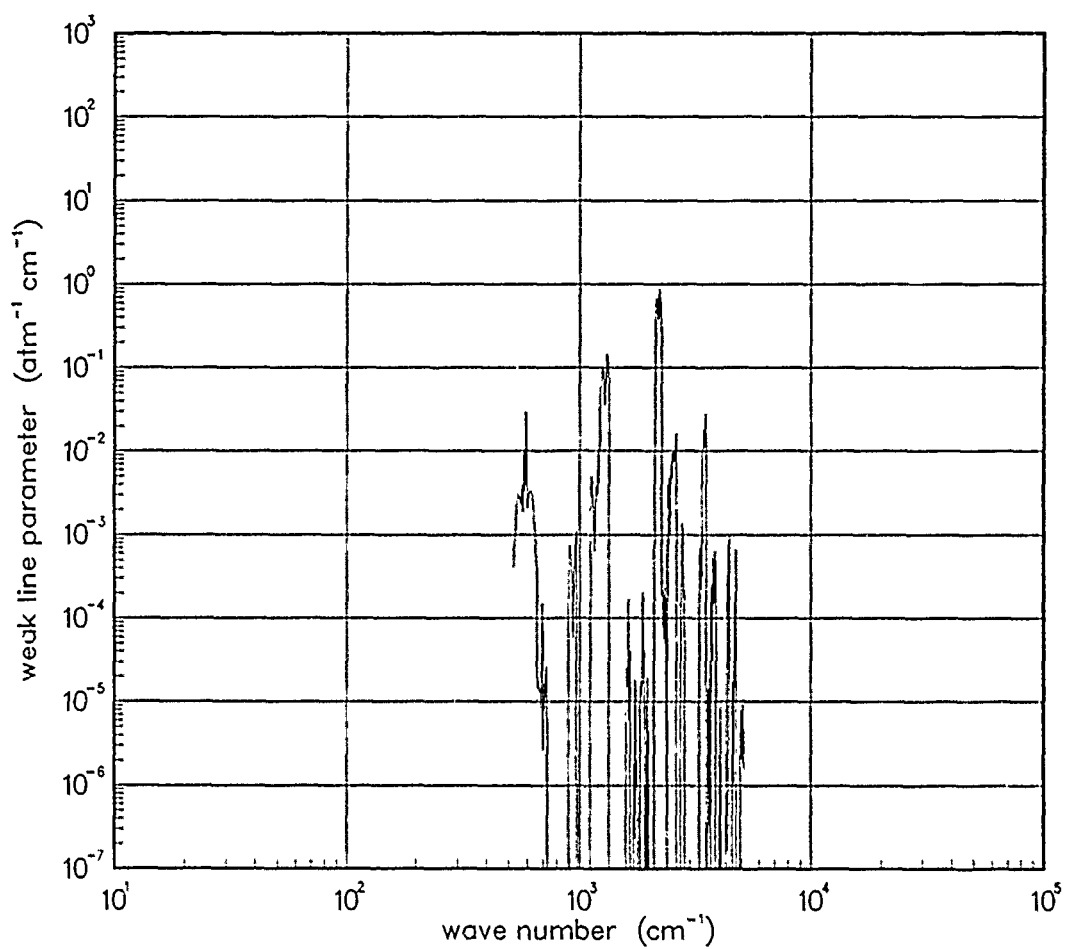


Figure 185. Weak-line parameter for N₂O at 3000°K.

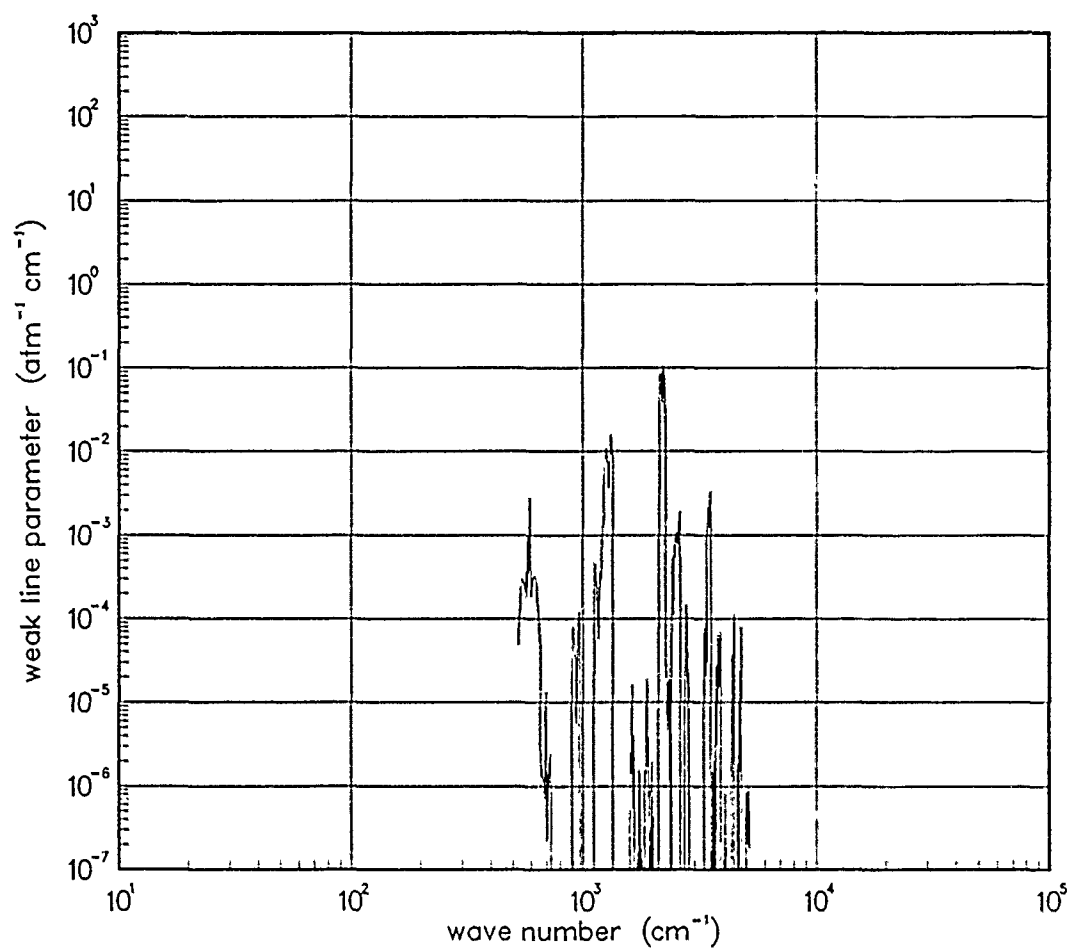


Figure 186. Weak-line parameter for N₂O at 5000°K.

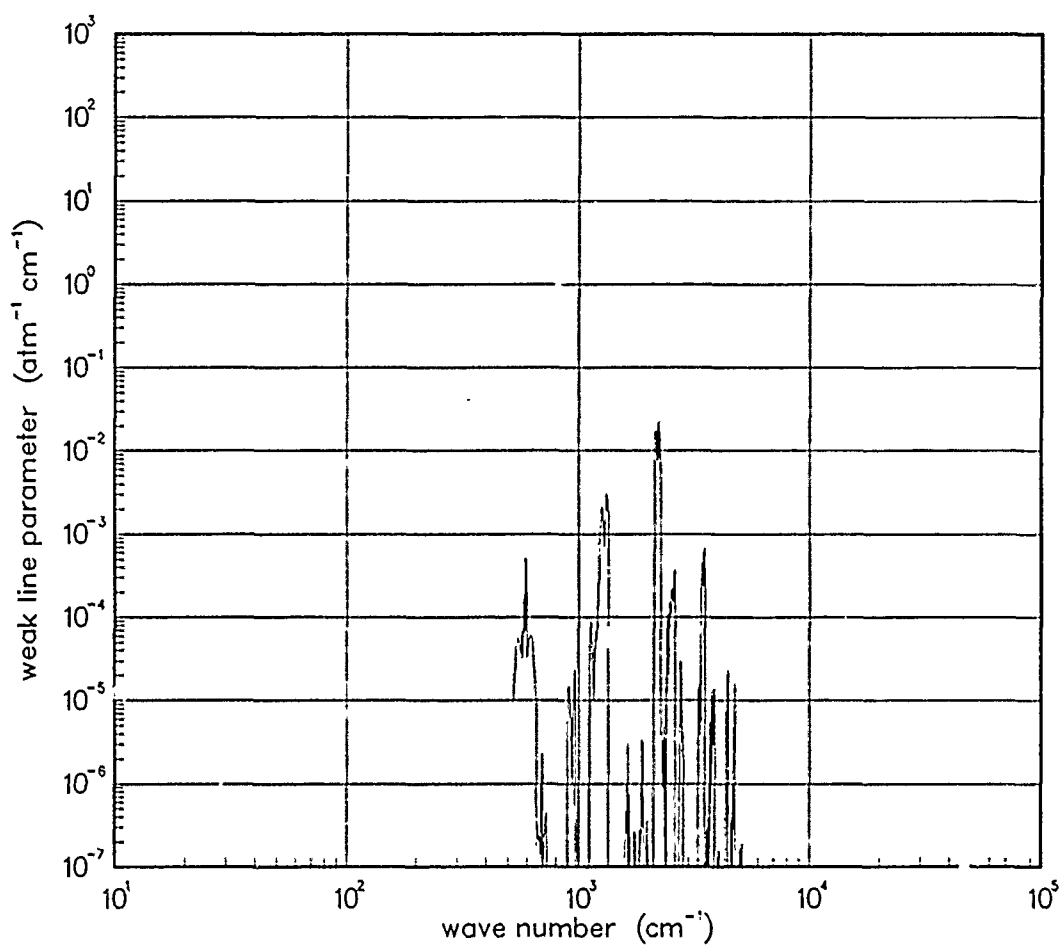


Figure 187. Weak-line parameter for N₂O at 7000°K.

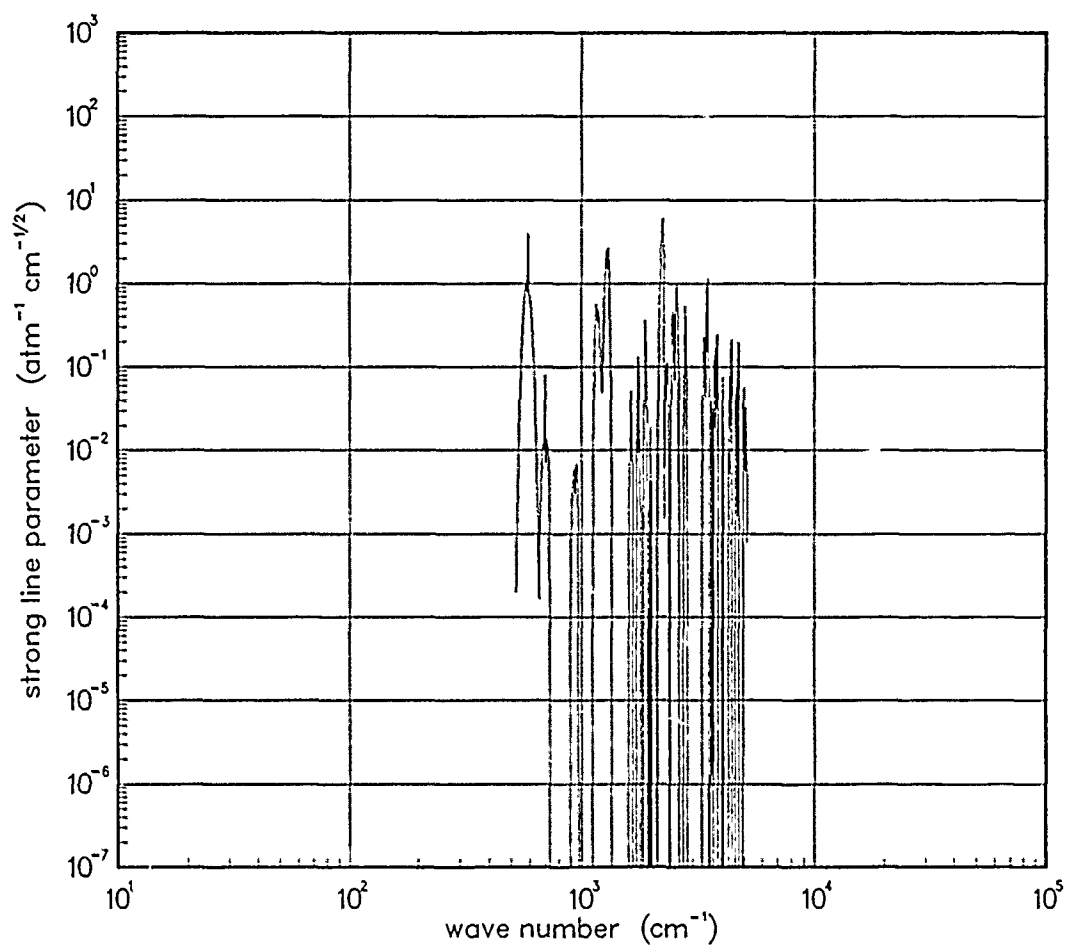


Figure 188. Strong-line parameter for N₂O at 200°K.

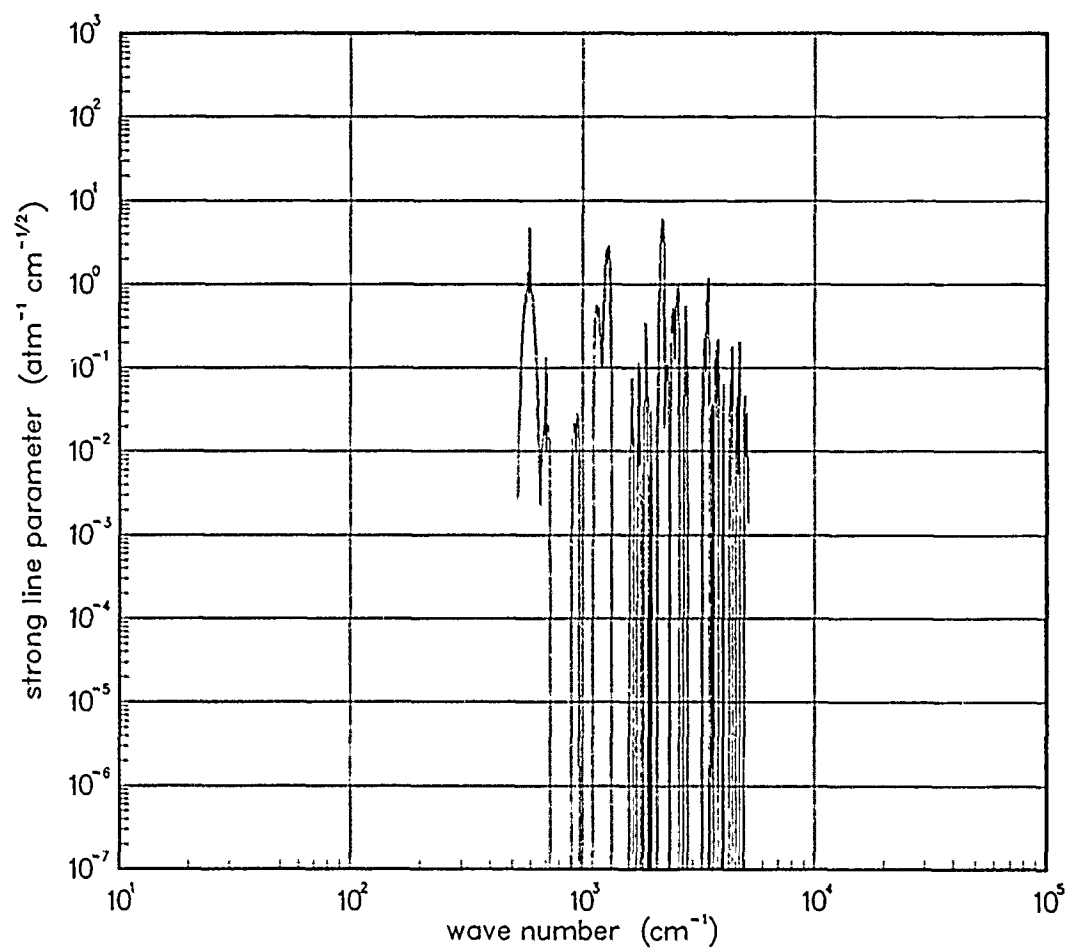


Figure 189. Strong-line parameter for N₂O at 300°K.

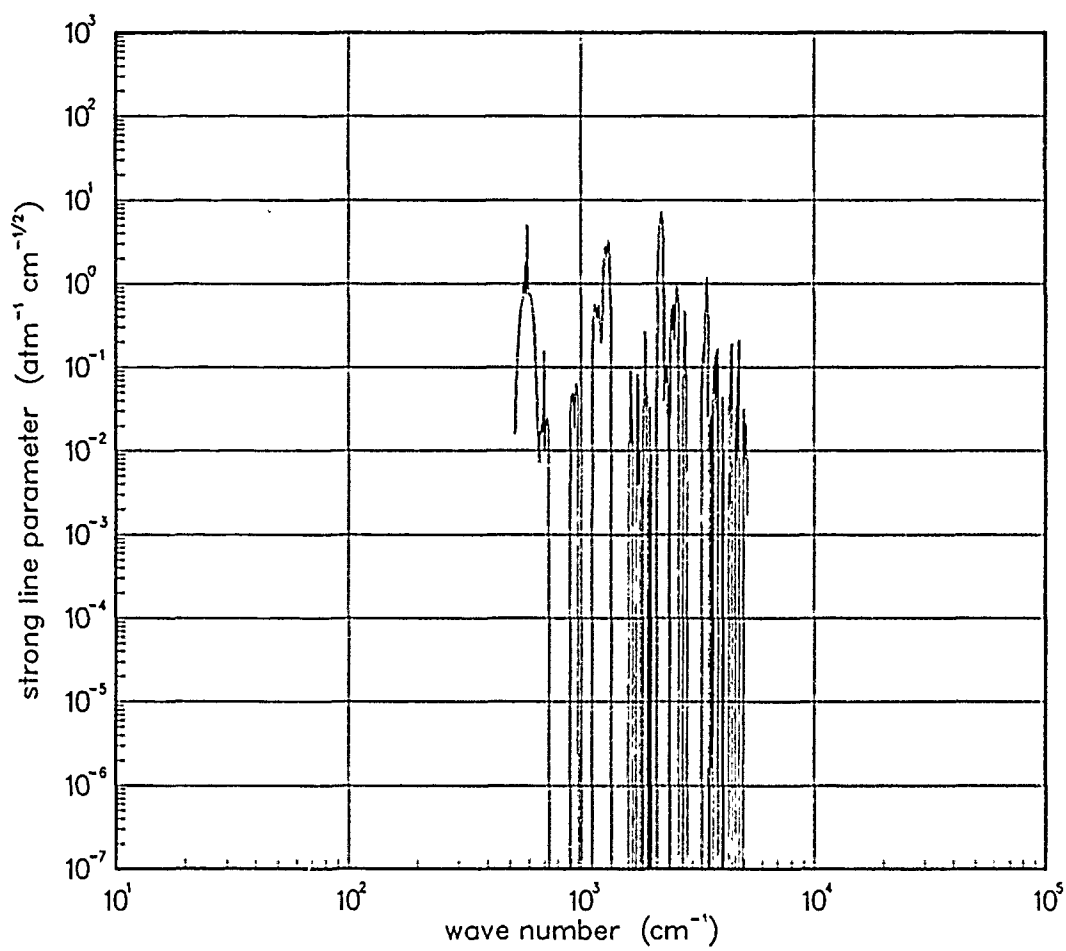


Figure 190. Strong-line parameter for N₂O at 500°K.

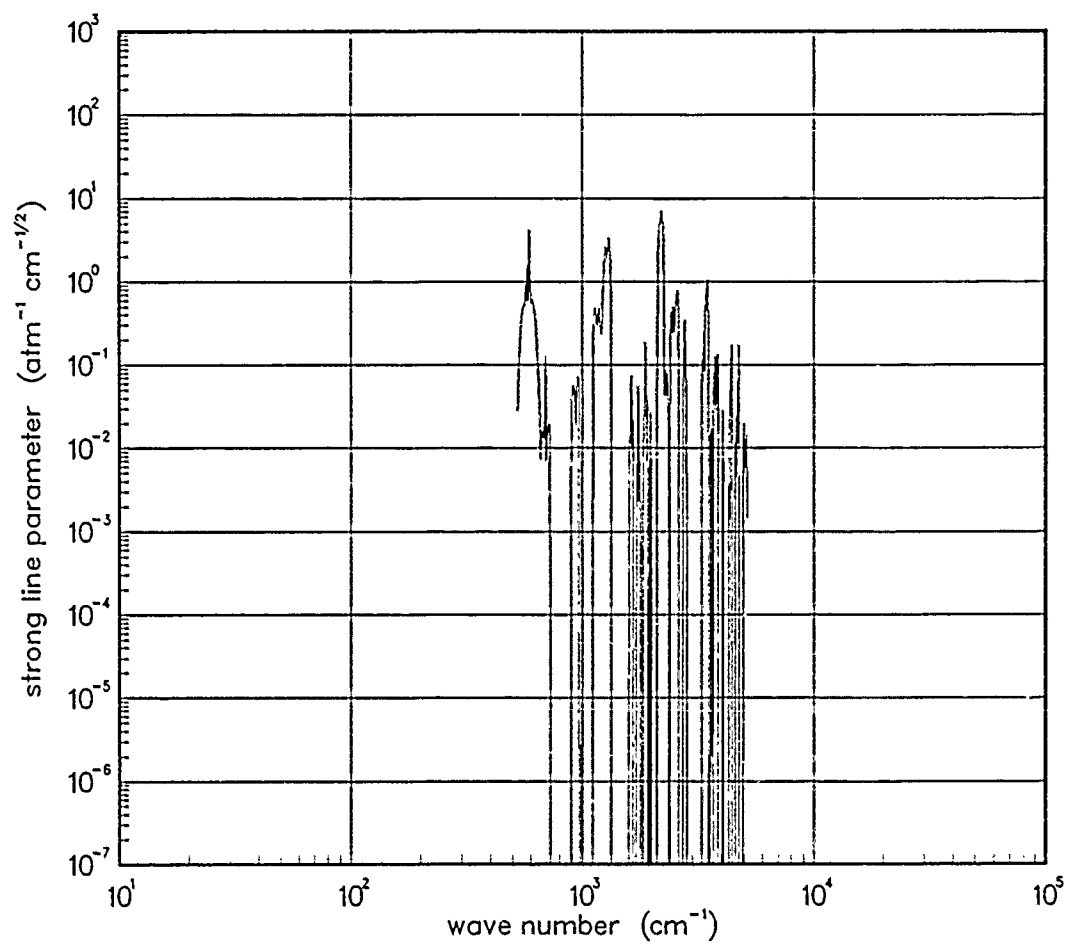


Figure 191. Strong-line parameter for N₂O at 750°K.

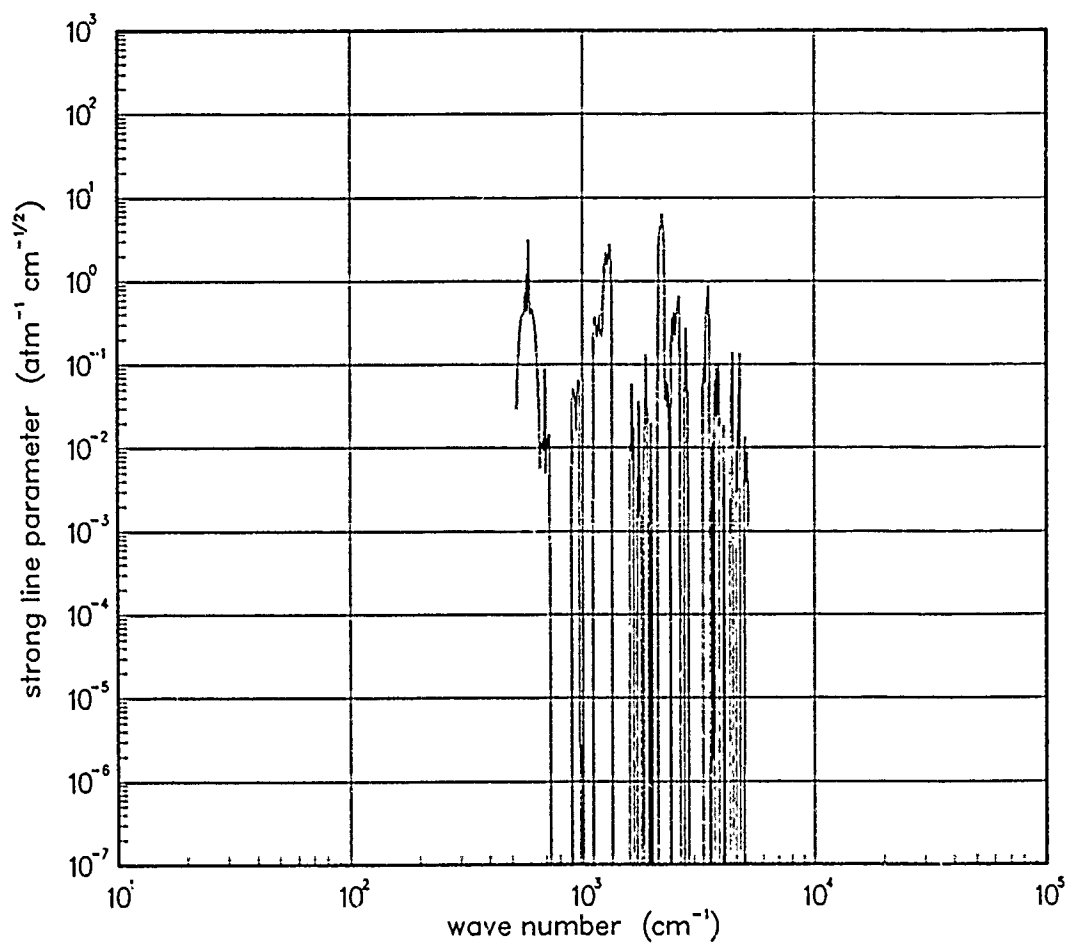


Figure 192. Strong-line parameter for N₂O at 1000°K.

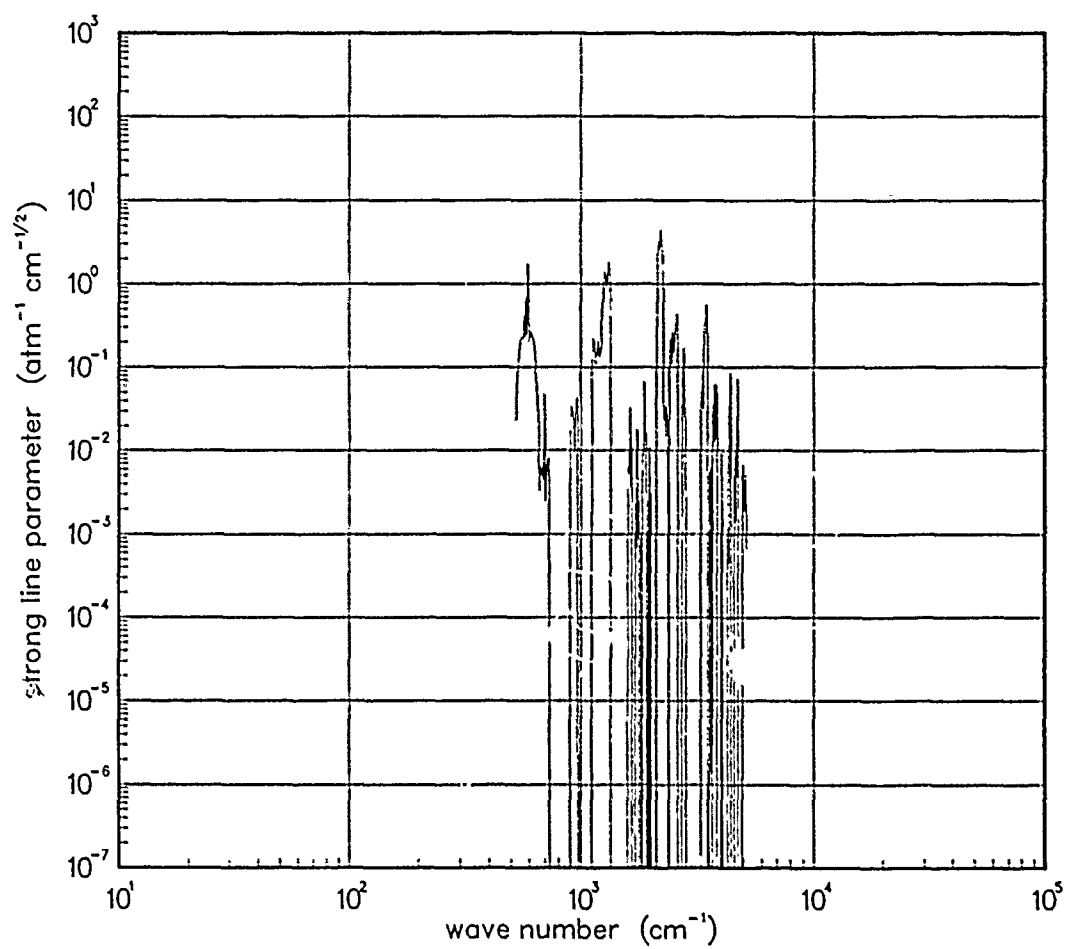


Figure 193. Strong-line parameter for N₂O at 1500°K.

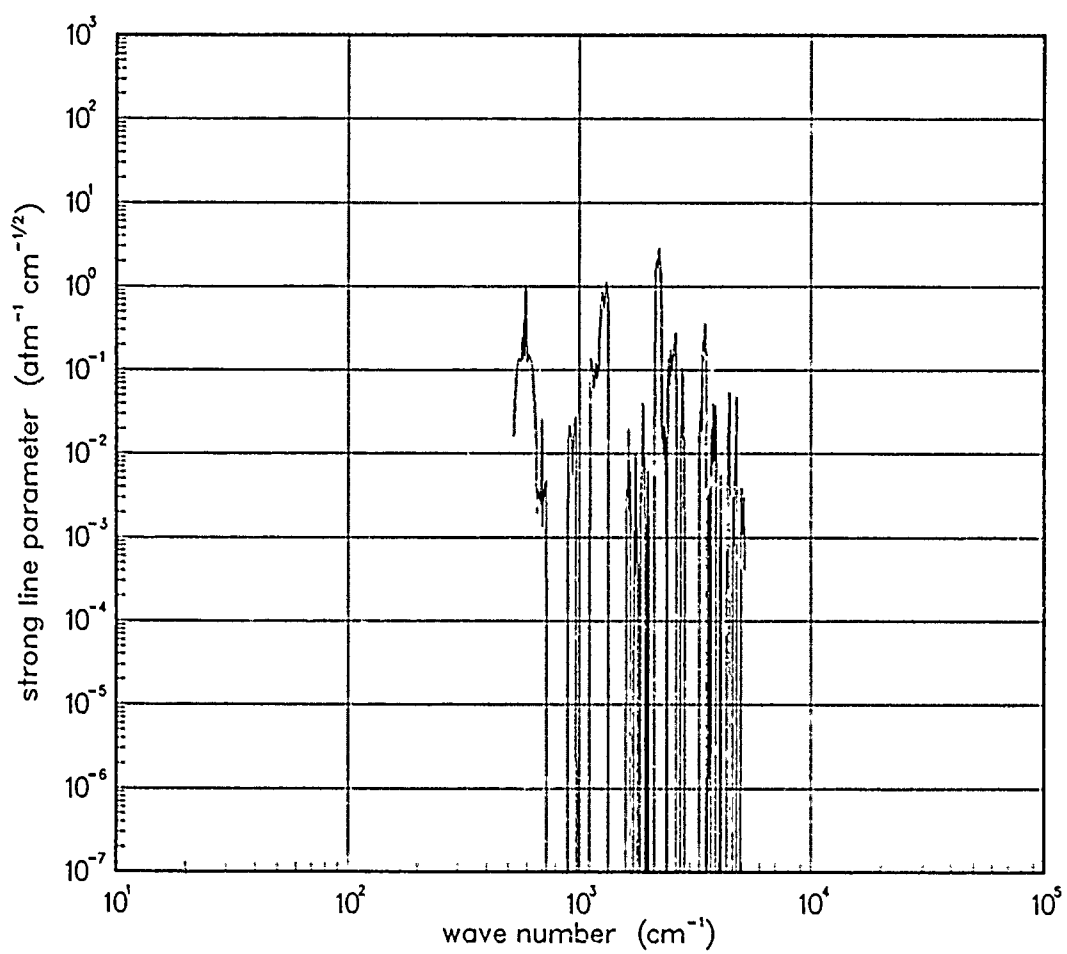


Figure 194. Strong-line parameter for N₂O at 2000°K.

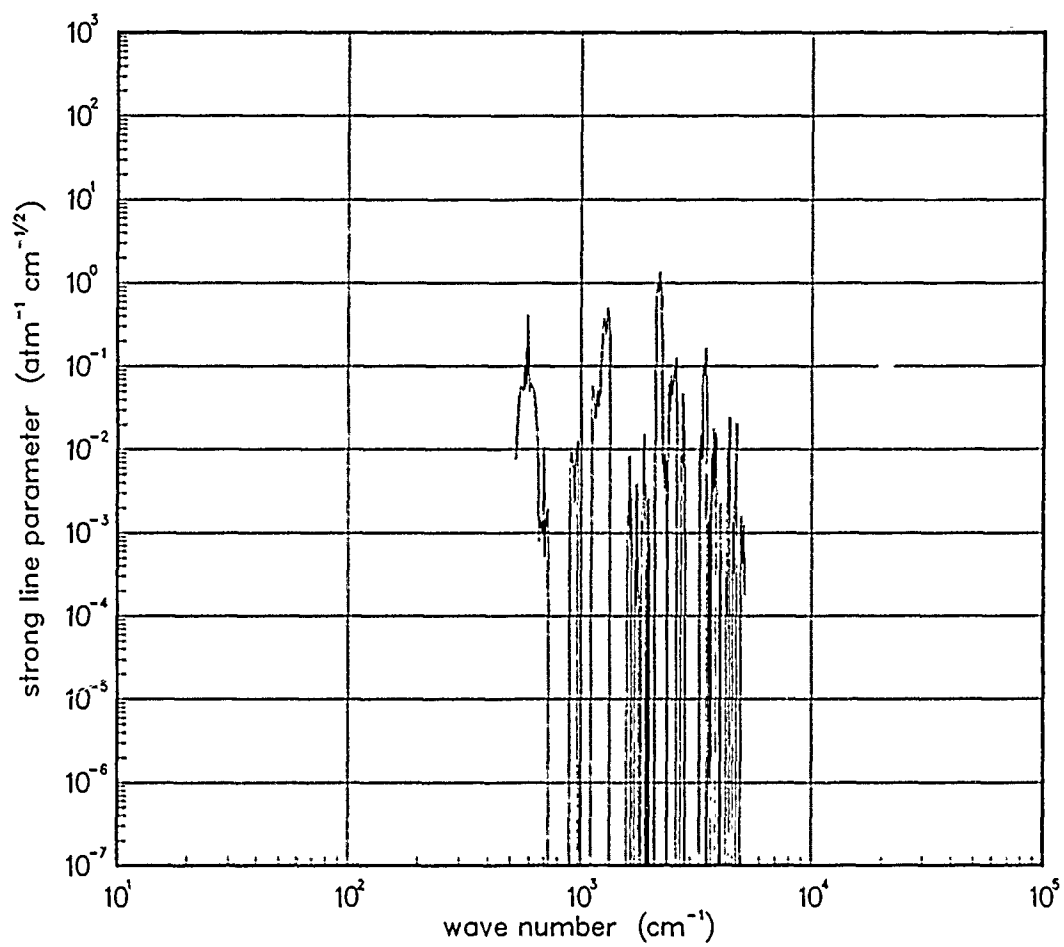


Figure 195. Strong-line parameter for N₂O at 3000°K.

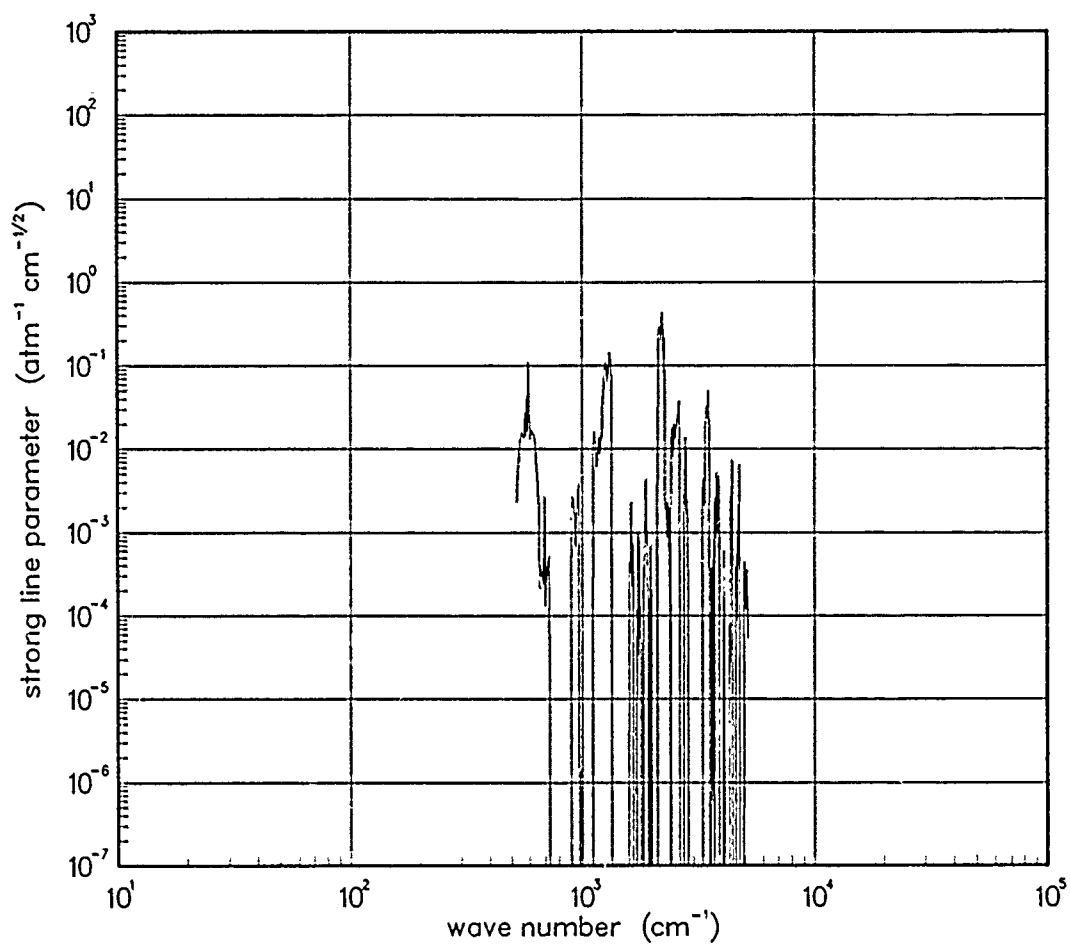


Figure 196. Strong-line parameter for N₂O at 5000°K.

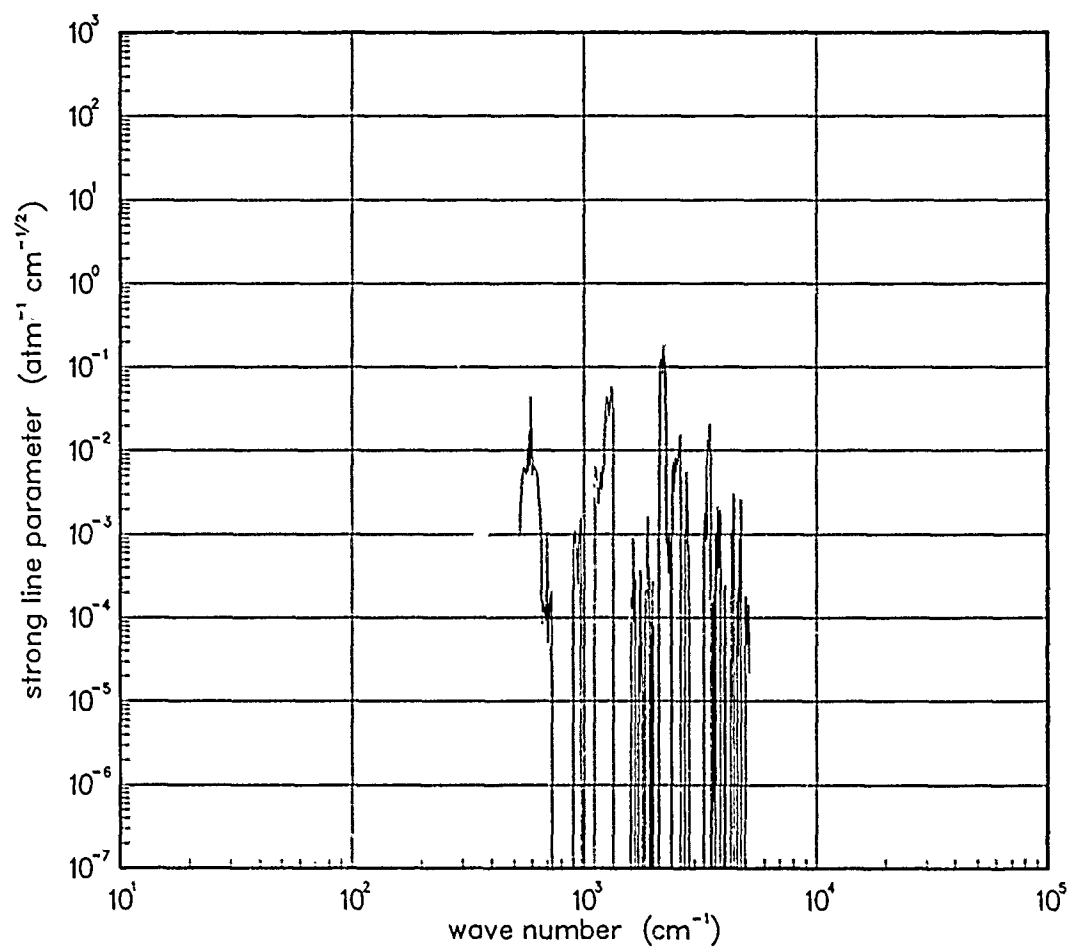


Figure 197. Strong-line parameter for N₂O at 7000°K.

5.4 METHANE (CH_4).

Local thermal equilibrium emission spectra for Methane has been developed from the Air Force Geophysical Laboratory line atlas for 200, 300, 500, 750, 1000 °K.

The CH_4 molecule has been included within the NORSE LTE data base because of its contribution to ambient atmospheric absorption. The inclusion of accurate parameters for this species above 1000 °K is felt to be of low priority.

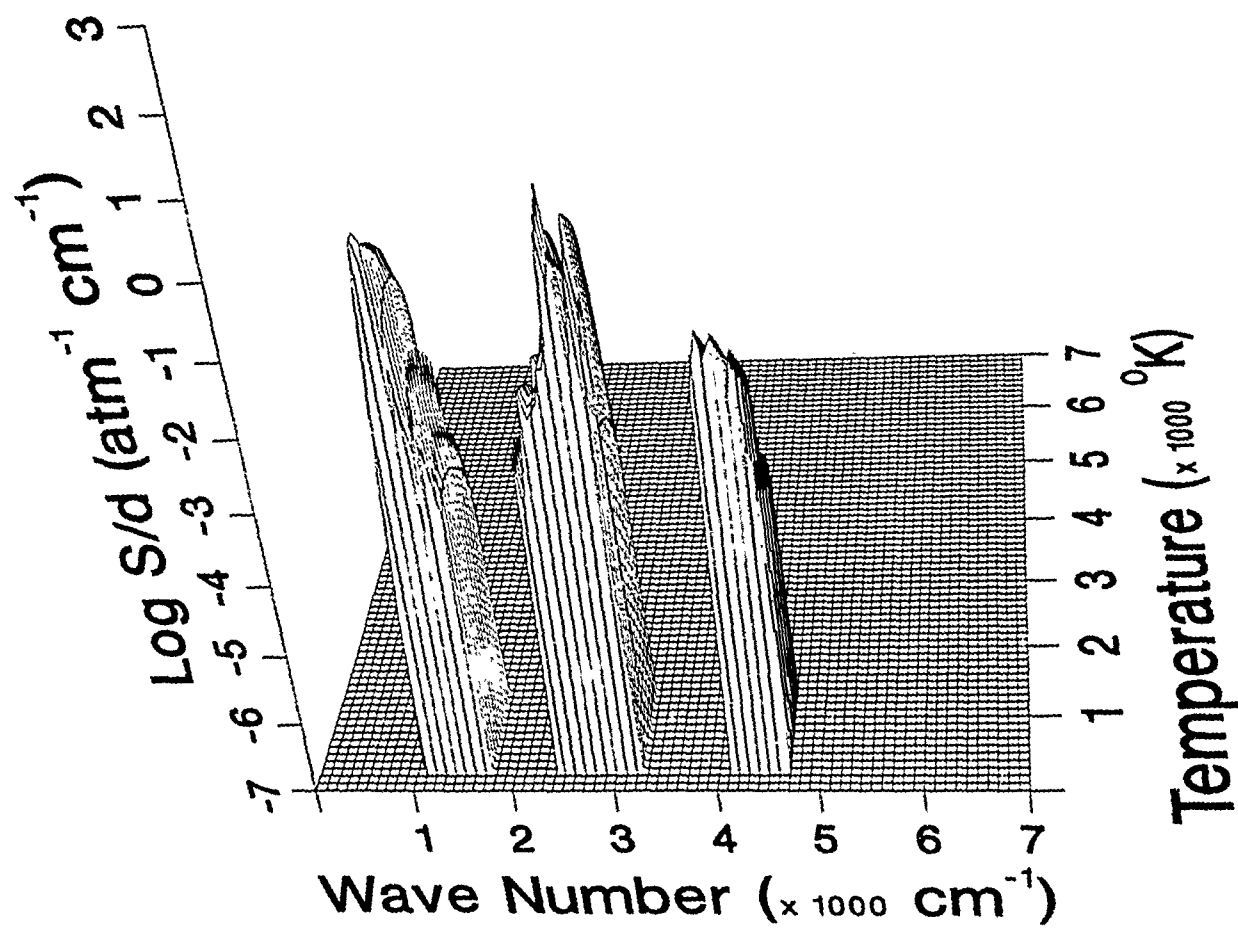


Figure 198. Weak-line parameter for CH_4 .

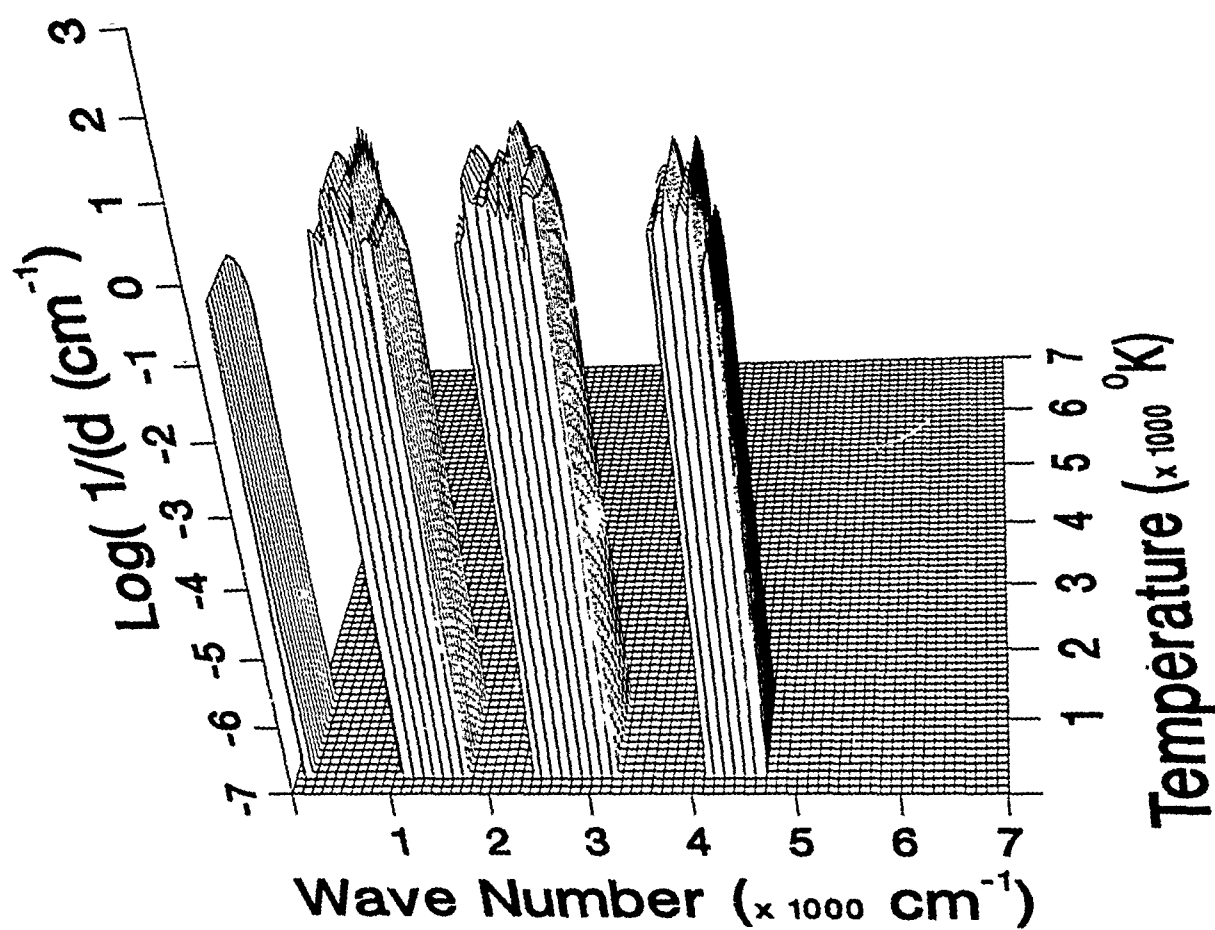


Figure 199. Inverse line spacing for CH_4 .

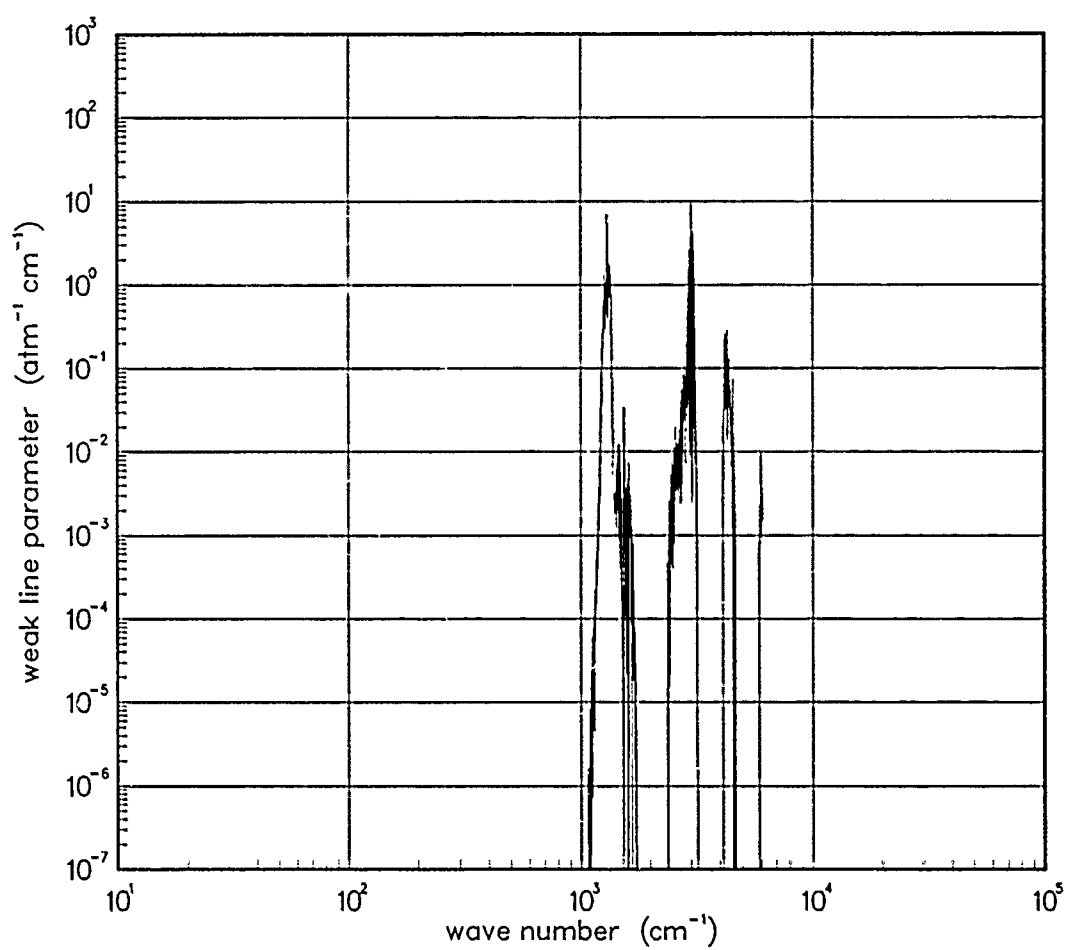


Figure 200. Weak-line parameter for CH₄ at 200°K.

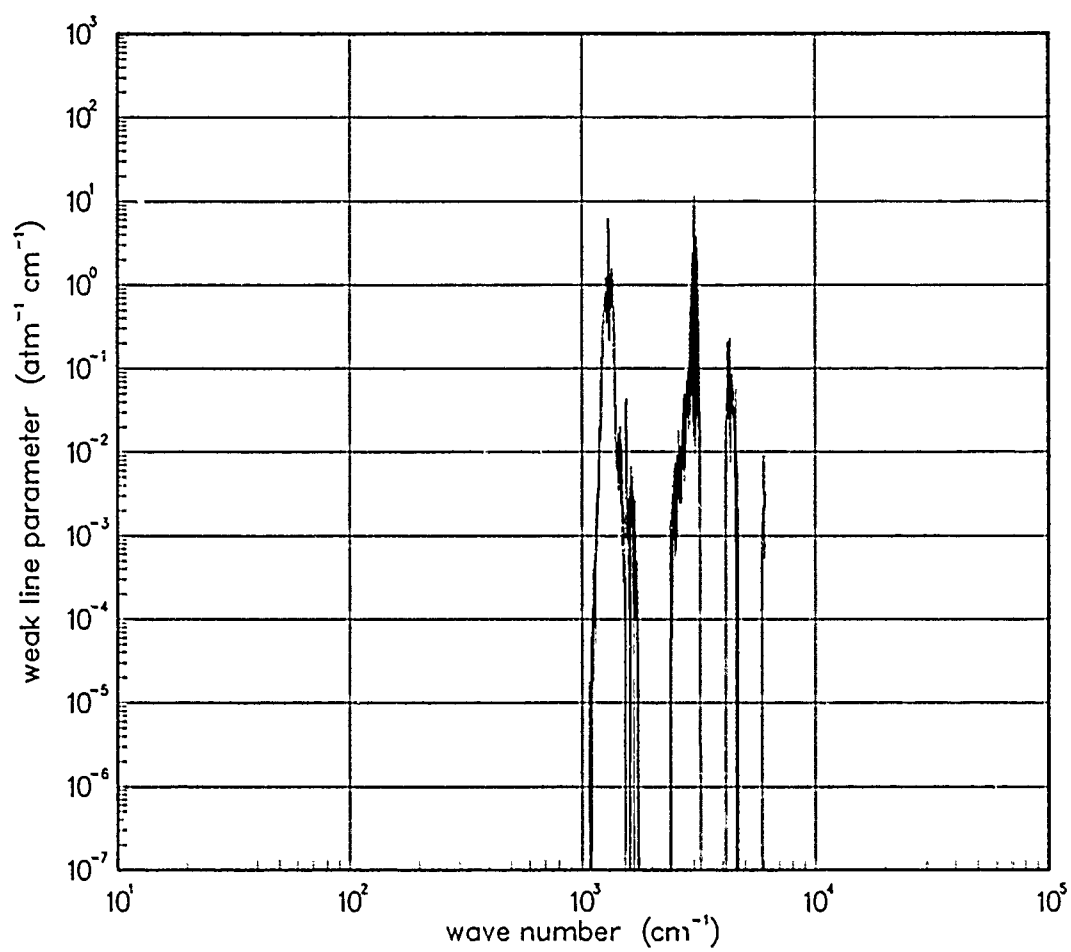


Figure 201. Weak-line parameter for CH₄ at 300°K.

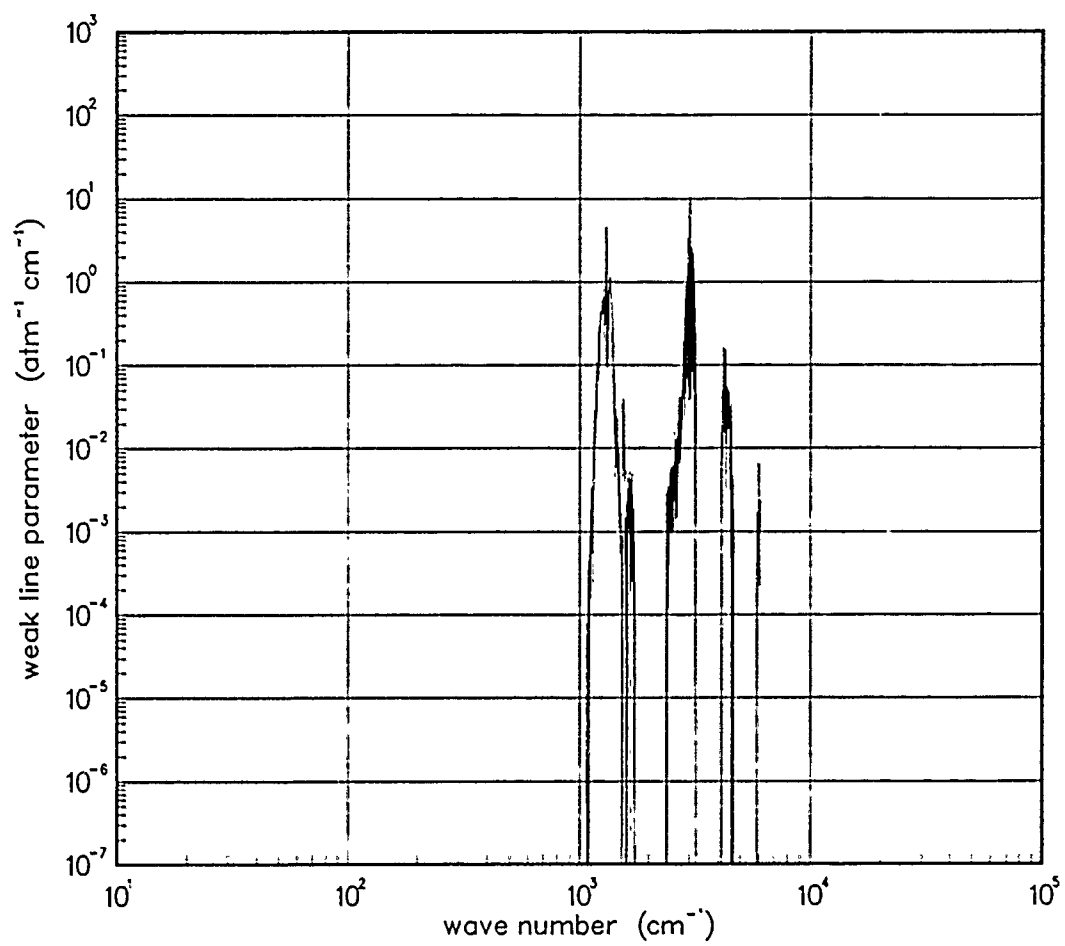


Figure 202. Weak-line parameter for CH₄ at 500°K.

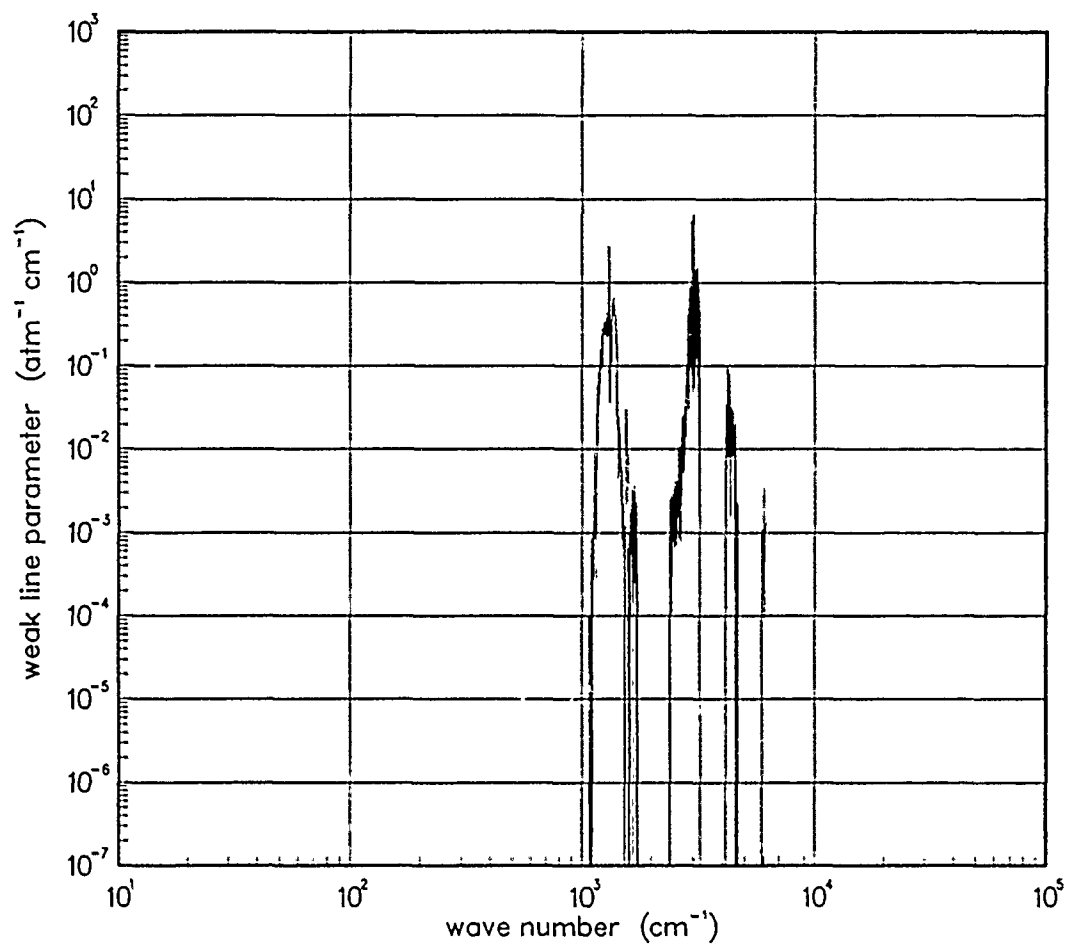


Figure 203. Weak-line parameter for CH₄ at 750°K.

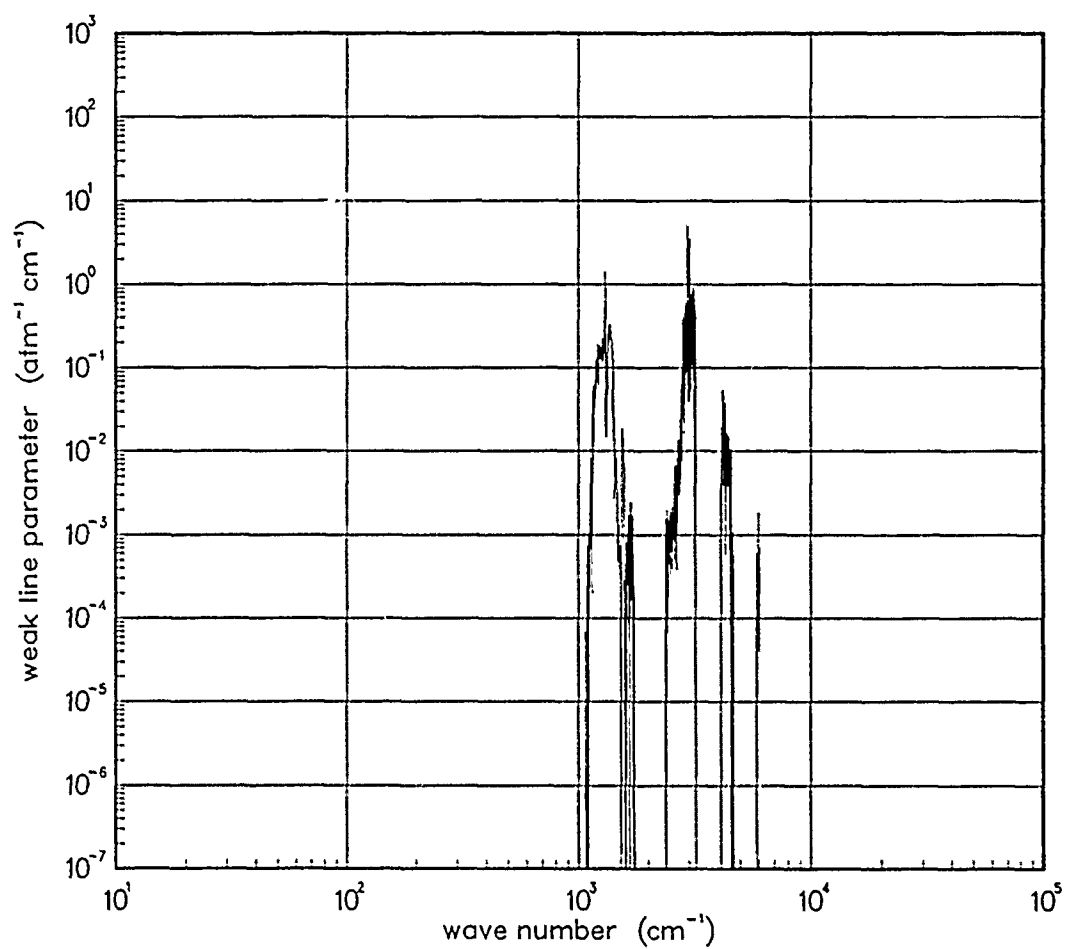


Figure 204. Weak-line parameter for CH_4 at 1000°K .

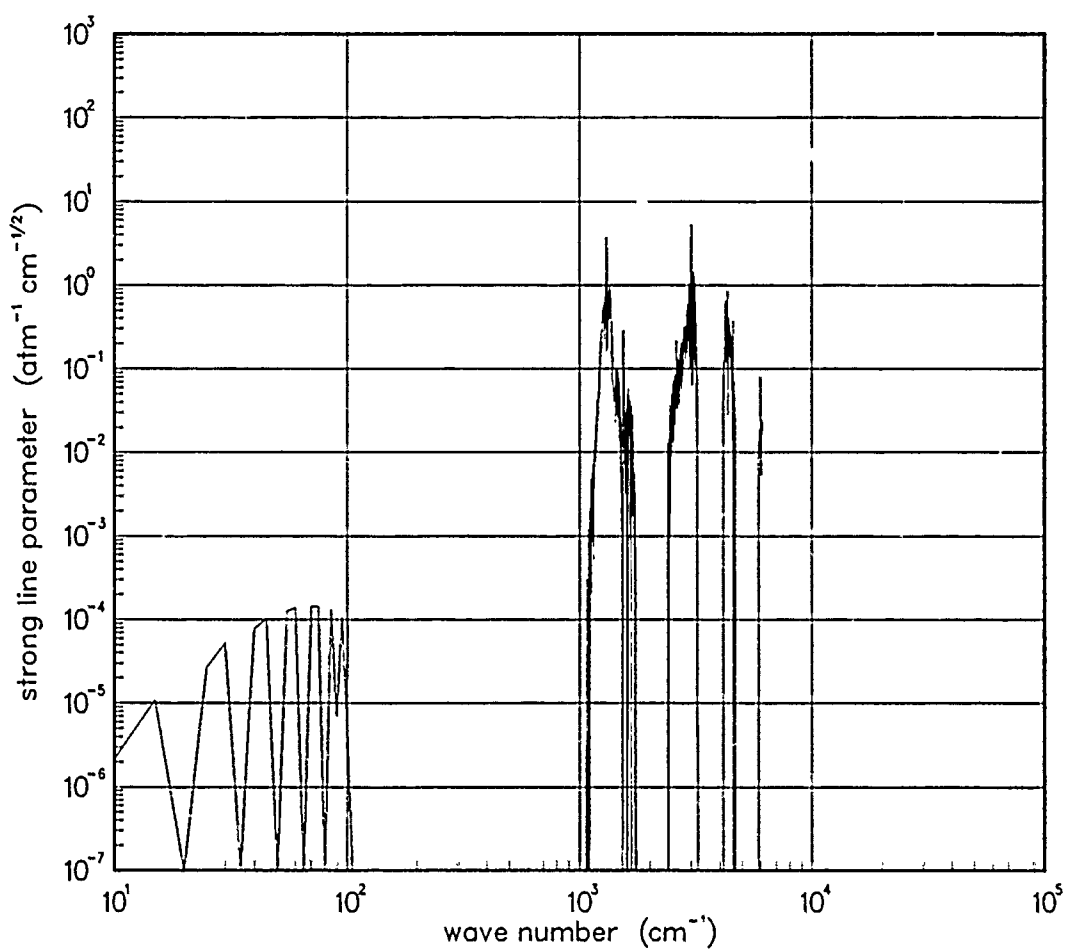


Figure 205. Strong-line parameter for CH₄ at 200°K.

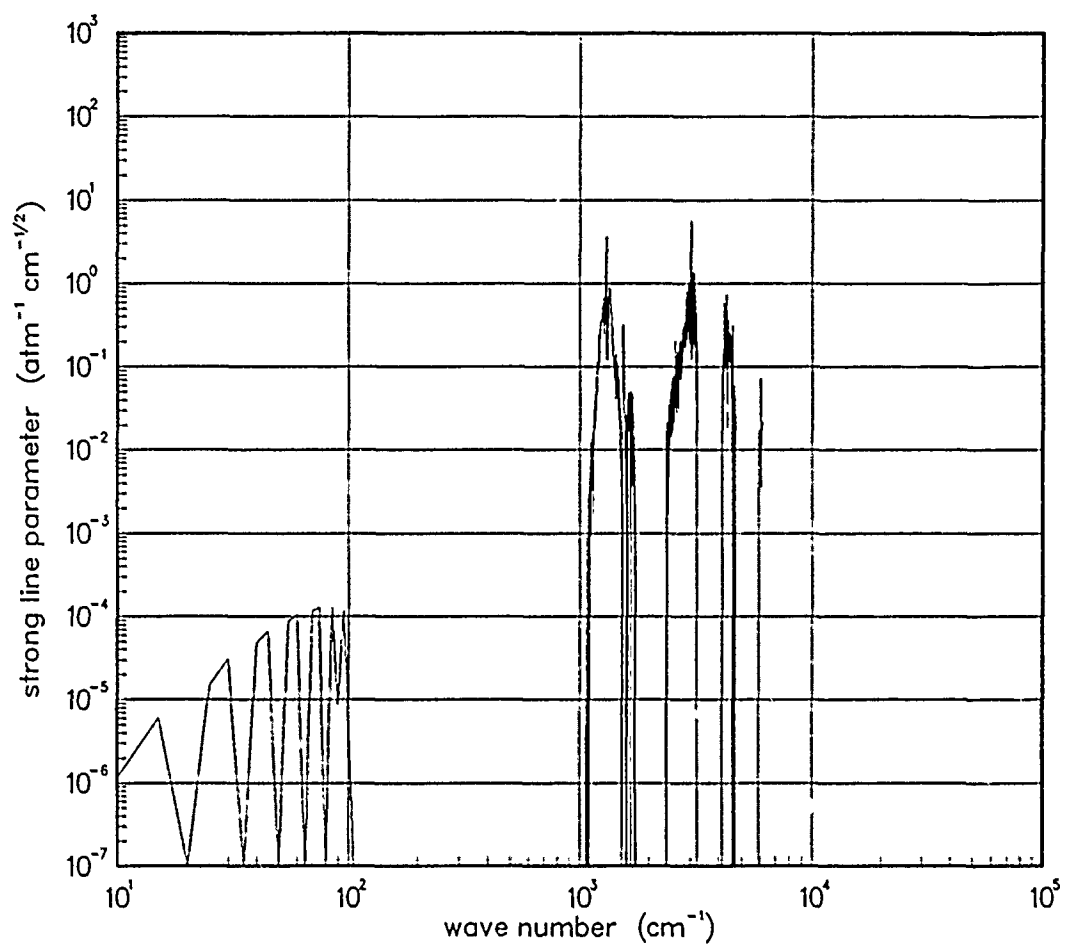


Figure 206. Strong-line parameter for CH₄ at 300°K.

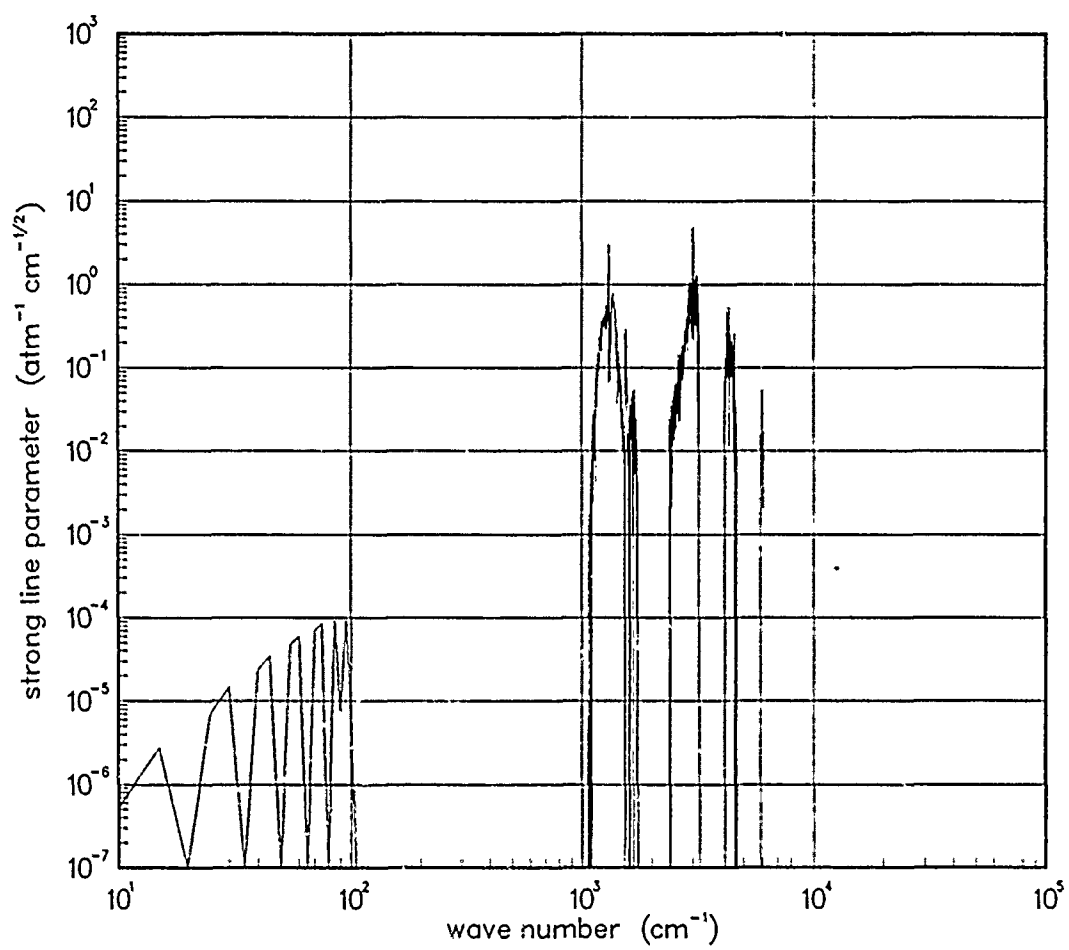


Figure 207. Strong-line parameter for CH₄ at 500°K.

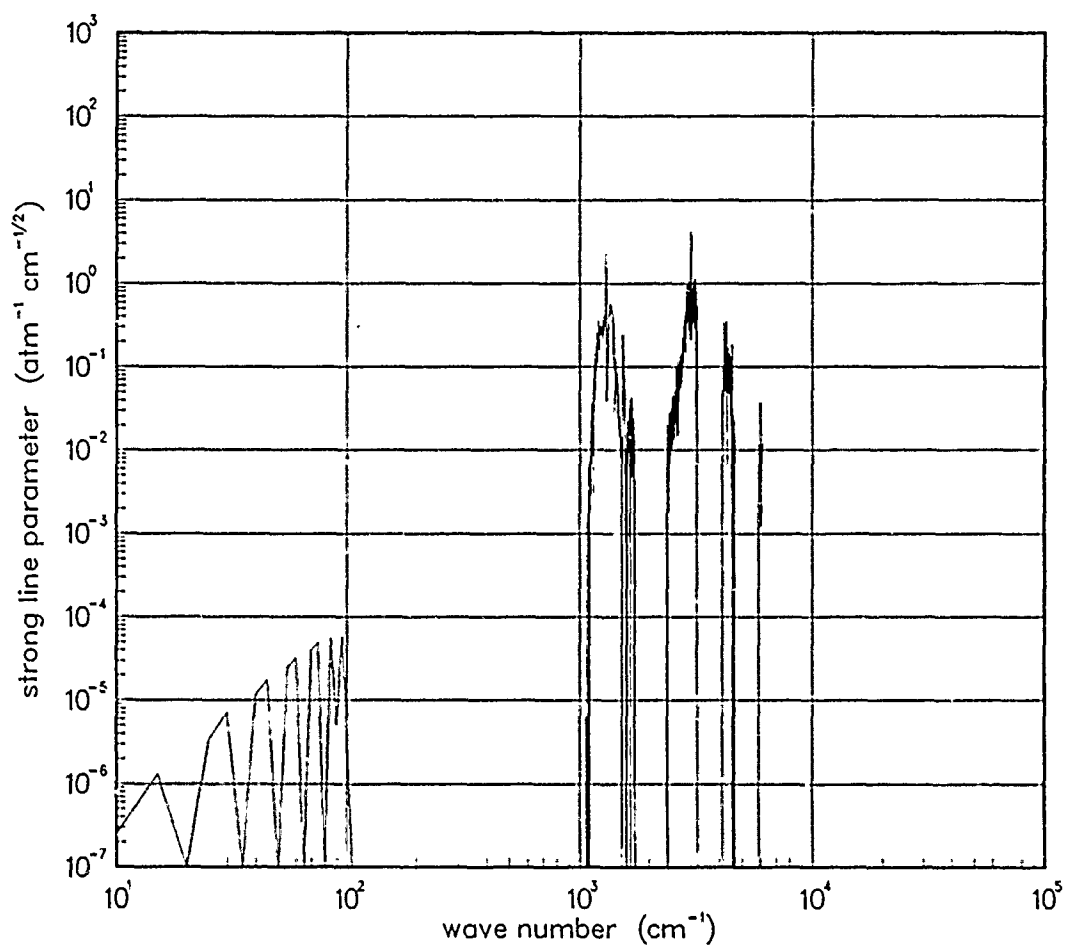


Figure 208. Strong-line parameter for CH₄ at 750°K.

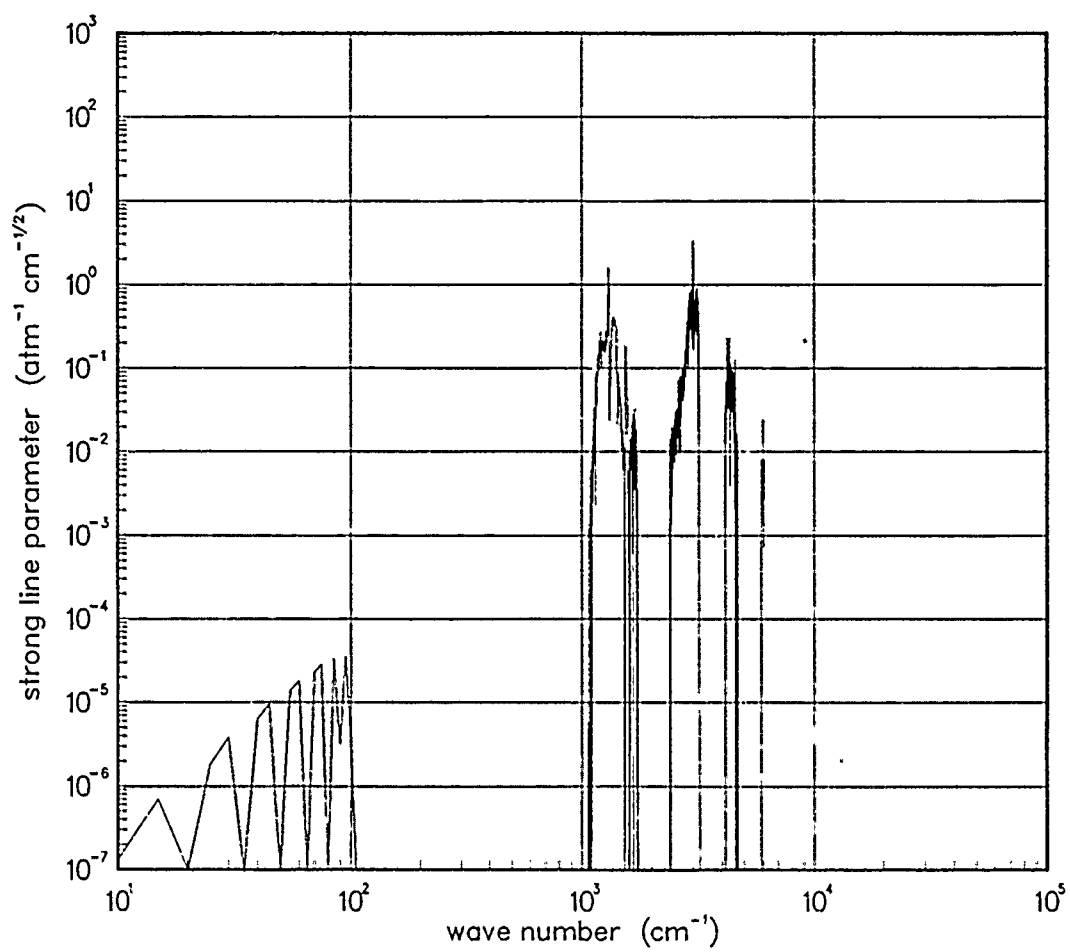


Figure 209. Strong-line parameter for CH_4 at 1000°K .

5.5 NITRIC ACID (HNO_3).

The local thermal equilibrium emission spectra for Nitric Acid has been developed from the 1982 Air Force Geophysical Laboratory Line Atlas for 300 °K.

The HNO_3 molecule has been included within the NORSE LTE data base because of its contribution to ambient atmospheric absorption. The inclusion of accurate parameters for this species at other temperatures is felt to be of low priority.

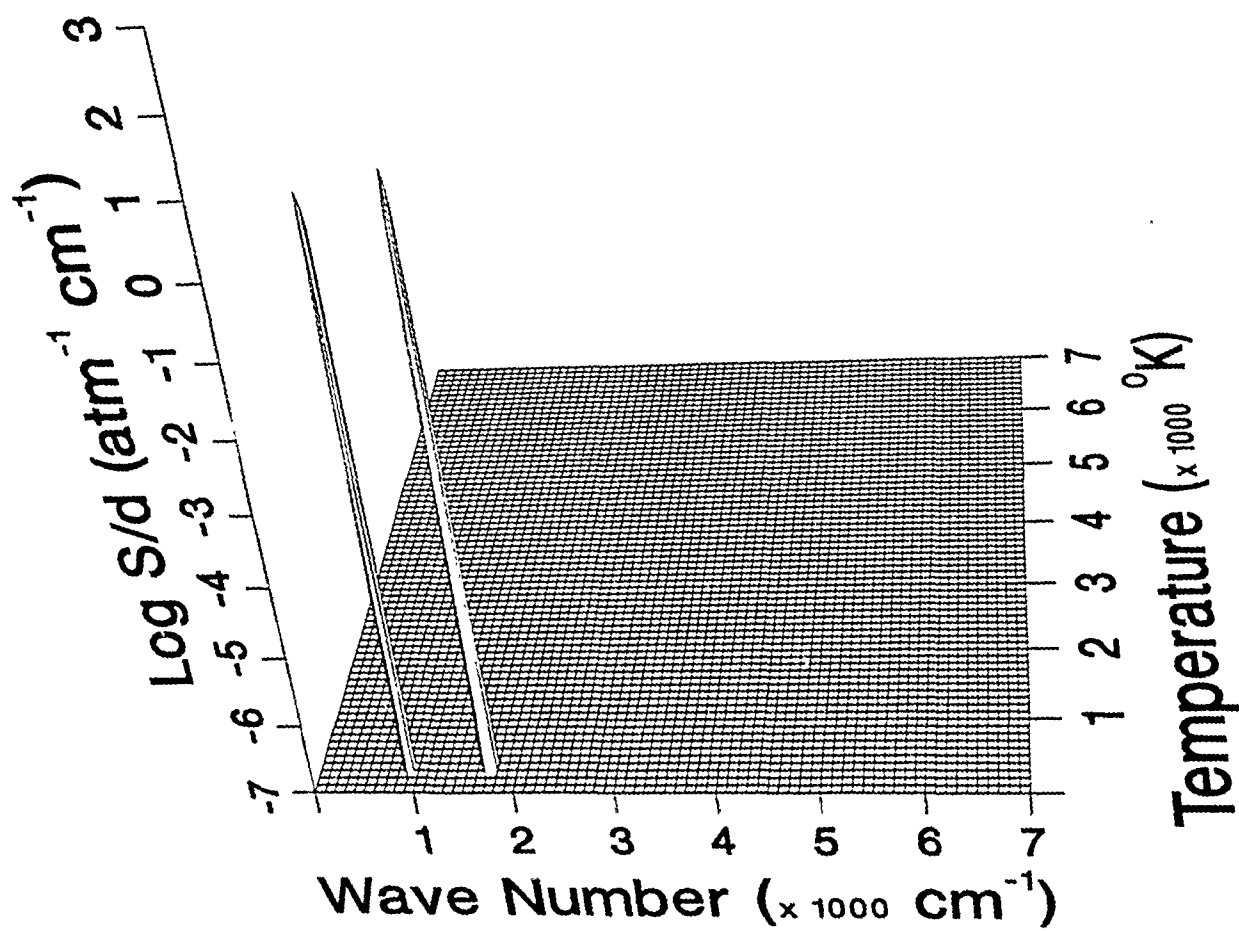


Figure 210. Weak-line parameter for HNO_3 .

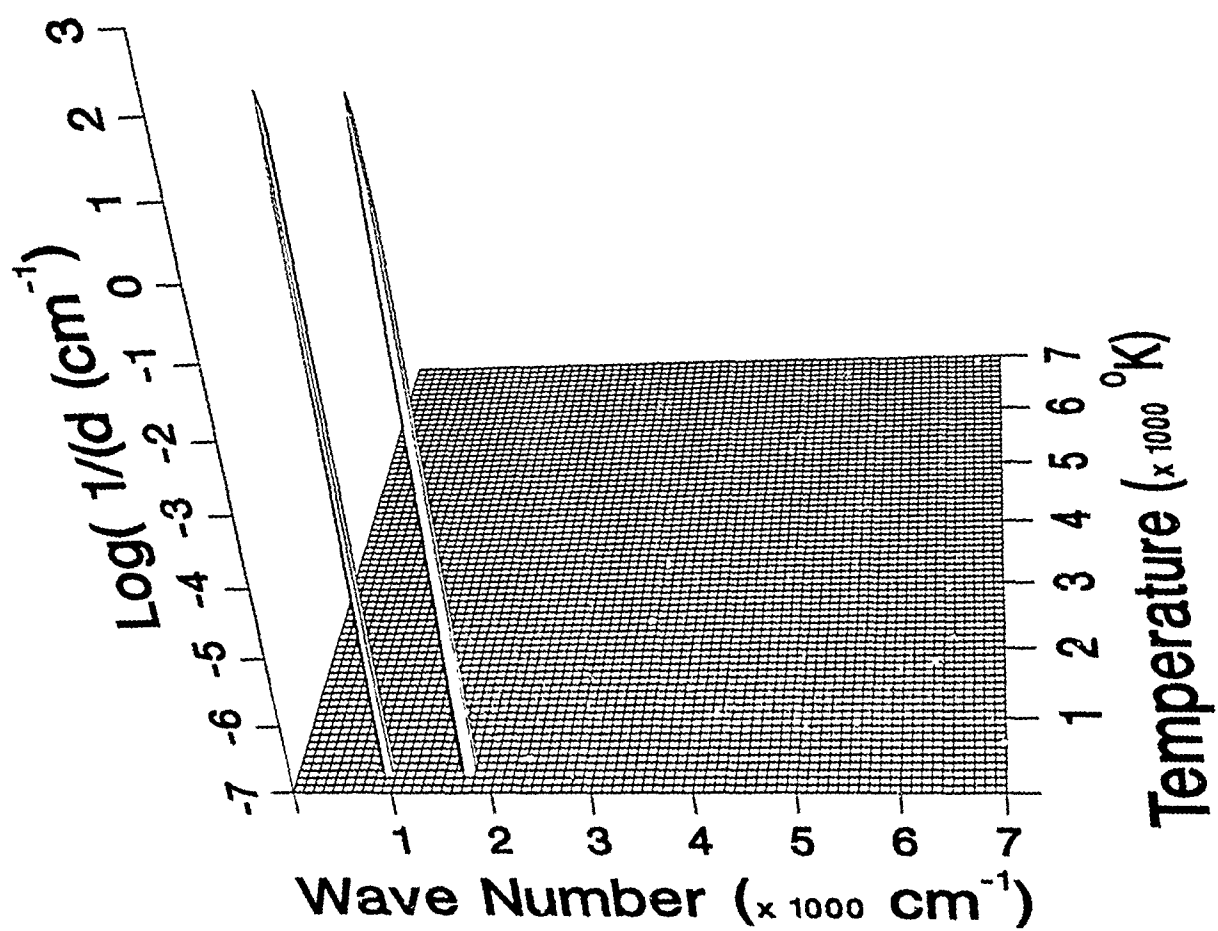


Figure 211. Inverse line spacing for HNO_3 .

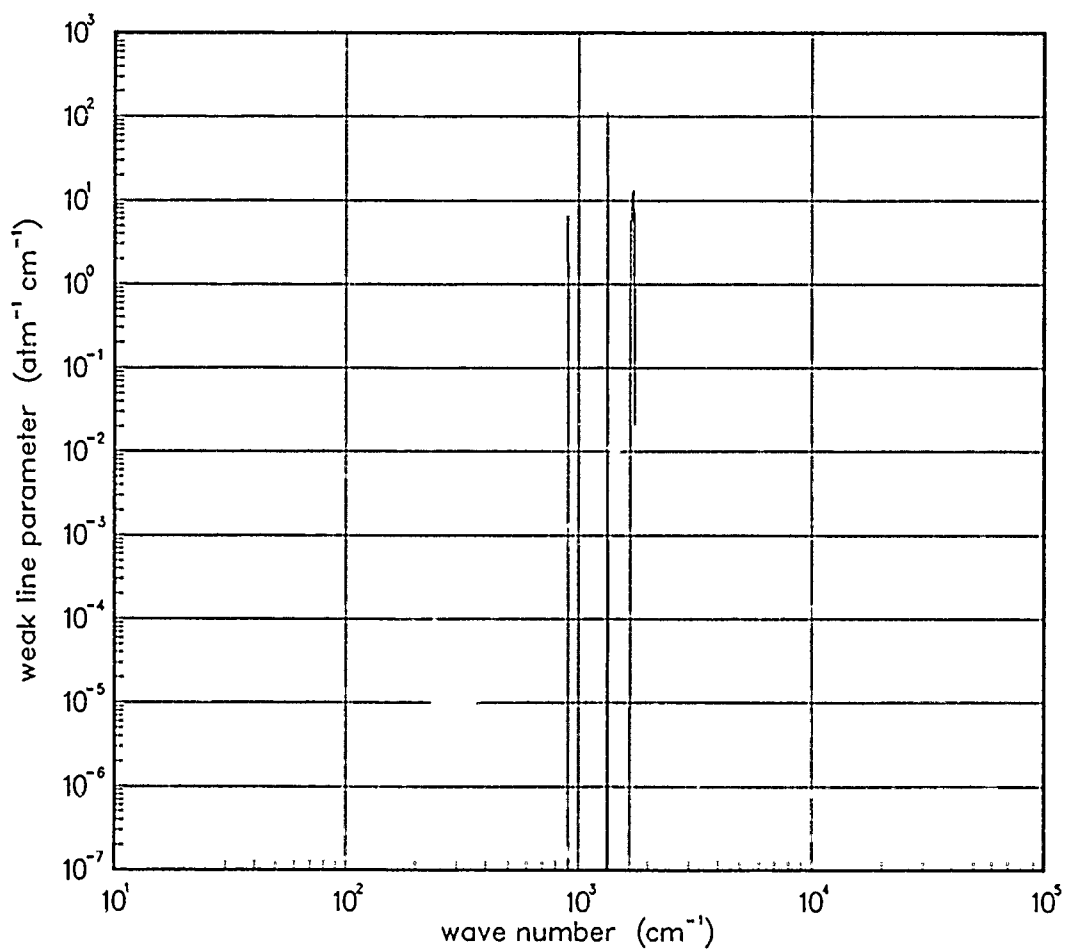


Figure 212. Weak-line parameter for HNO₃ at 300°K.

5.6 NITROGEN PEROXIDE (NO₂).

The local thermal equilibrium emission spectra for Nitrogen Peroxide was taken from the Roscoe IR database for the spectral region $< 5,000 \text{ cm}^{-1}$. In the spectral region of 5,000 to 100,000 cm^{-1} the data was developed by the VisiDyne Corporation^{||} using a Air Force Weapons Laboratory database developed in the late sixties.

The calculation of the LTE NO₂ curves is discussed in ROSCOE Manual Volume 28*. The calculations ($< 5,000 \text{ cm}^{-1}$) were performed with the TATE Code[†].

Table 5. Spectroscopic data for NO₂.

Ground Electronic State		
$\omega_1 = 1326.8$	$\omega_2 = 751.3^{\S}$	$\omega_3 = 1632.8$
$\chi_{11} = -7.9$	$\chi_{22} = -1.6^{\S}$	$\chi_{33} = -16.0$
$\chi_{12} = -8.6^{\S}$	$\chi_{13} = -29.5$	$\chi_{23} = -11.3^{\S}$
$A_e = 8.0012$	$B_e = 0.43364$	$C_e = 0.41040$
$\gamma_t(300 \text{ }^{\circ}\text{K}) = 0.10^{\dagger}$		

Data Source:

*J.G. DeVore, and T.L. Stephens, Band Model Parameters for Thermal Emission (U) , .72TMP-20, General Electric - TEMPO, (June 1972) (Secret).

[†]T.L. Stephens, V.R. Stull, A.L. Klein, and J.D. Losse, The ROSCOE Manual, Volume 28-Molecular Band Models for Thermal and Optically Pumped emissions (U) , GE78TMP-52, General Electric -- TEMPO (June 1978) (Confidential).

[†]Estimate.

[§]Inferred (See The ROSCOE Manual Volume 28, GE78TMP-52).

^{||}H. Smith, T. Keneshea, VisiDyne Corporation, private communication (1986).

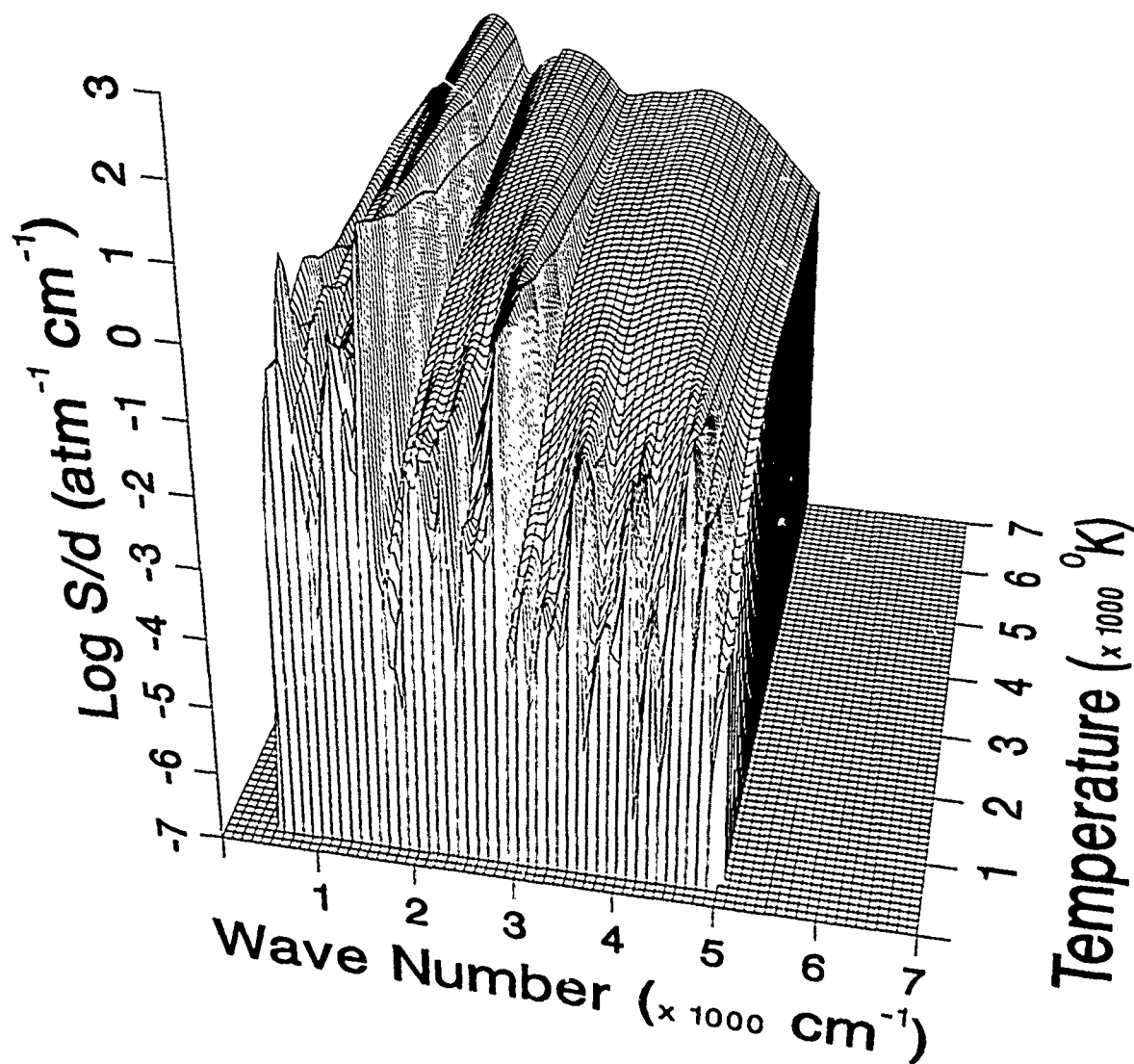


Figure 213. Weak-line parameter for NO₂.

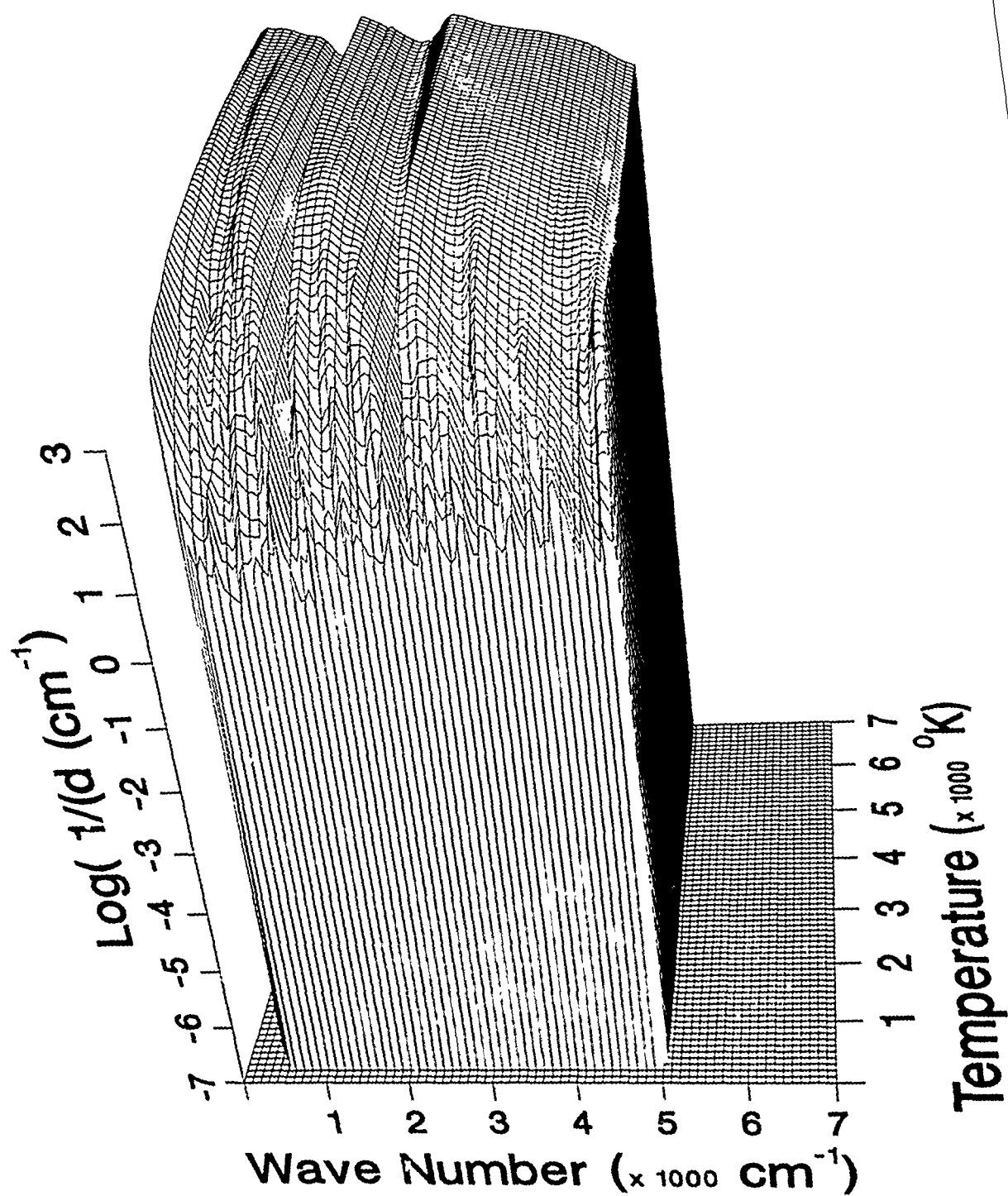


Figure 214. Inverse line spacing for NO_2 .

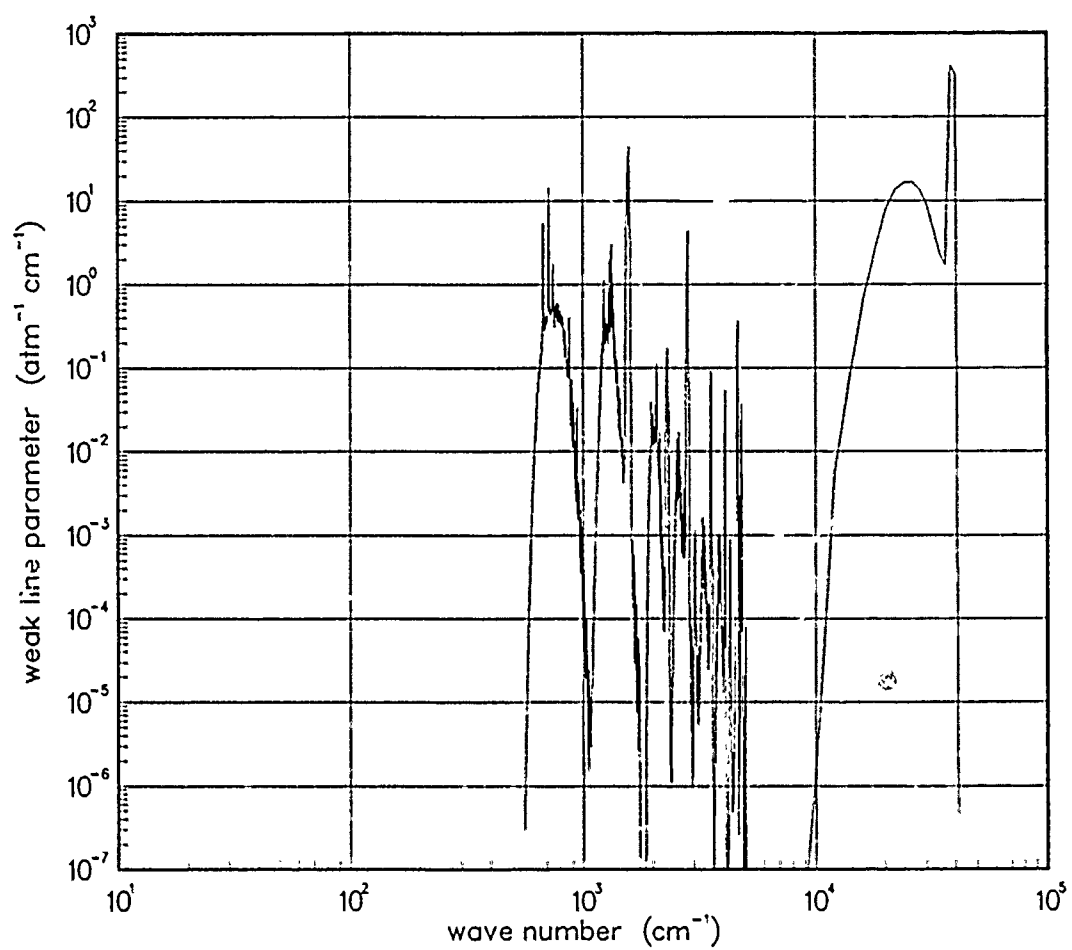


Figure 215. Weak-line parameter for NO₂ at 200°K.

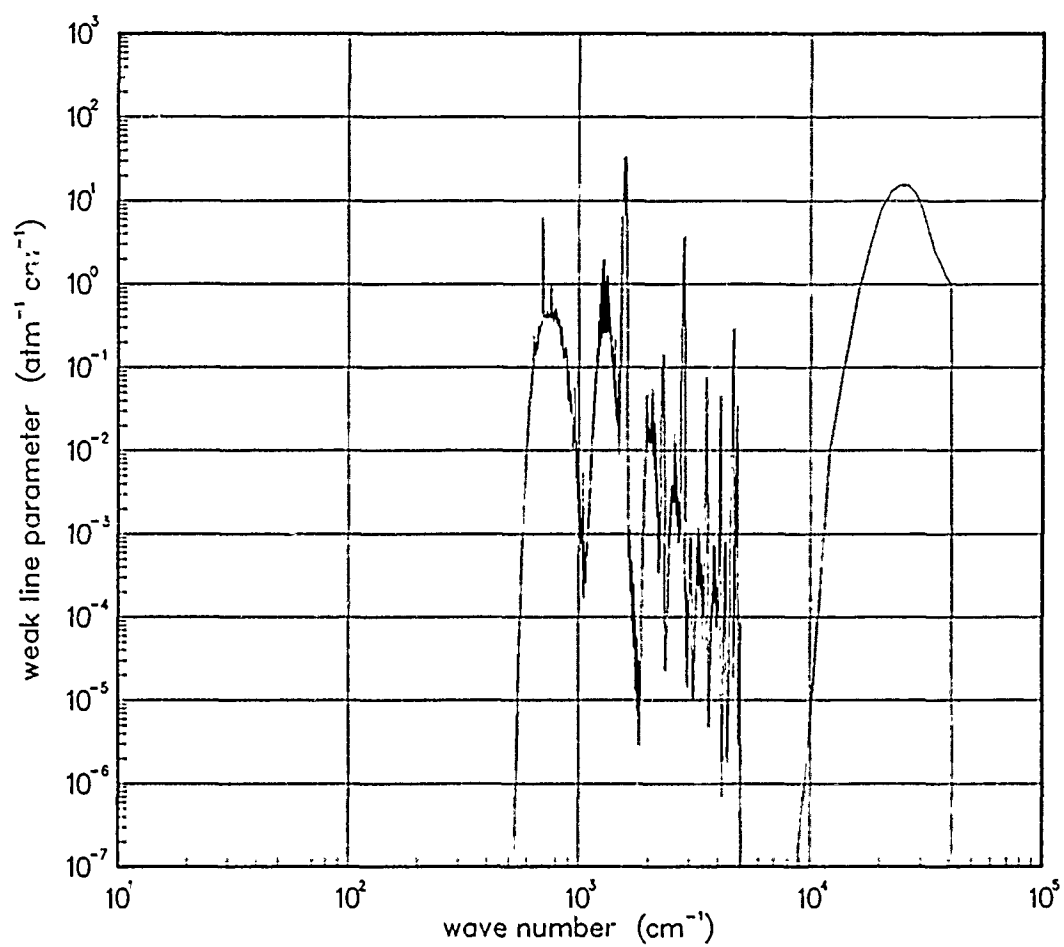


Figure 216. Weak-line parameter for NO₂ at 300°K.

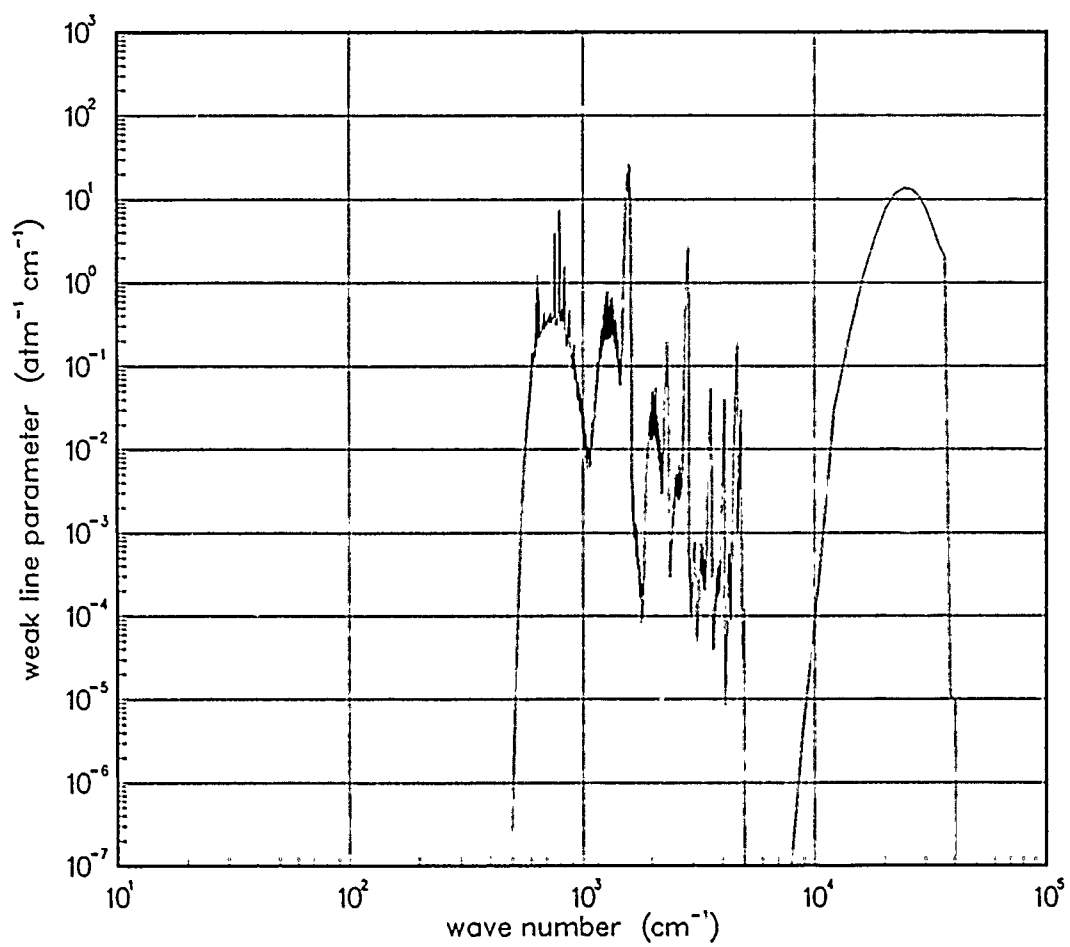


Figure 217. Weak-line parameter for NO₂ at 500°K.

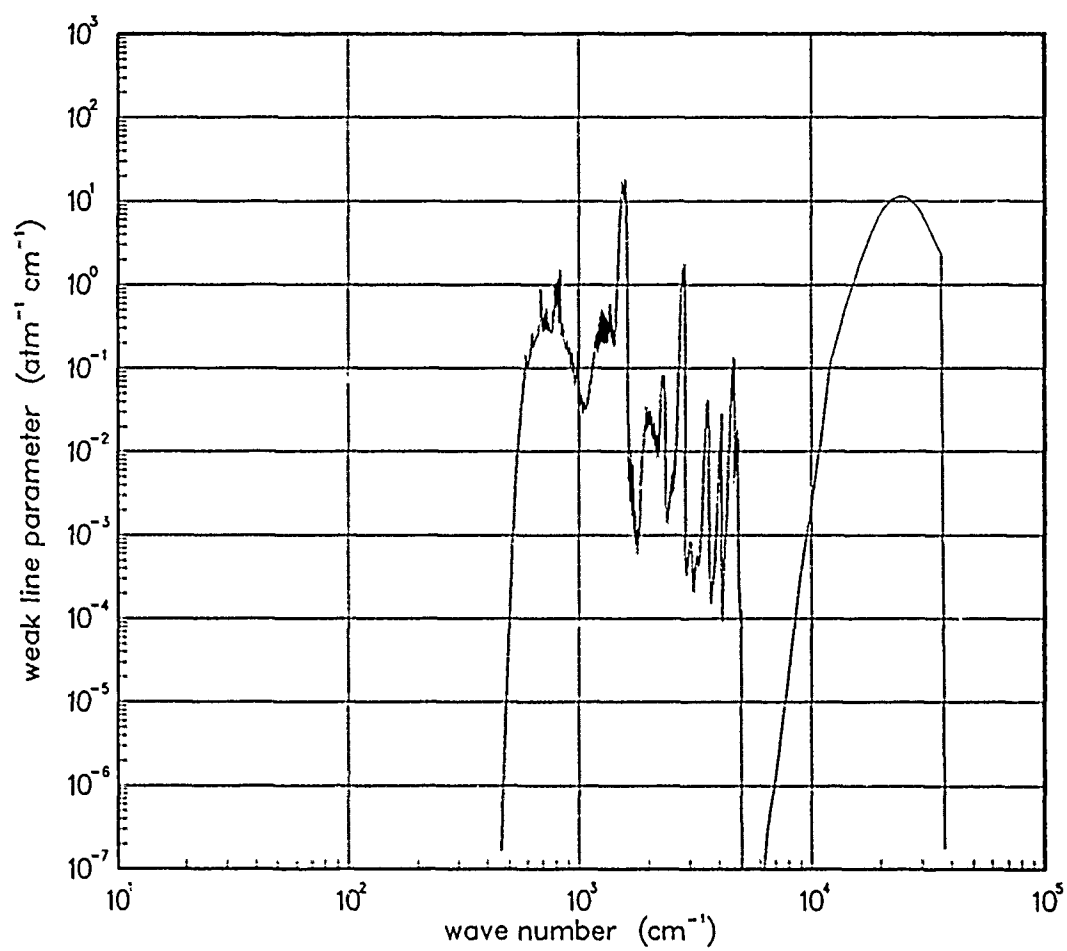


Figure 218. Weak-line parameter for NO₂ at 750°K.

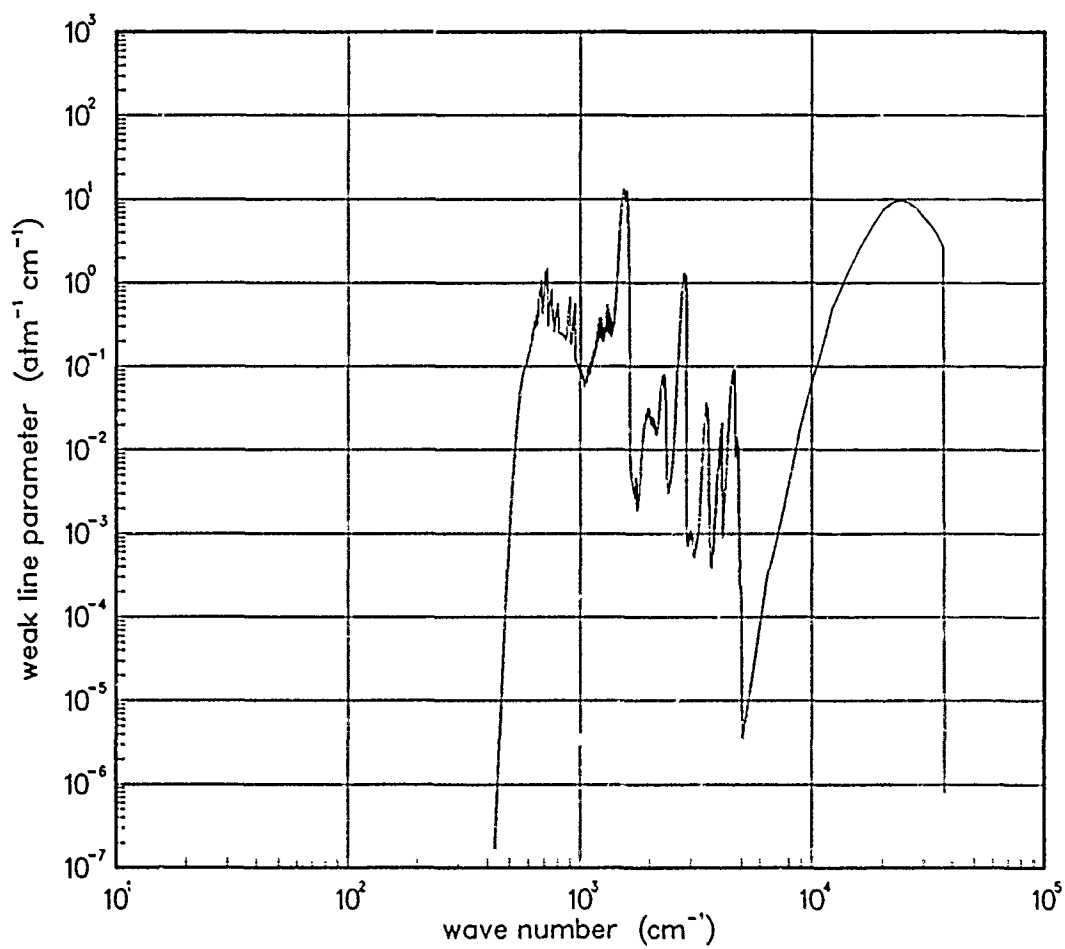


Figure 219. Weak-line parameter for NO₂ at 10° K.

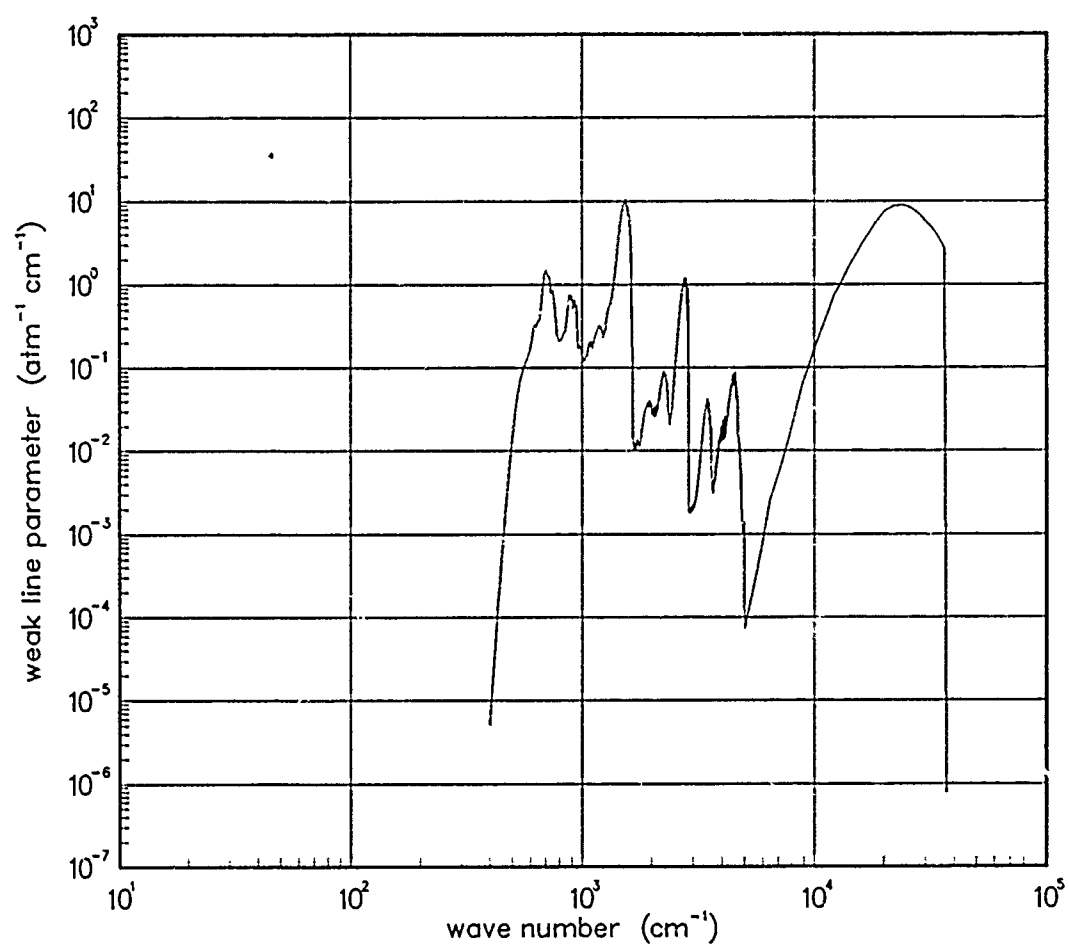


Figure 220. Weak-line parameter for NO₂ at 1500°K.

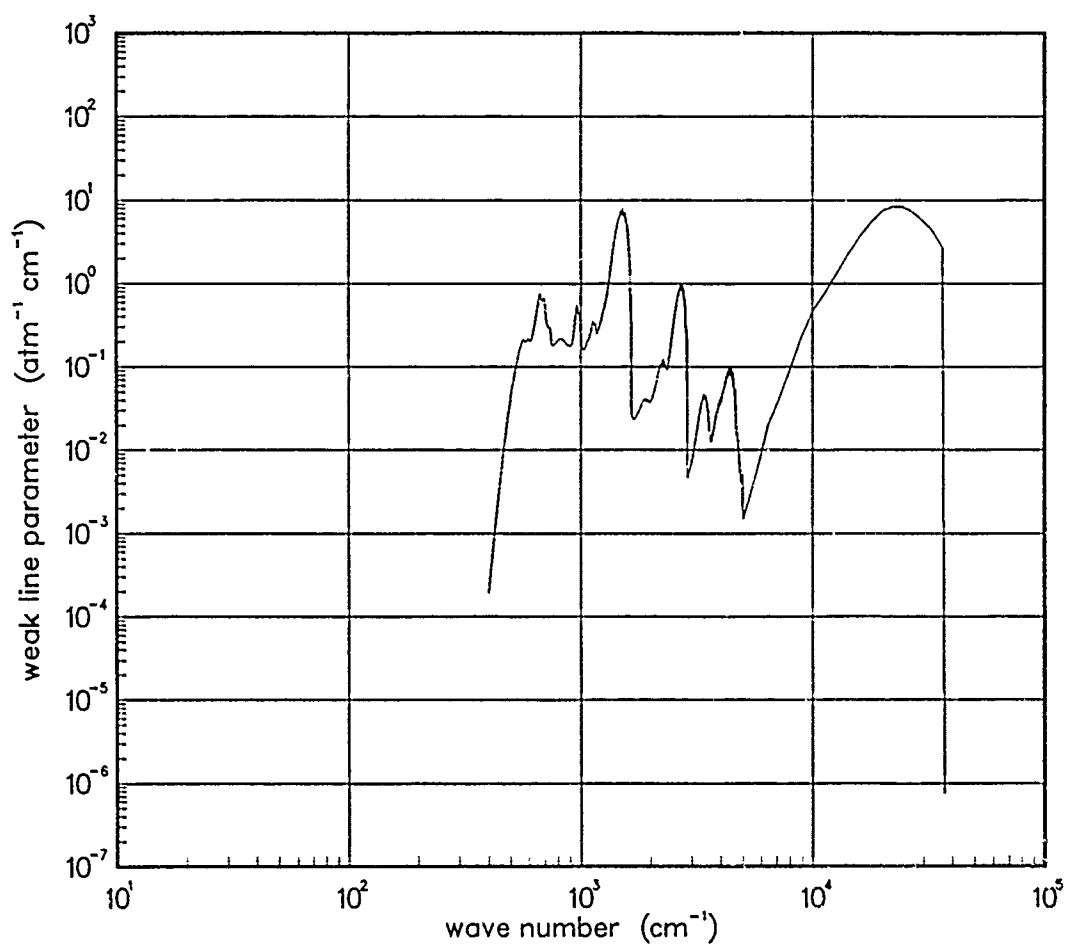


Figure 221. Weak-line parameter for NO₂ at 2000°K.

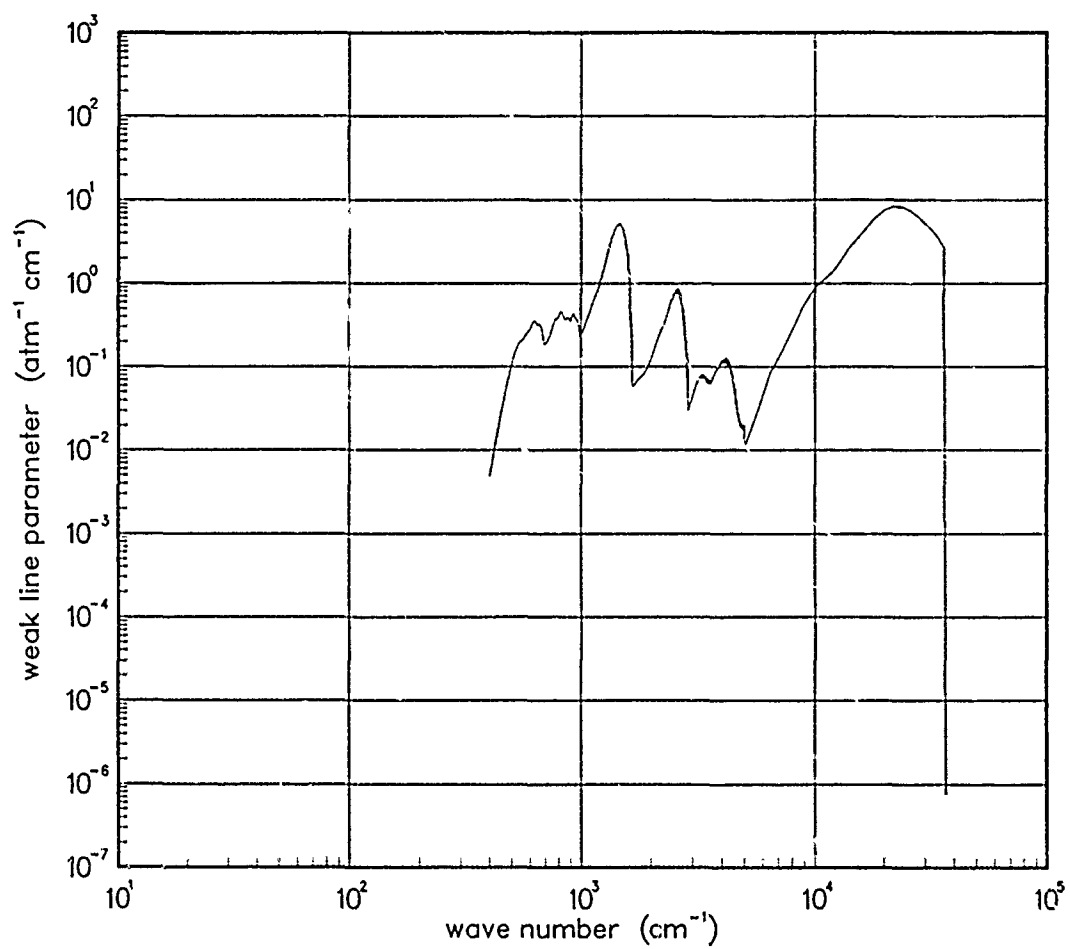


Figure 222. Weak-line parameter for NO₂ at 3000°K.

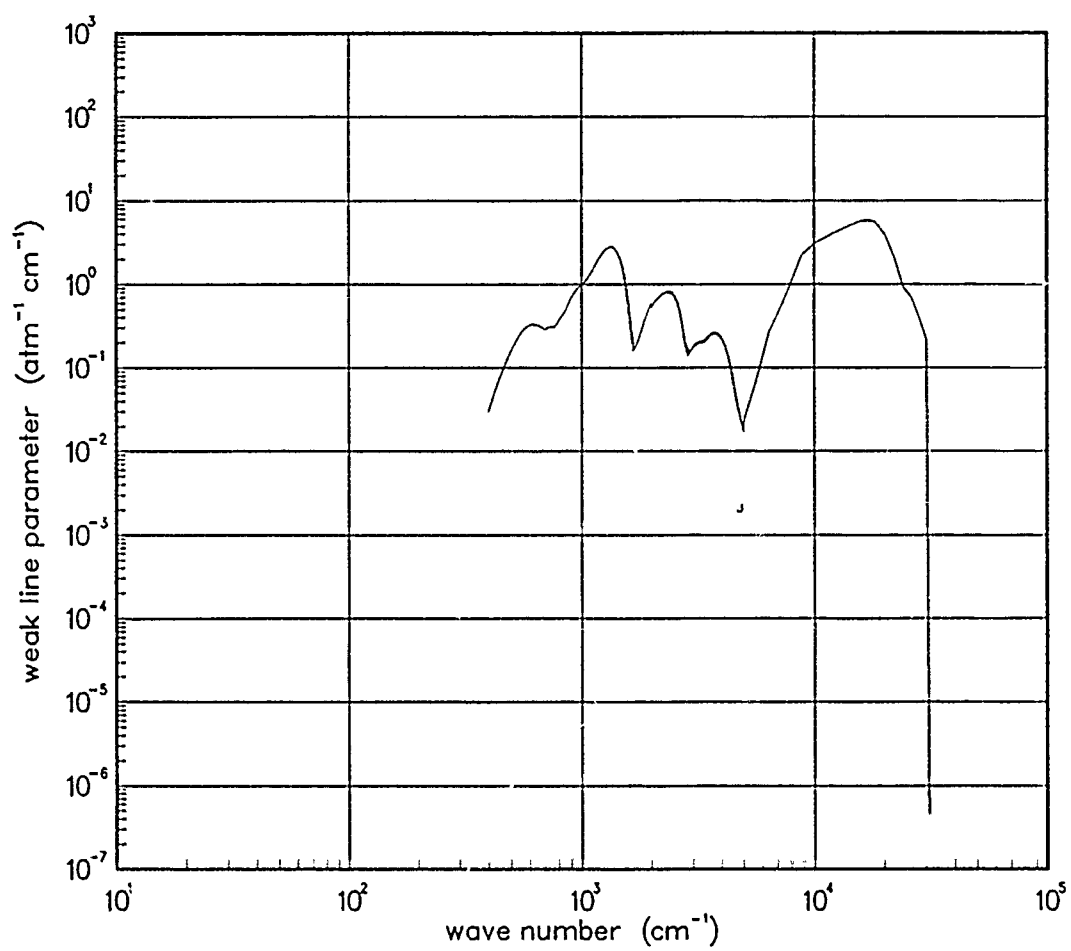


Figure 223. Weak-line parameter for NO₂ at 5900°K.

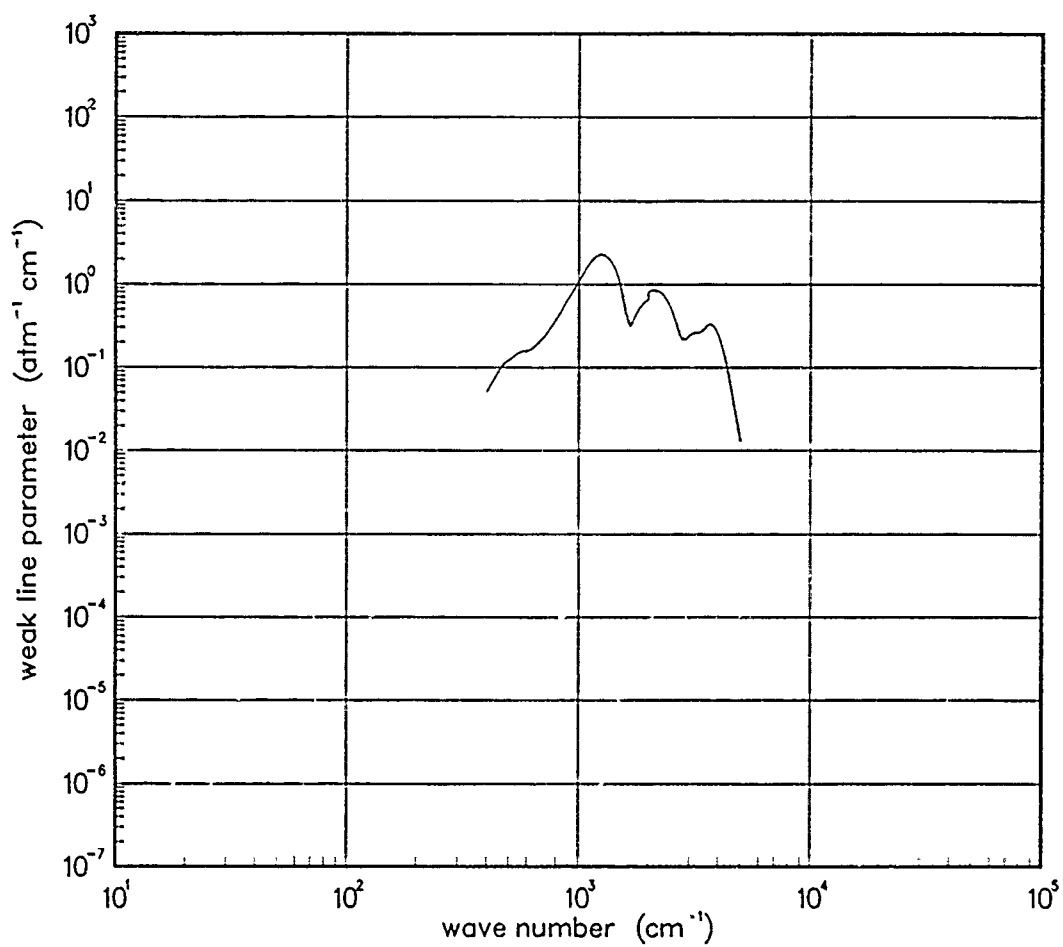


Figure 224. Weak-line parameter for NO₂ at 7000°K.

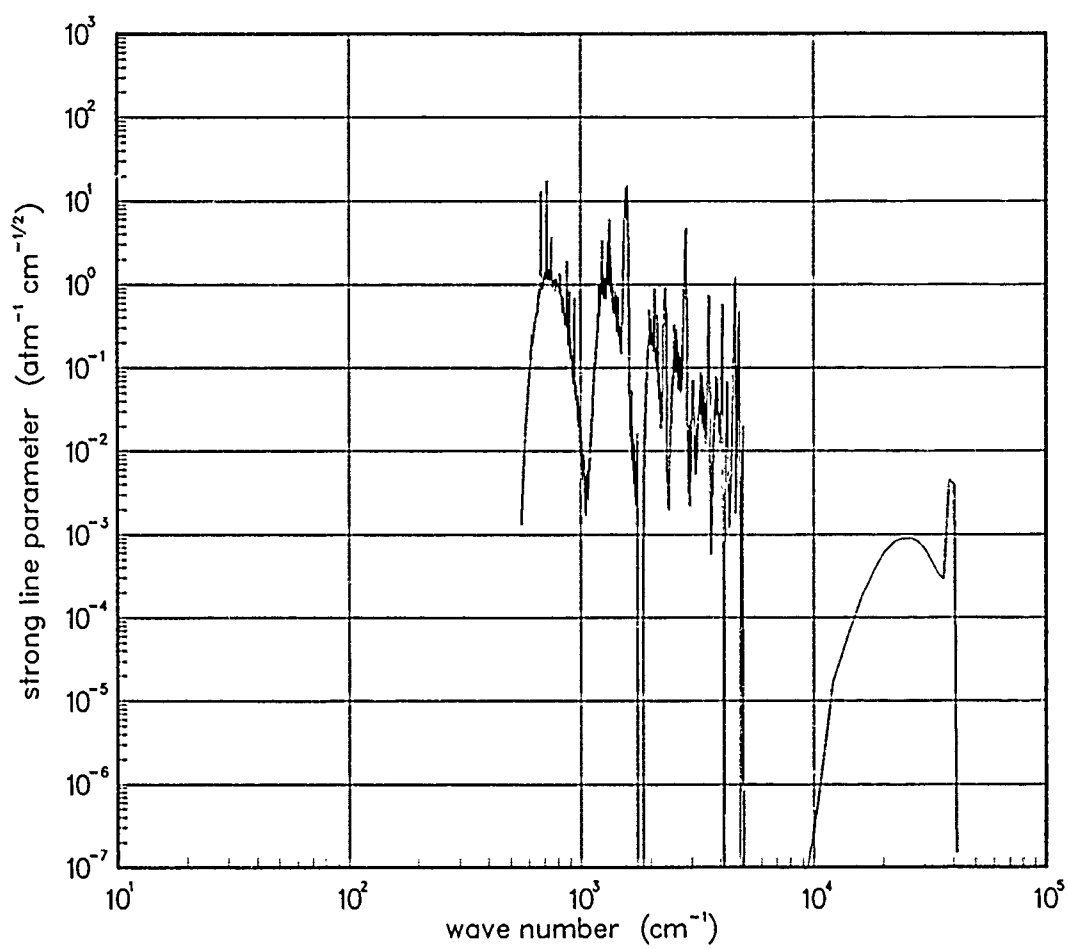


Figure 225. Strong-line parameter for NO₂ at 200°K.

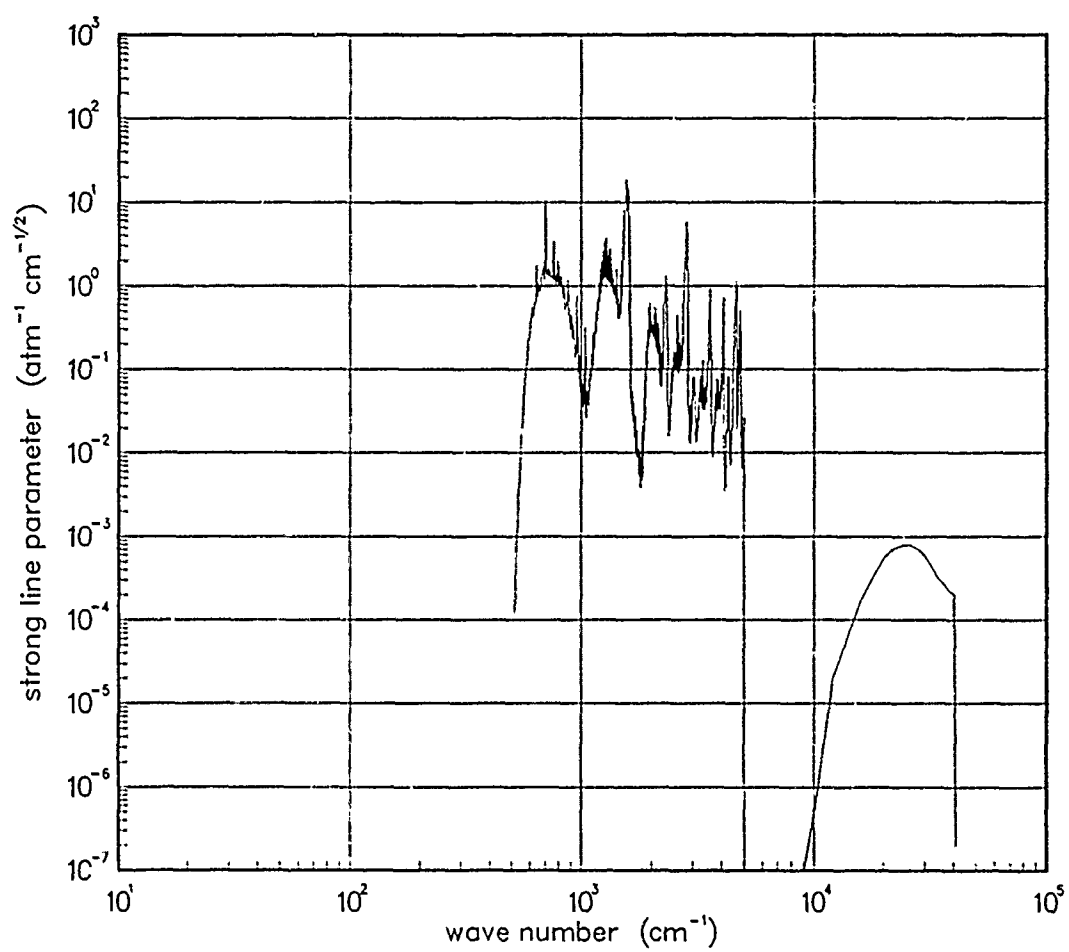


Figure 226. Strong-line parameter for NO₂ at 300°K.

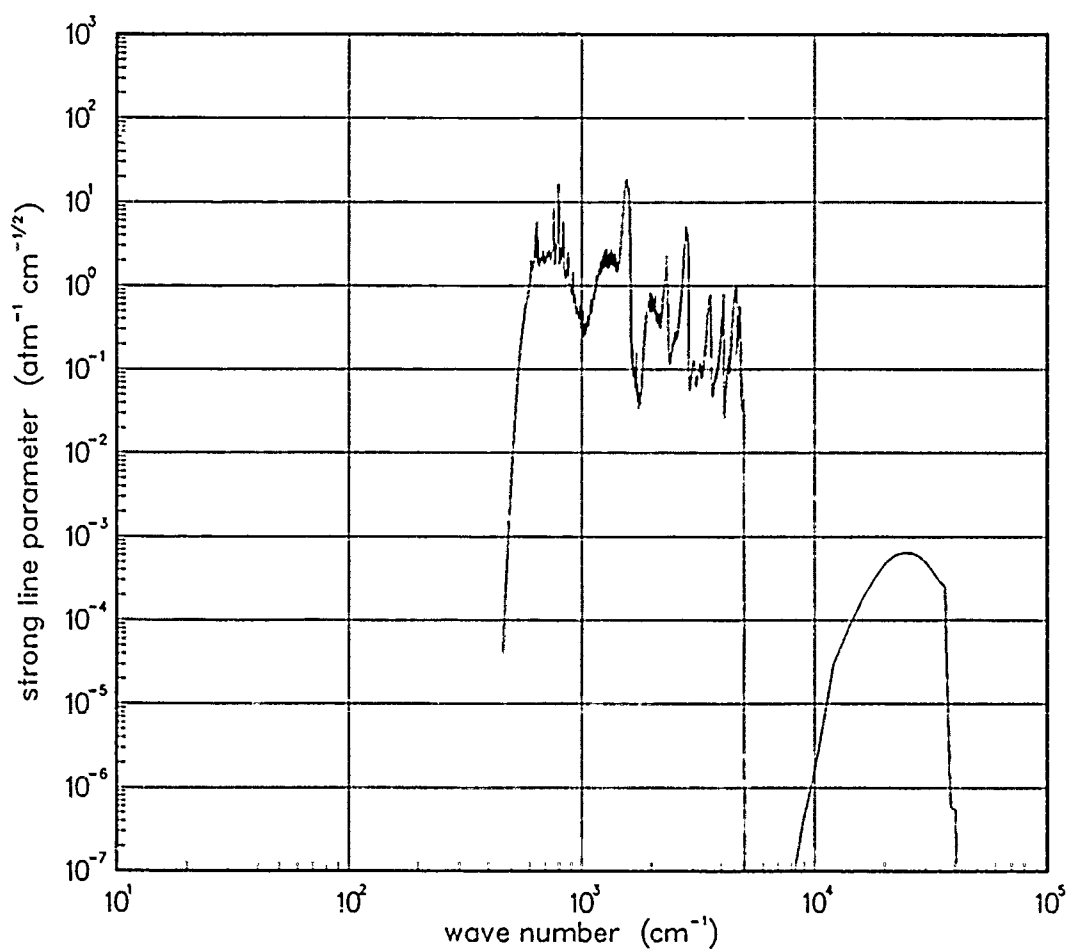


Figure 227. Strong-line parameter for NO₂ at 500°K.

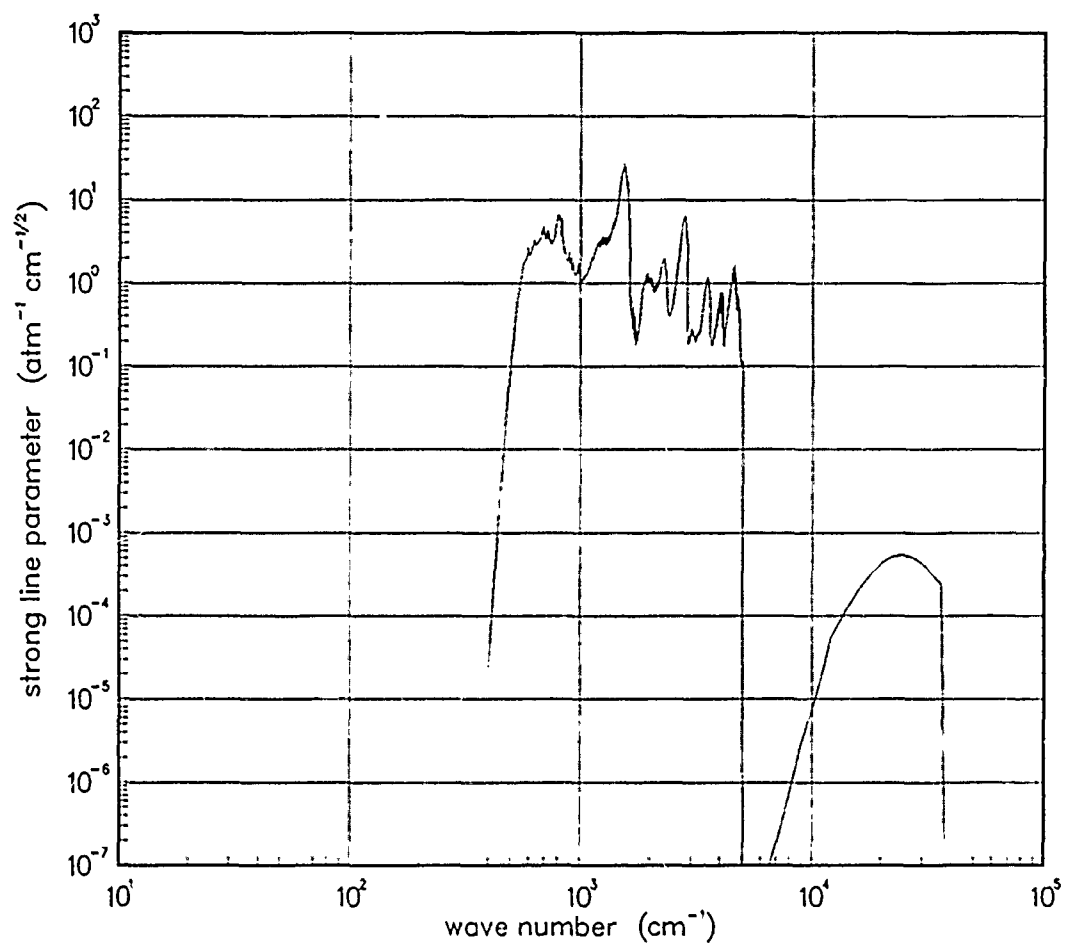


Figure 228. Strong-line parameter for NO₂ at 750°K.

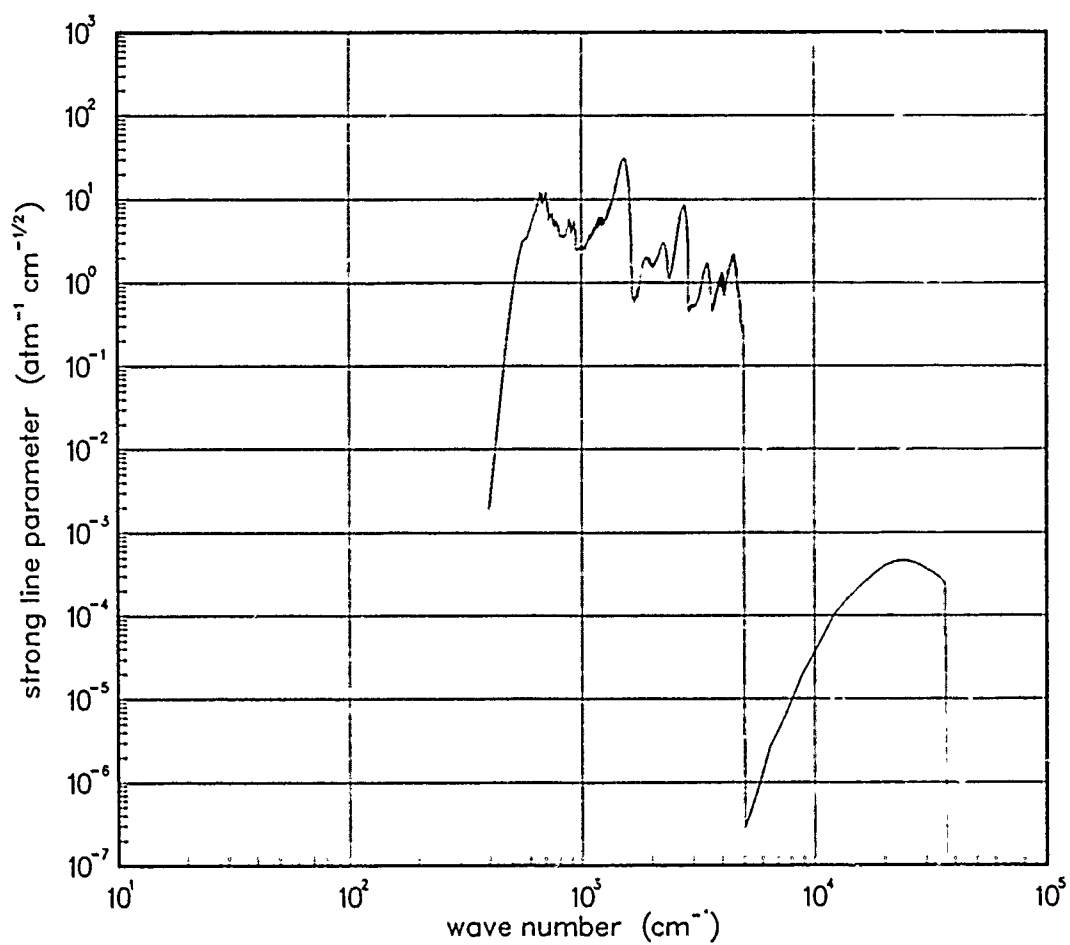


Figure 229. Strong-line parameter for NO₂ at 1000°K.

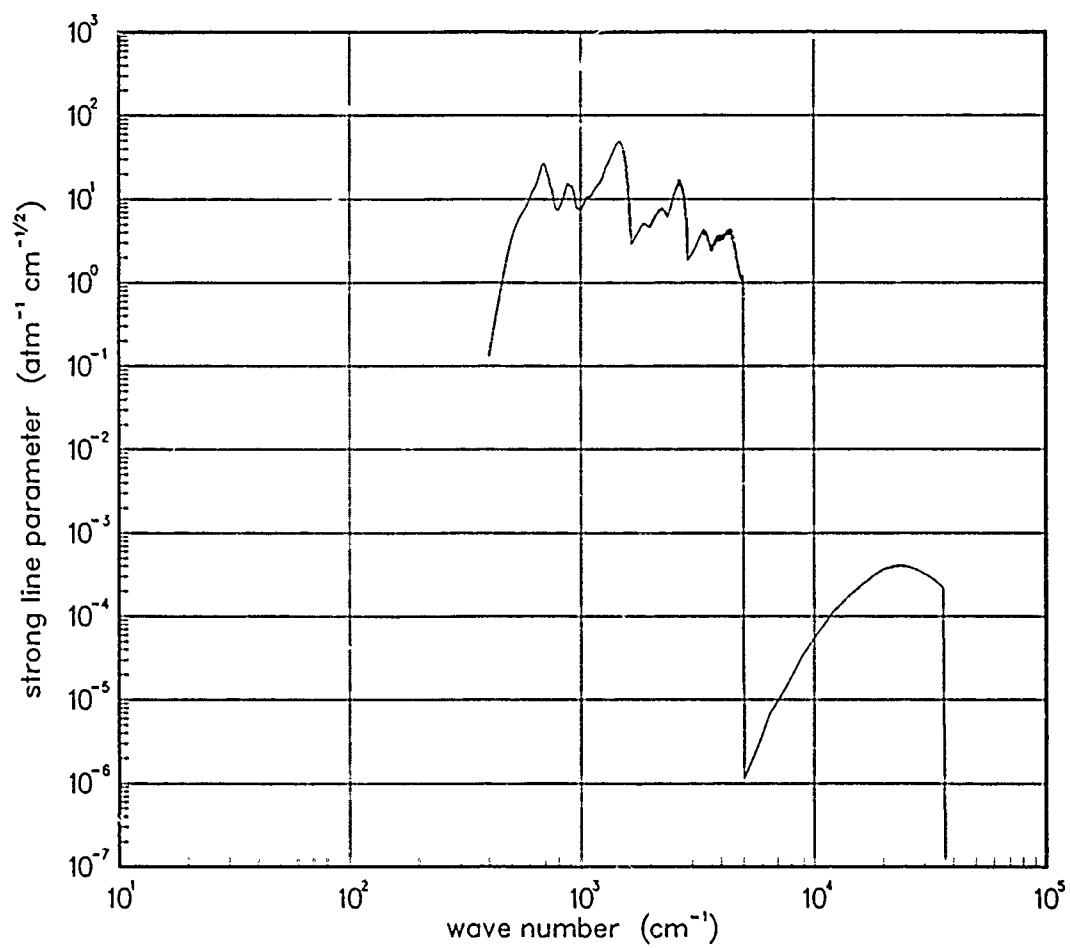


Figure 230. Strong-line parameter for NO₂ at 1500°K.

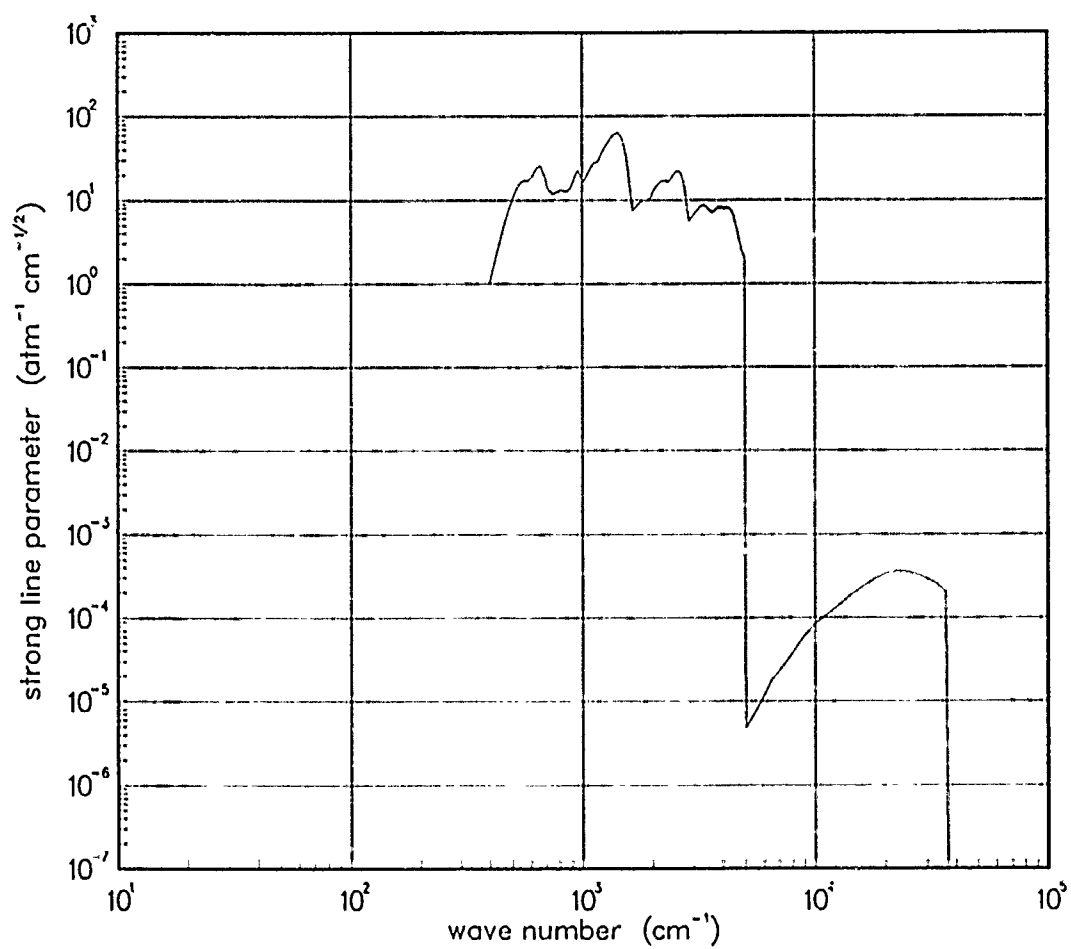


Figure 231. Strong-line parameter for NO₂ at 2000°K.

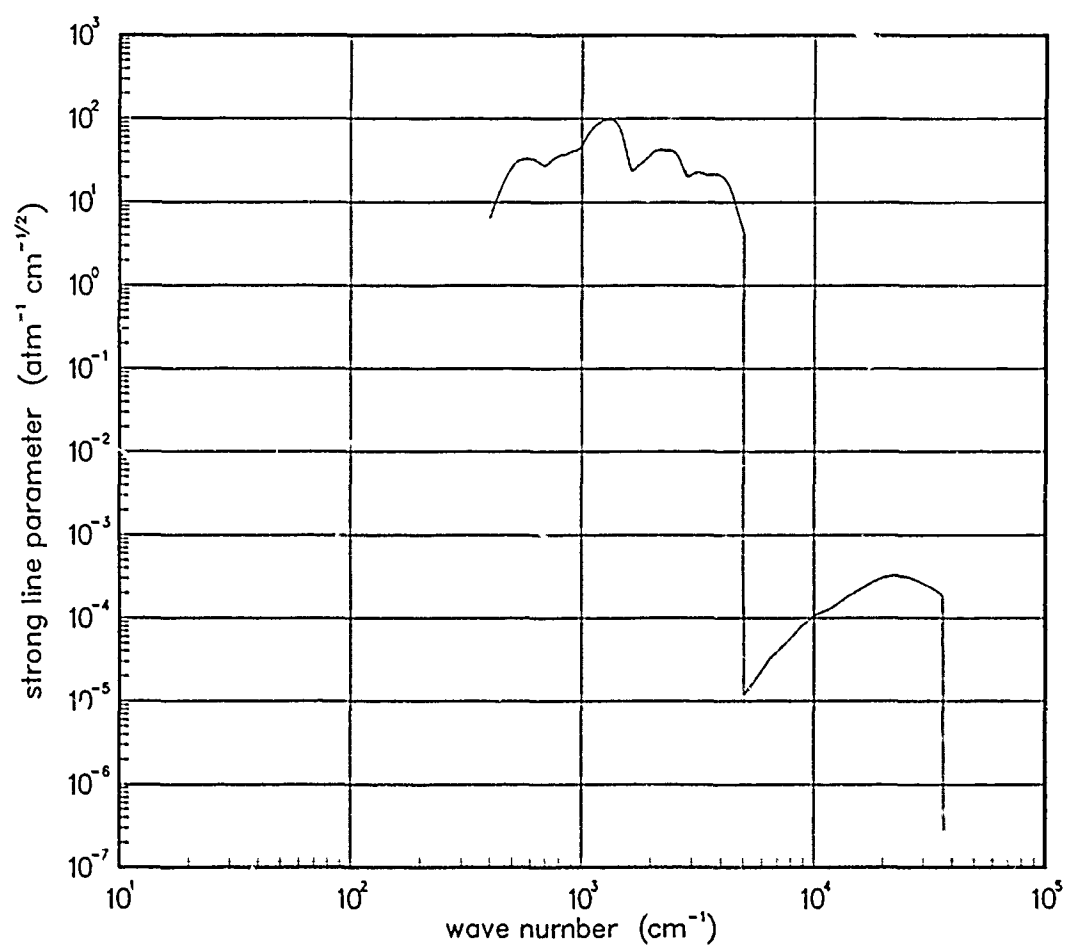


Figure 232. Strong-line parameter for NO₂ at 3000°K.

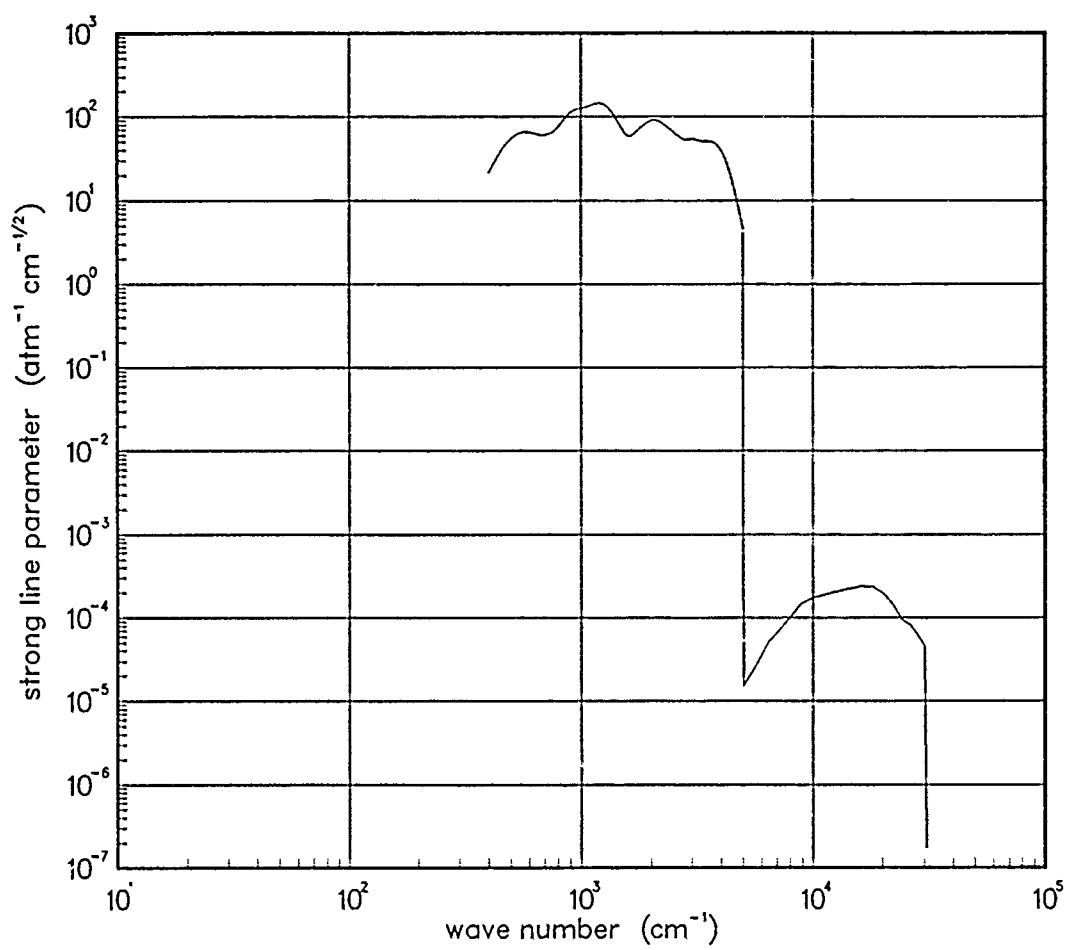


Figure 233. Strong-line parameter for NO₂ at 5000°K.

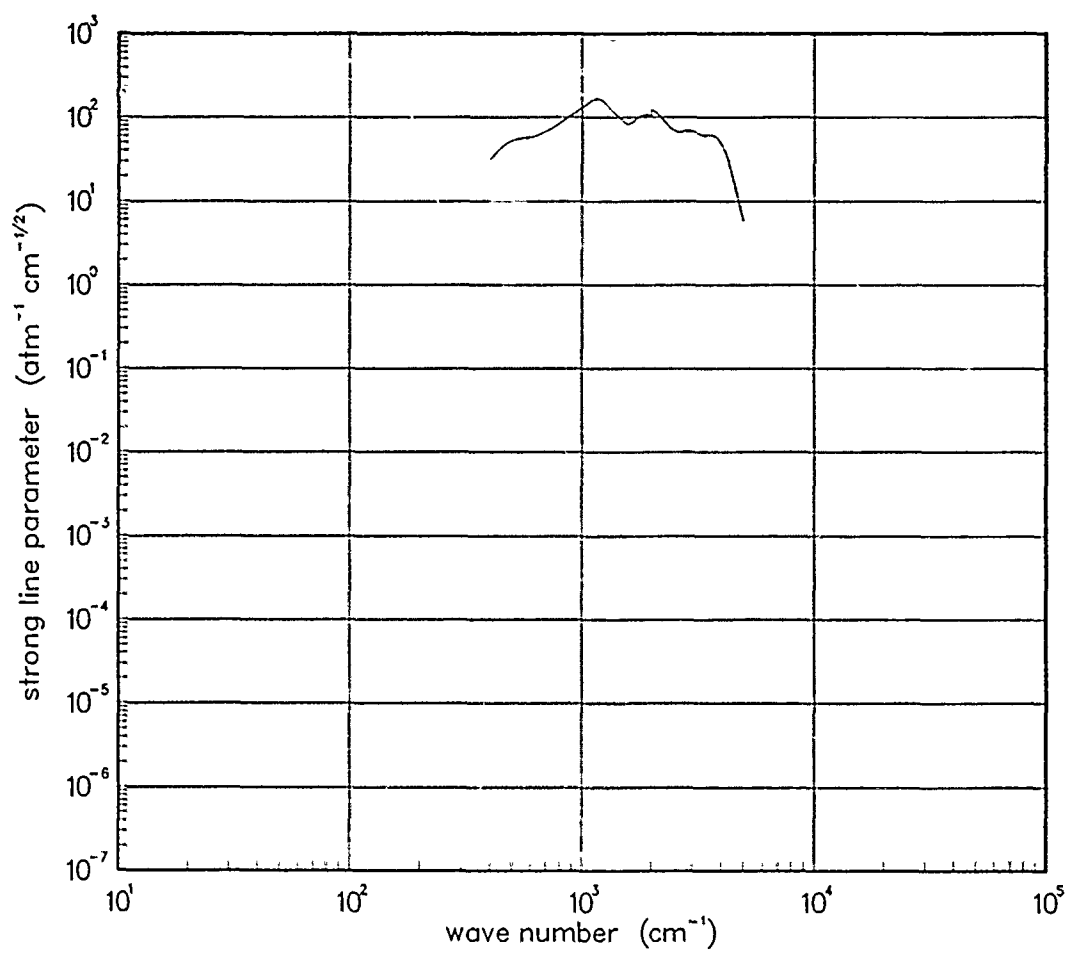


Figure 234. Strong-line parameter for NO₂ at 7000°K.

5.7 OZONE (O₃).

The local thermal equilibrium emission spectra for O₃ was taken from the ROSCOE LTE data base.

The computation of this data was performed with the TATE code*. The calculations are described in The ROSCOE Manual, Volume 28†.

Table 6. Spectroscopic data for O₃.

Ground Electronic State		
$\omega_1 = 1123.1$	$\omega_2 = 719.4$	$\omega_3 = 1101.1$
$\chi_{11} = 2.0$	$\chi_{22} = -1.0$	$\chi_{33} = -15.$
$\chi_{12} = -11.$	$\chi_{13} = -39.$	$\chi_{23} = -21.$
$A_e = 3.55196$	$B_e = 0.444917$	$C_e = 0.39476$
$\gamma_e(300^\circ\text{K}) = 0.11$		

Data Source:

*J.G. DeVore, and T.L. Stephens, Band Model Parameters for Thermal Emission (U) , 72TMP-20, General Electric - TEMPO (June 1972) (Secret).

†T.L. Stephens, V.R. Stull, A.L. Klein, and J.D. Losse, The ROSCOE Manual, Volume 28-Molecular Band Models for Thermal and Optically Pumped Emissions (U) , GE78TMP-52, General Electric -- TEMPO (June 1978) (Confidential).

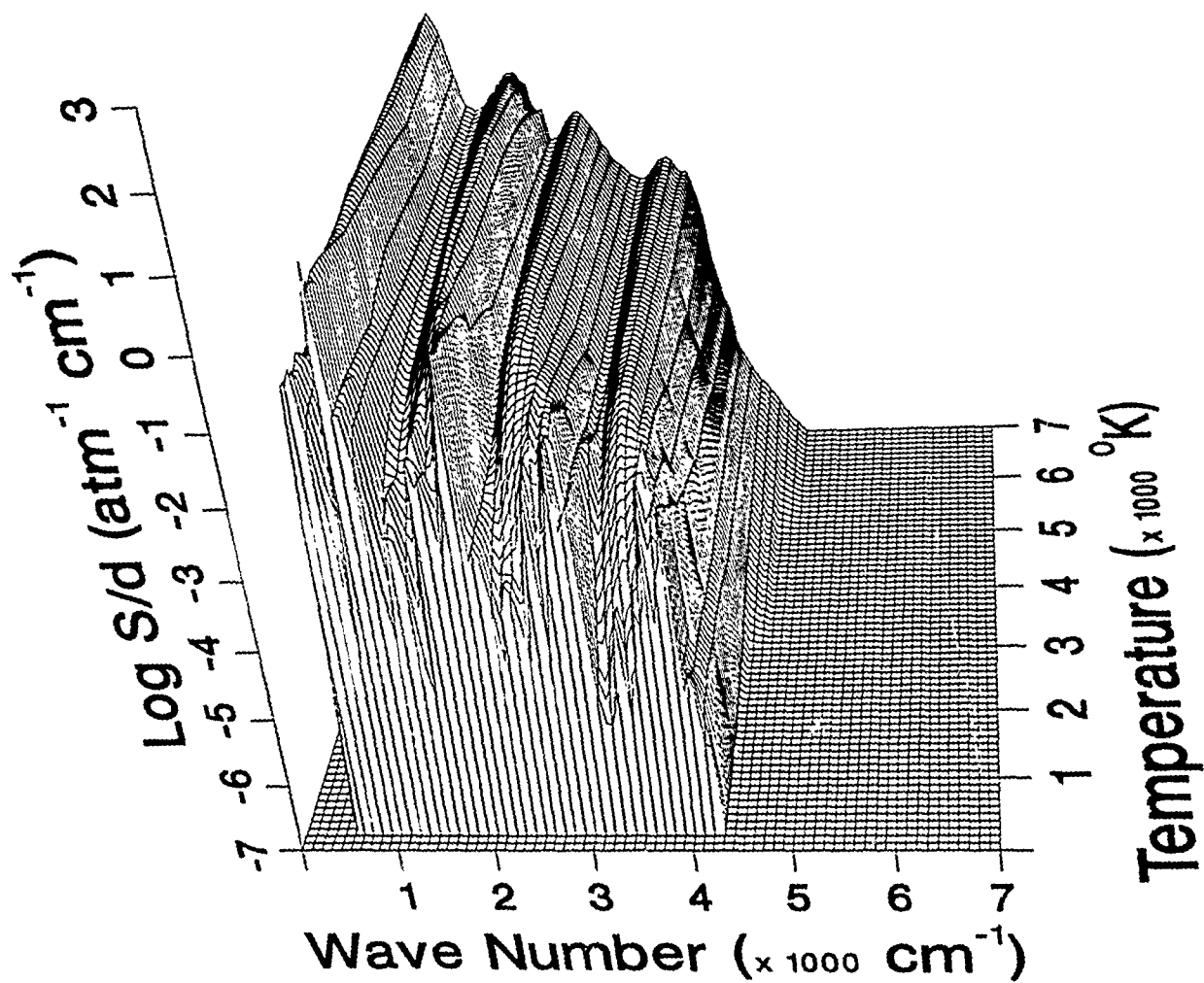


Figure 235. Weak-line parameter for O_3 .

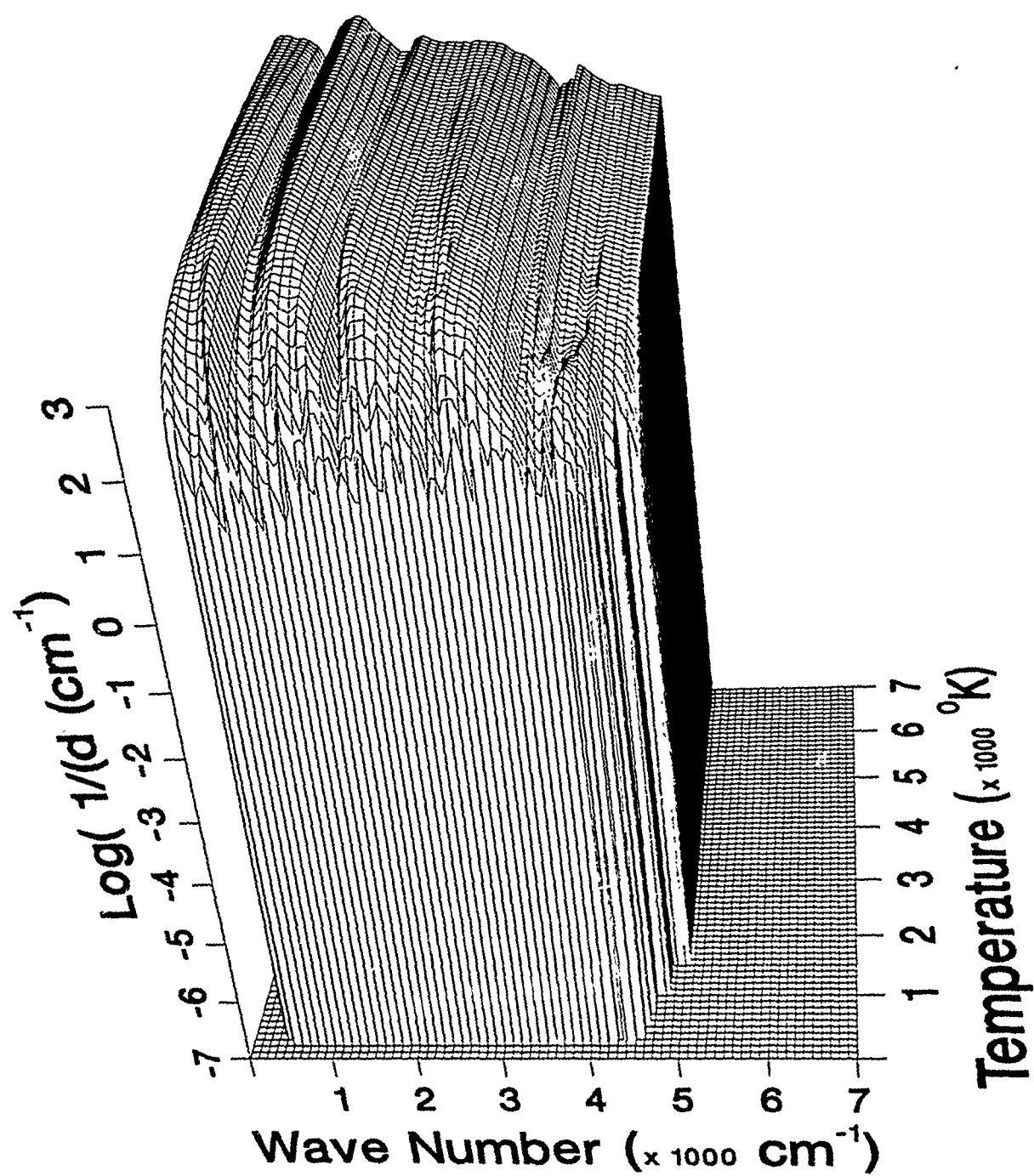


Figure 236. Inverse line spacing for O_3 .

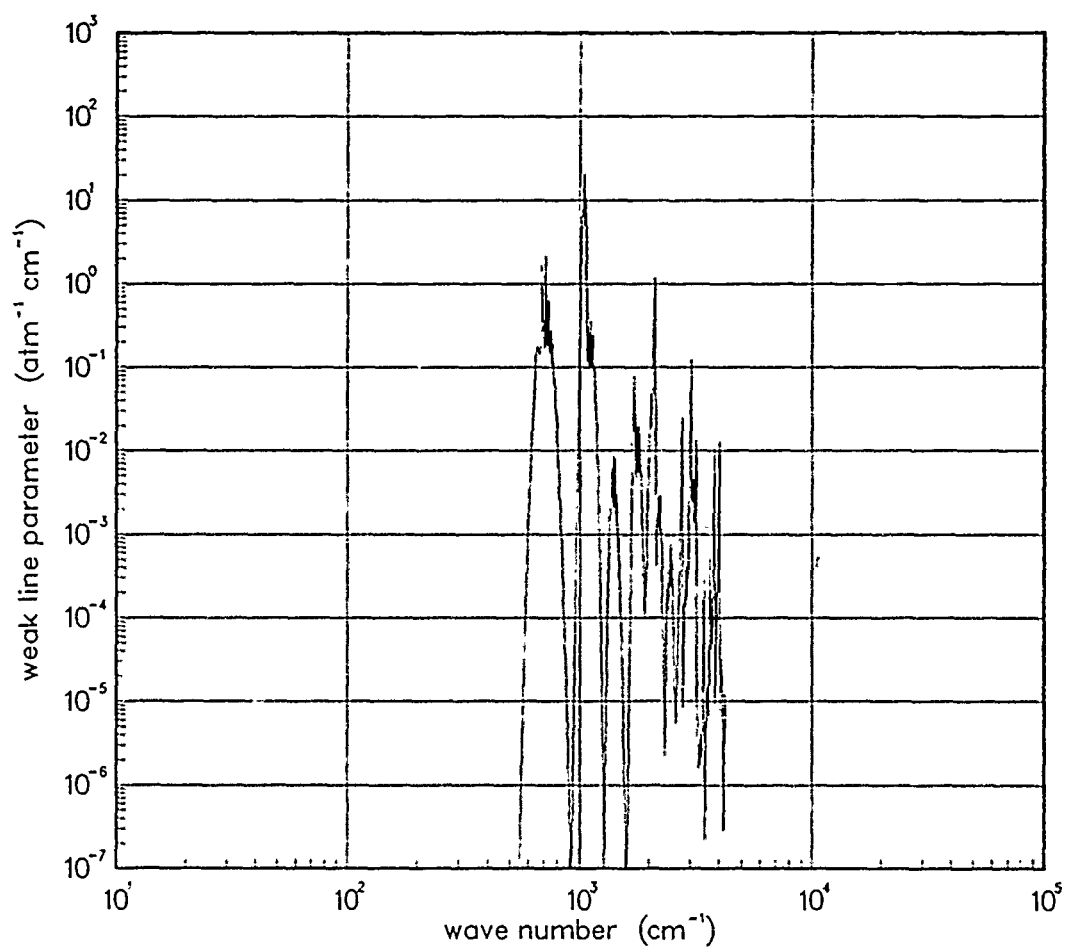


Figure 237. Weak-line parameter for O₃ at 200°K.

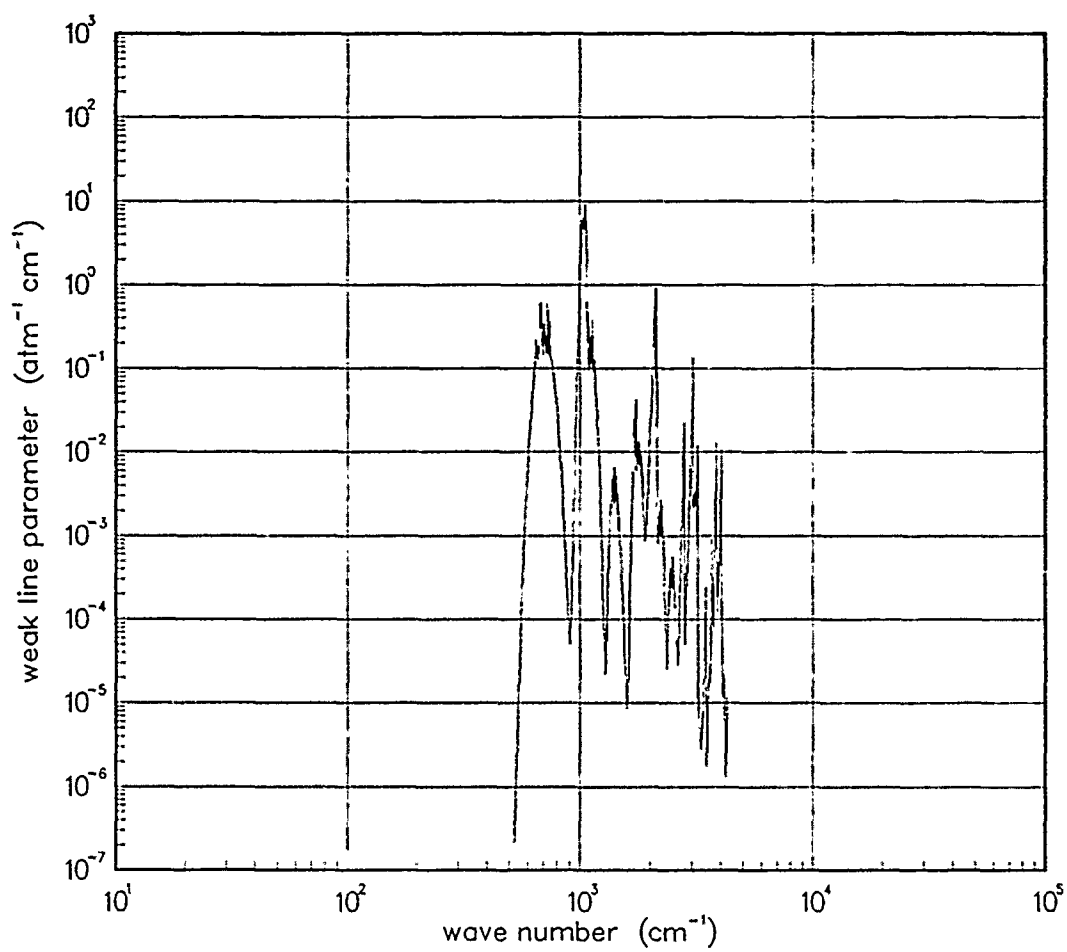


Figure 238. Weak-line parameter for O₃ at 300°K.

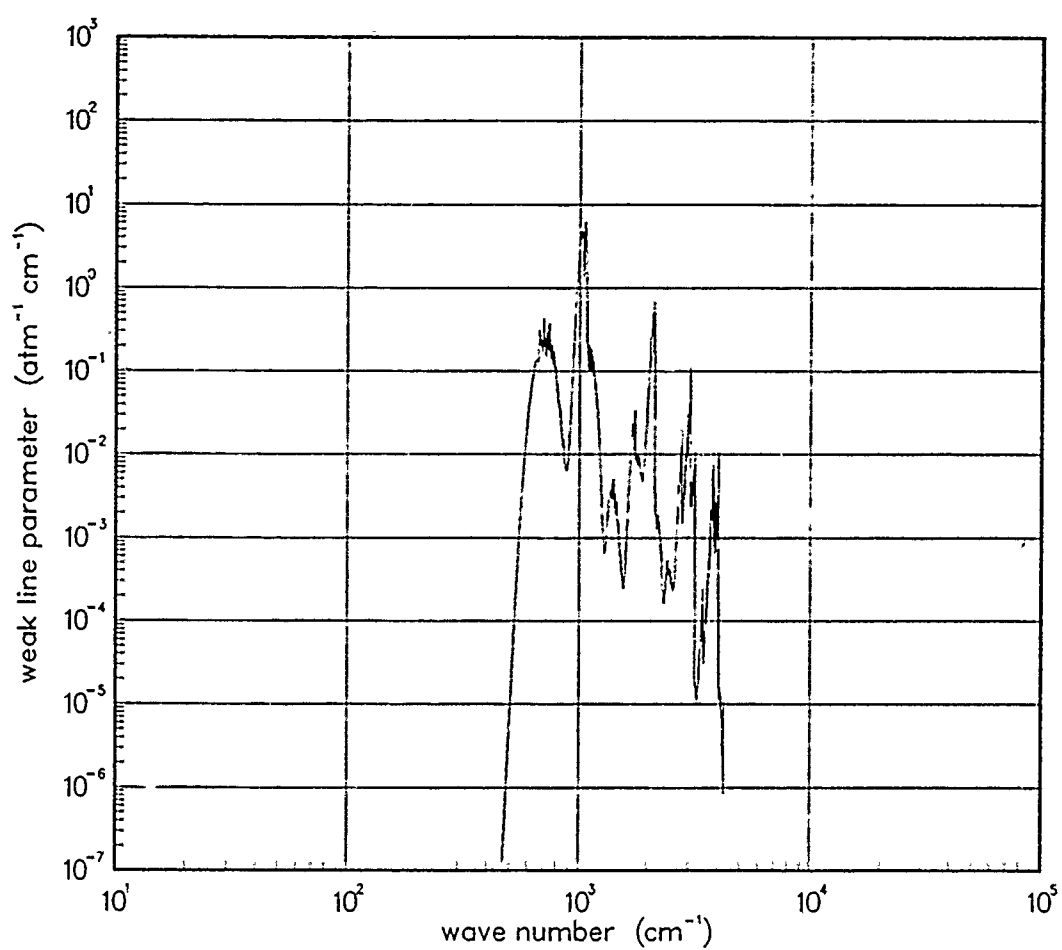


Figure 239. Weak-line parameter for O₃ at 500°K.

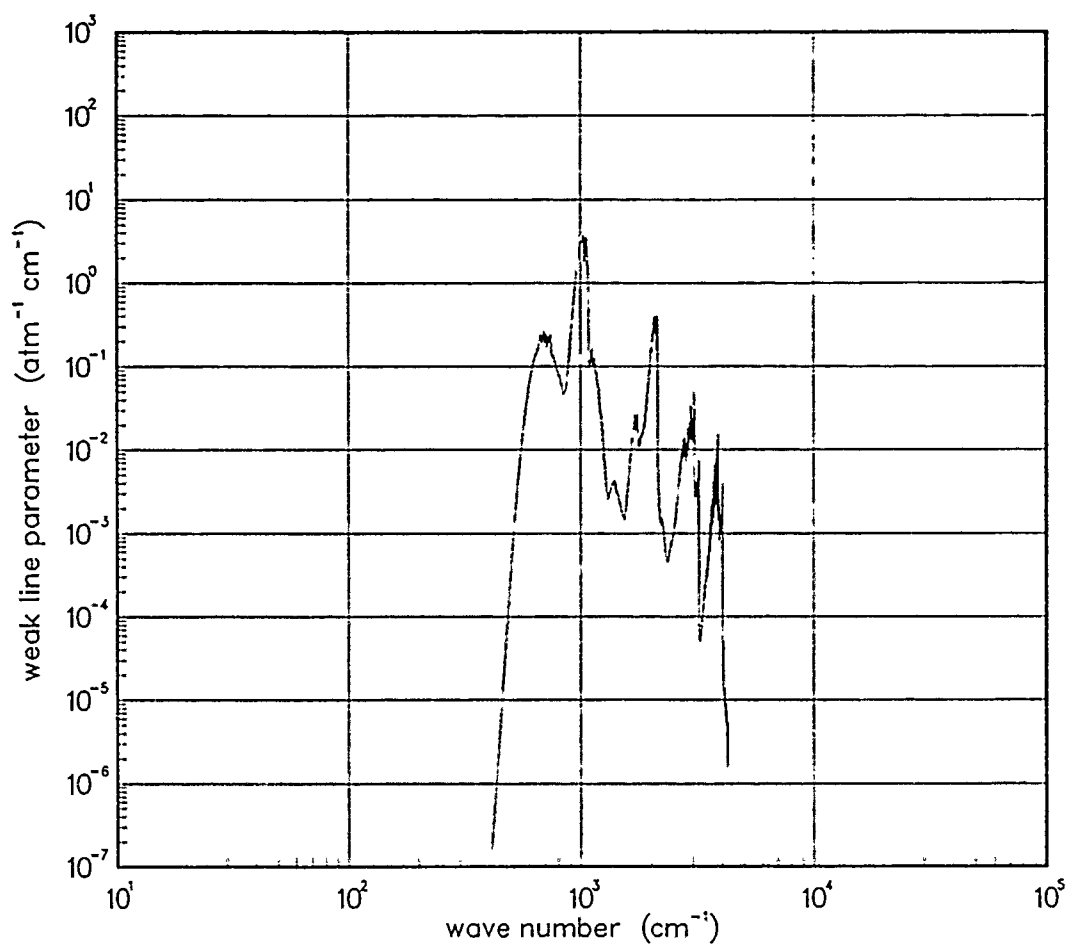


Figure 240. Weak-line parameter for O₃ at 750°K.

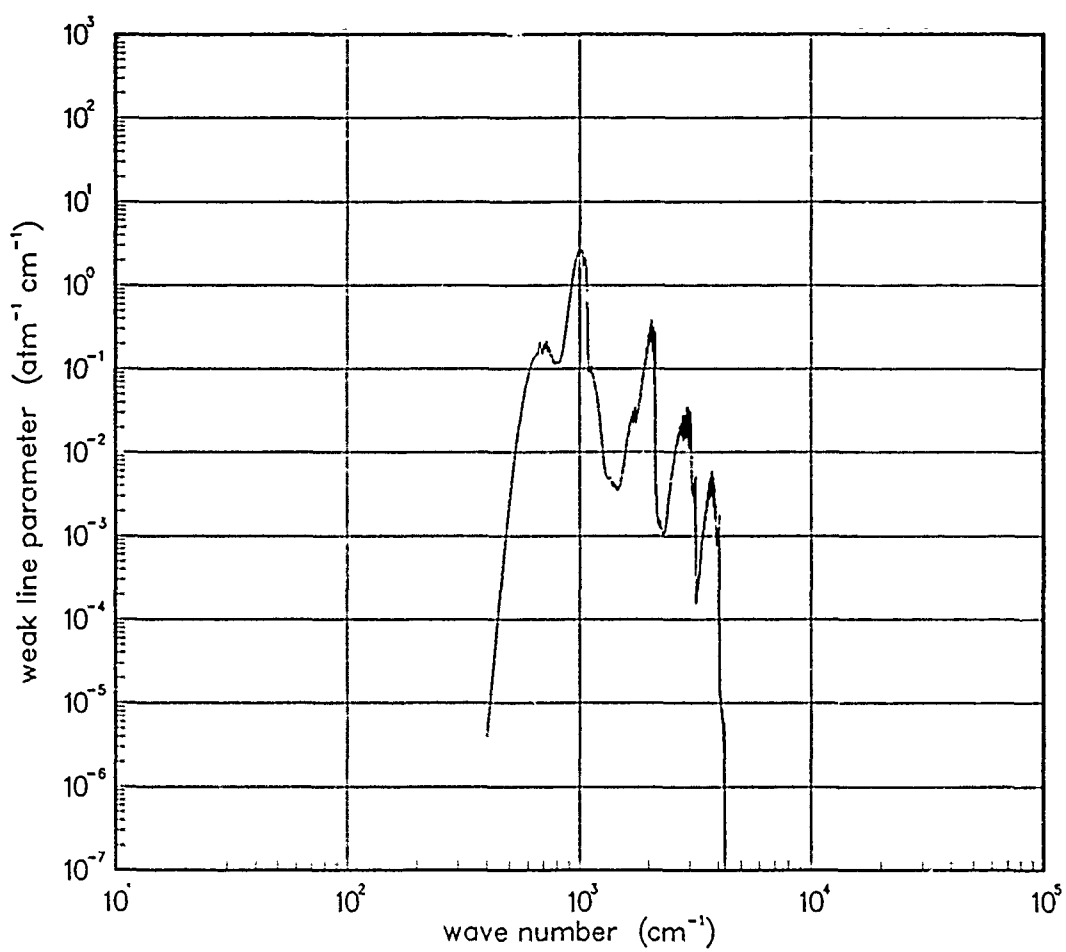


Figure 241. Weak-line parameter for O₃ at 1000°K.

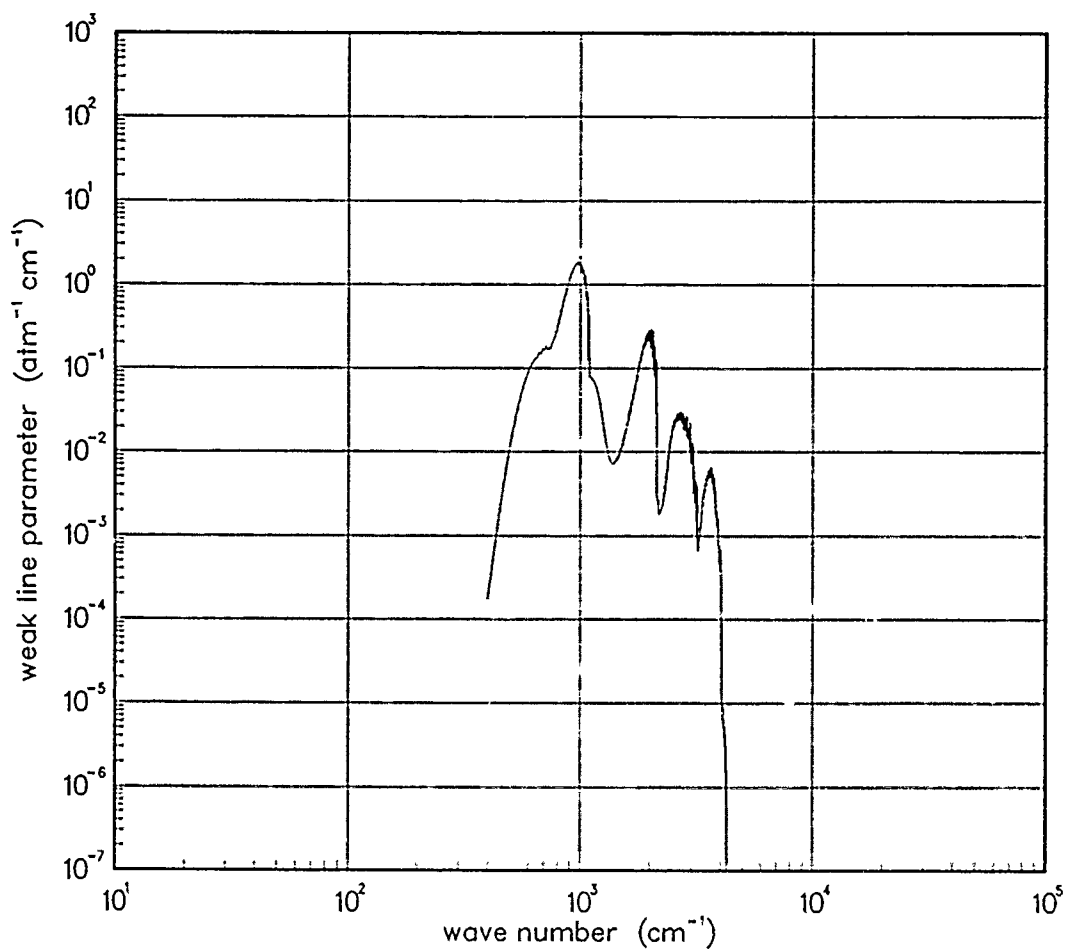


Figure 242. Weak-line parameter for O₃ at 1500°K.

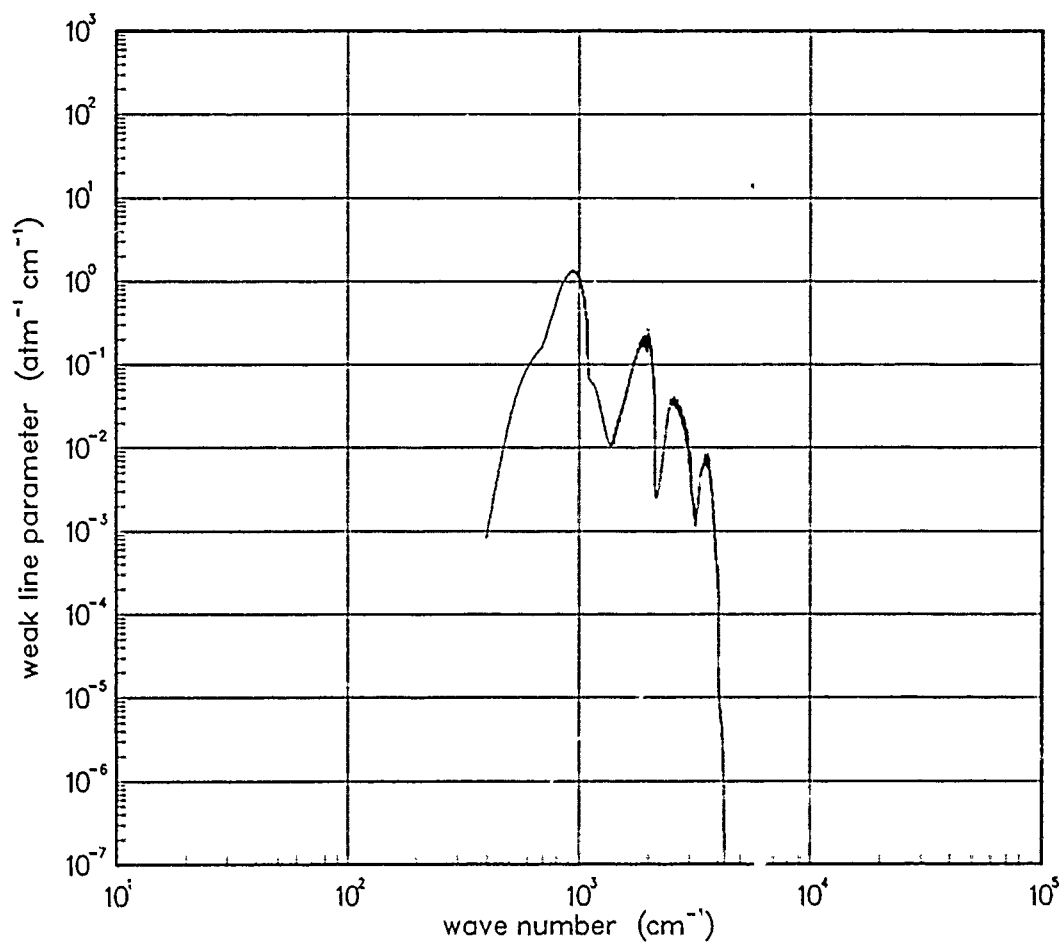


Figure 243. Weak-line parameter for O₃ at 2000°K.

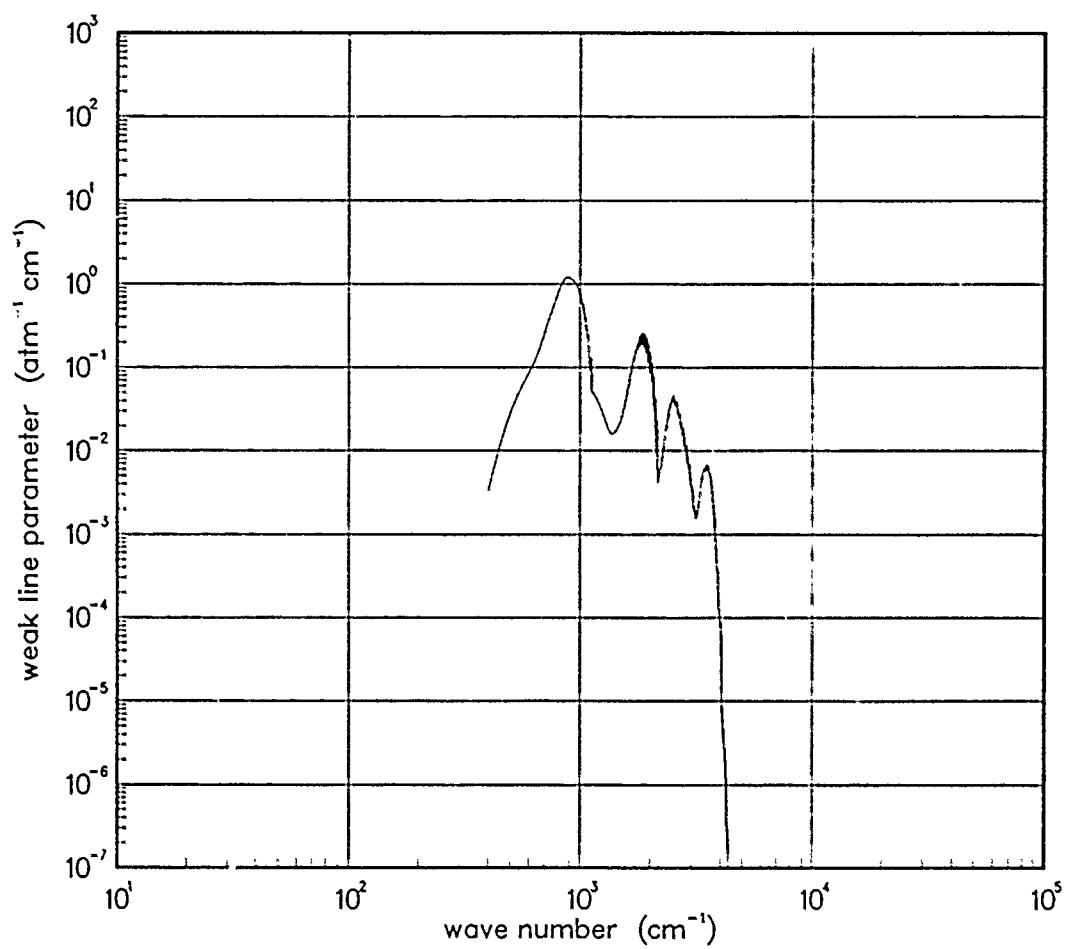


Figure 244. Weak-line parameter for O_3 at $3000^\circ K$.

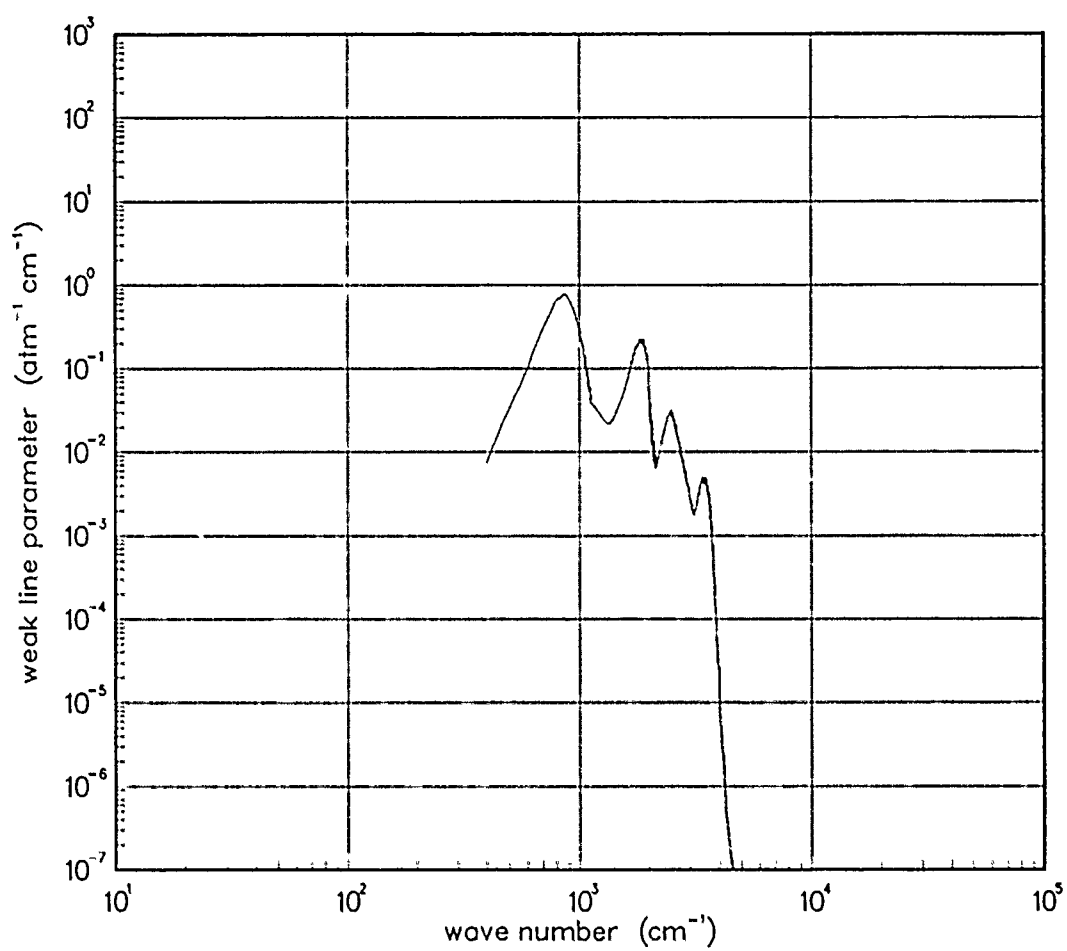


Figure 245. Weak-line parameter for O_3 at $5000^\circ K$.

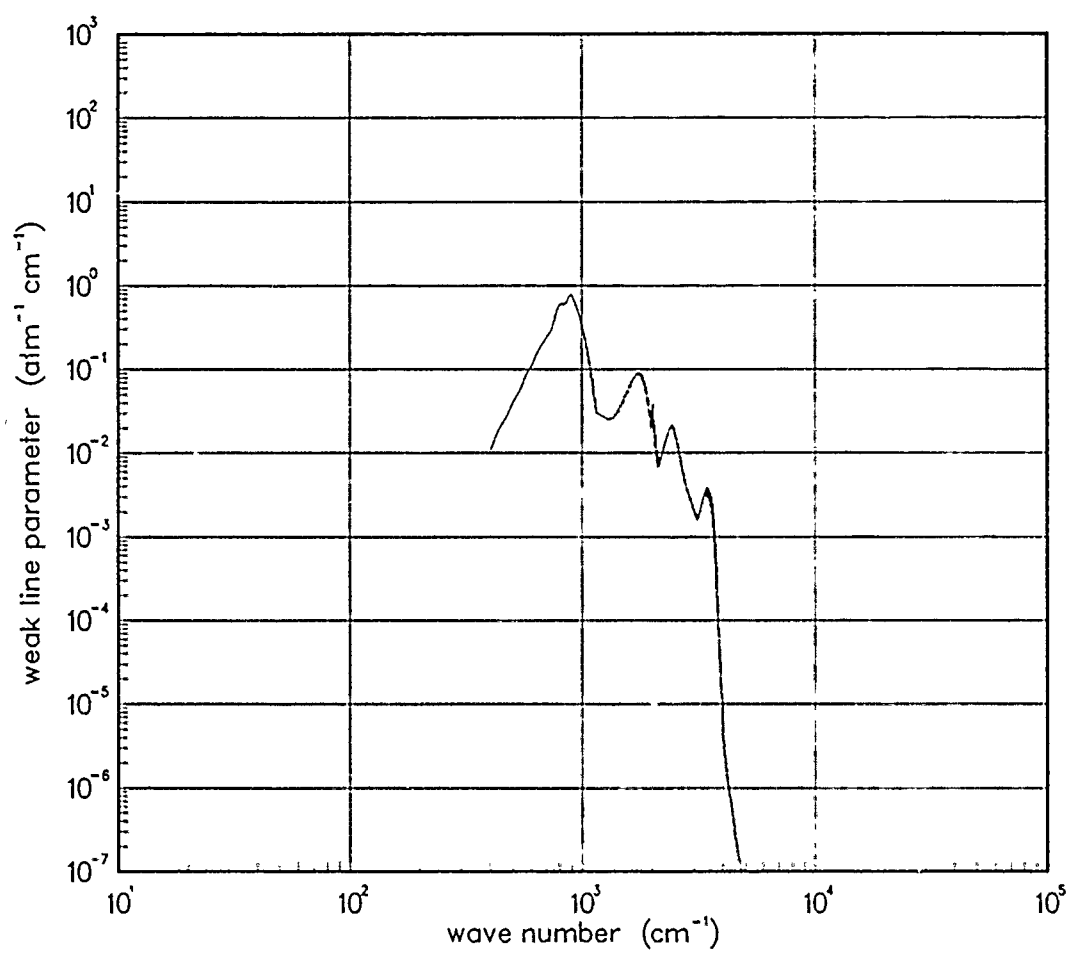


Figure 246. Weak-line parameter for O₃ at 7000°K.

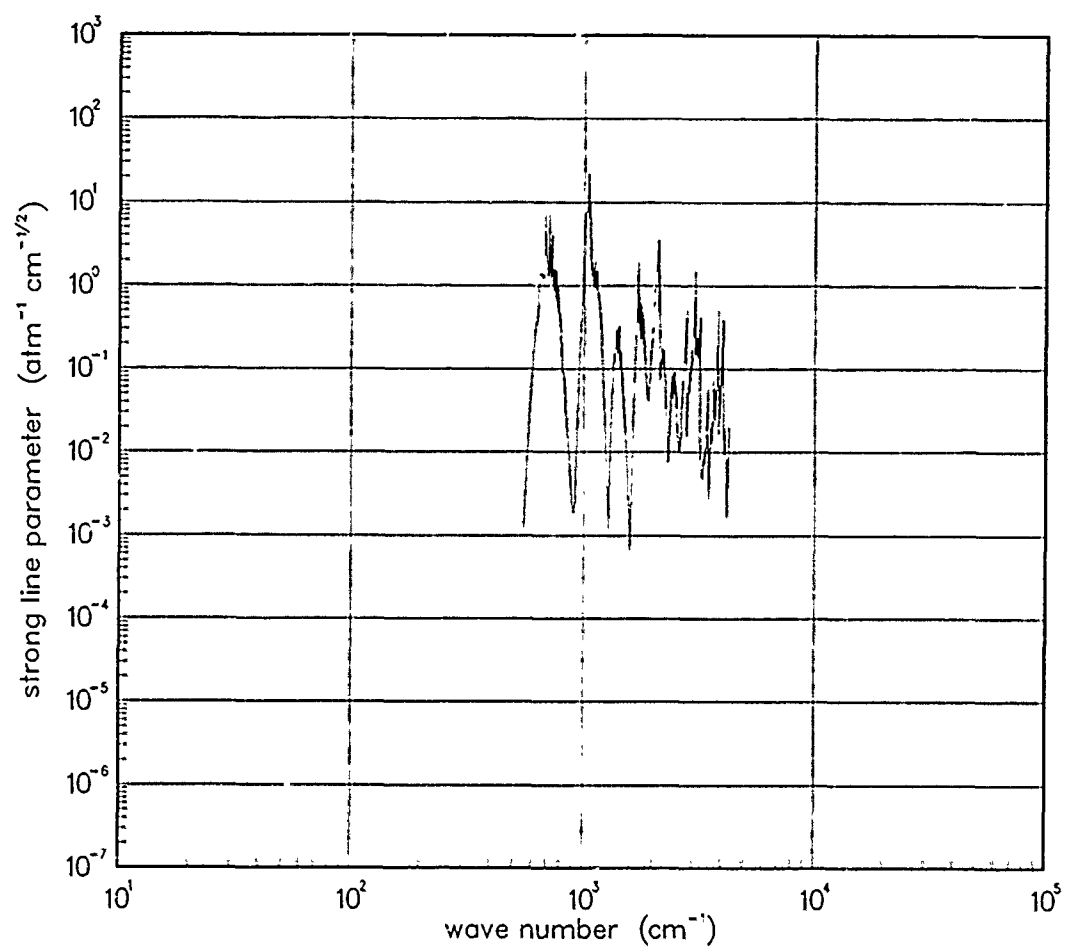


Figure 247. Strong-line parameter for O_3 at $200^\circ K$.

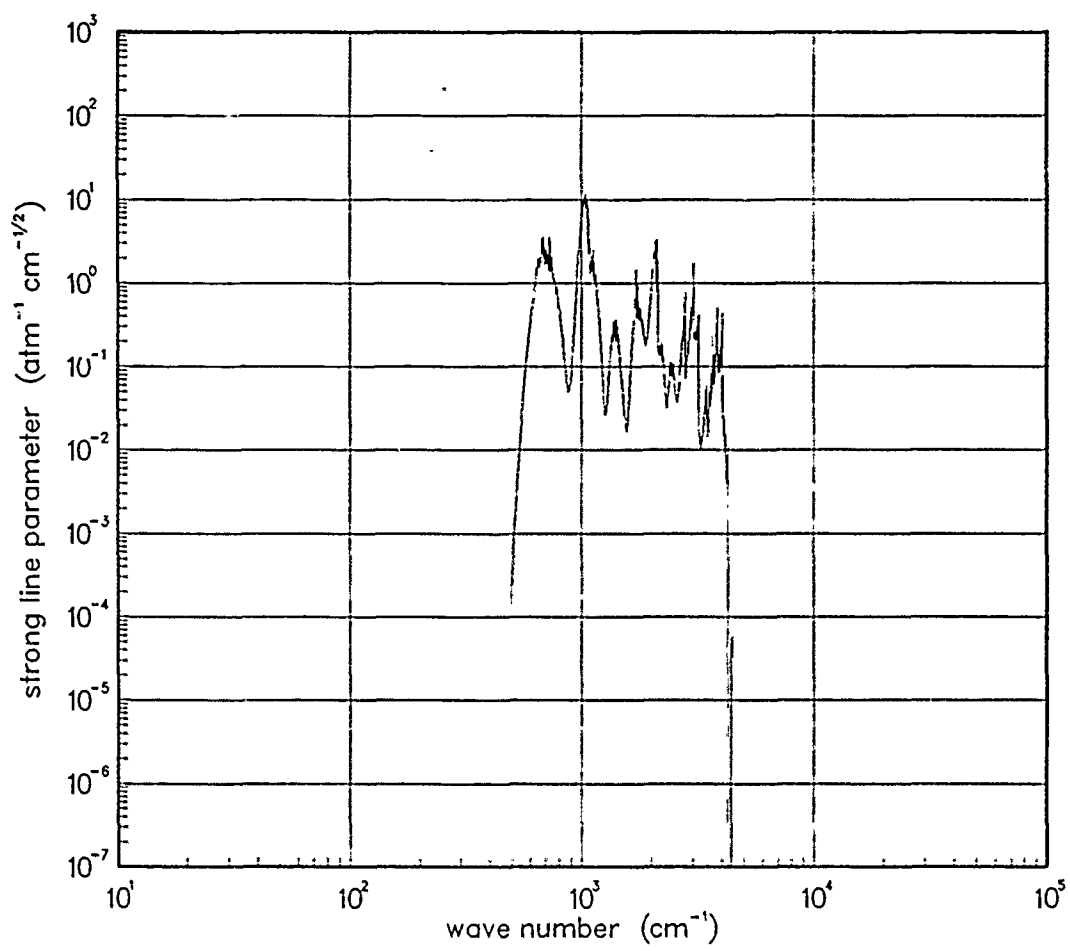


Figure 248. Strong-line parameter for O₃ at 300°K.

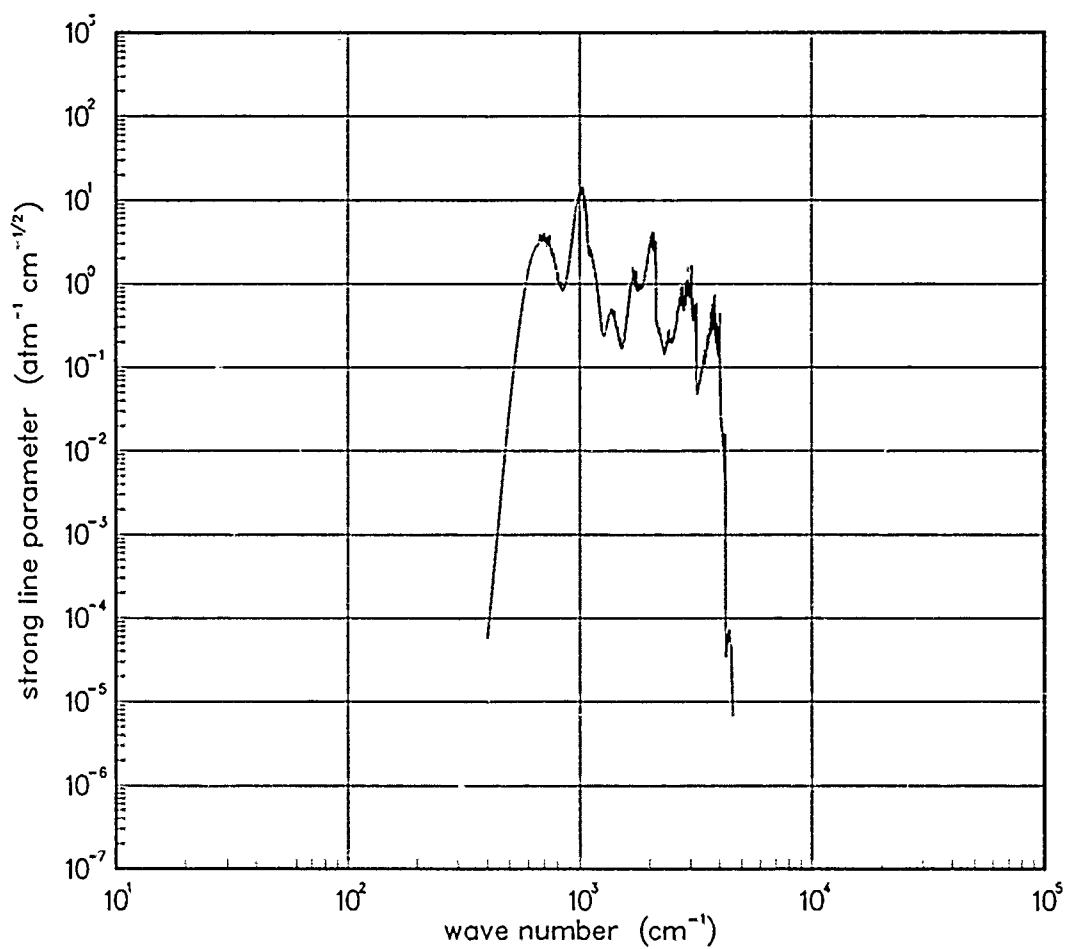


Figure 249. Strong-line parameter for O₃ at 500°K.

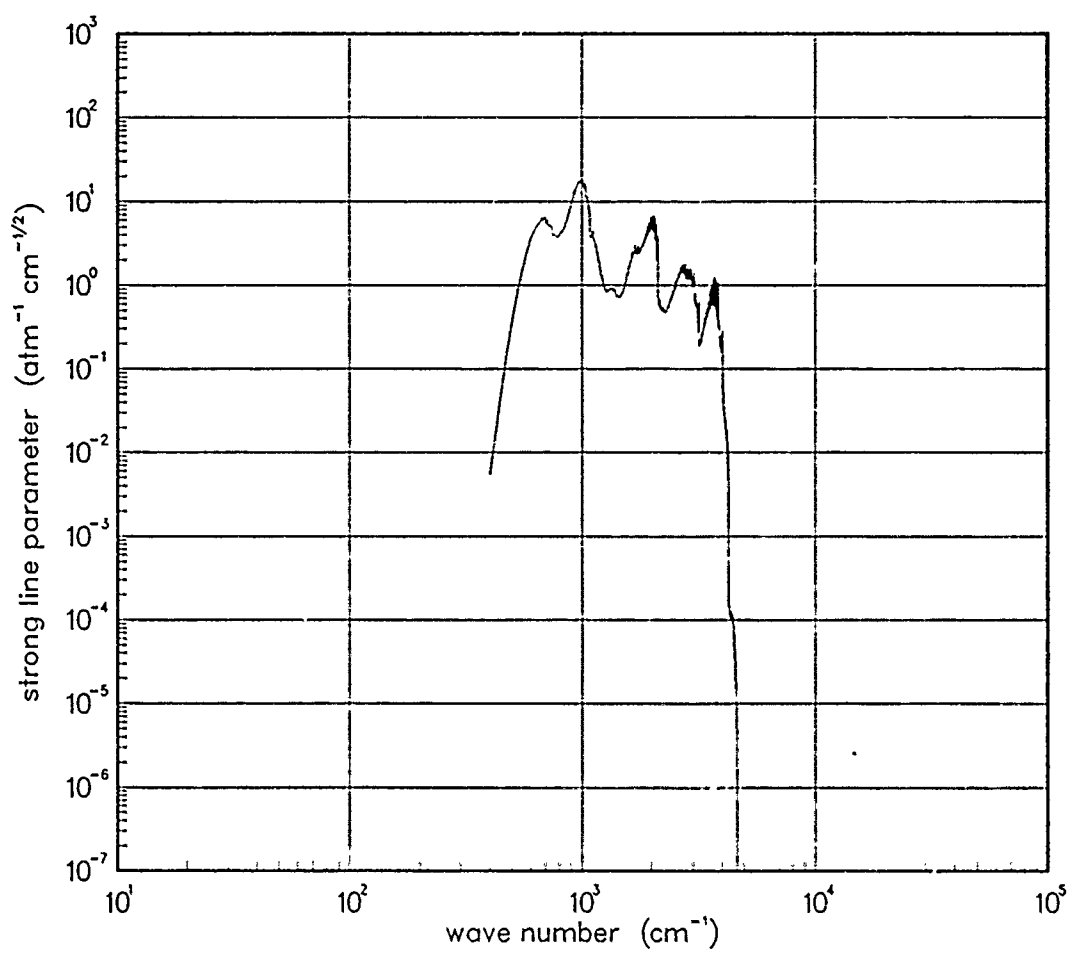


Figure 250. Strong-line parameter for O₃ at 750°K.

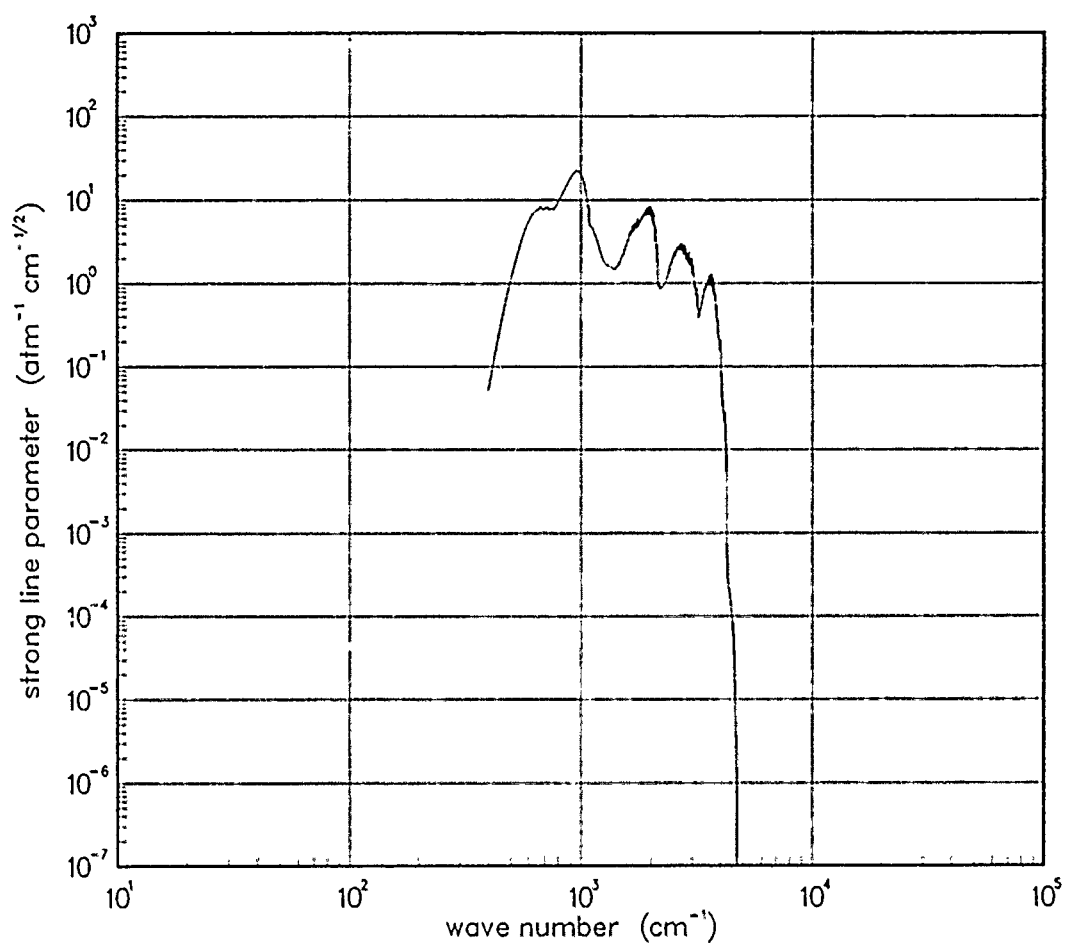


Figure 251. Strong-line parameter for O_3 at $1000^\circ K$.

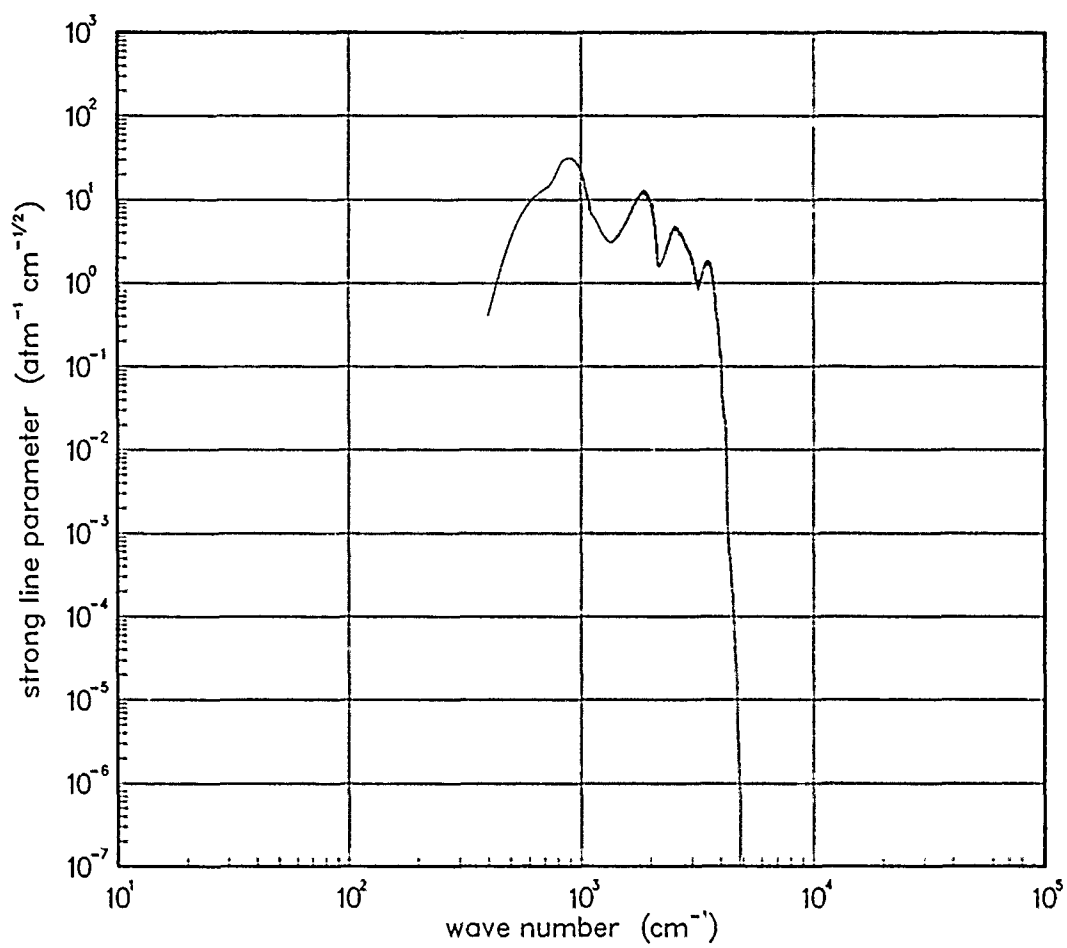


Figure 252. Strong-line parameter for O_3 at $1500^\circ K$.

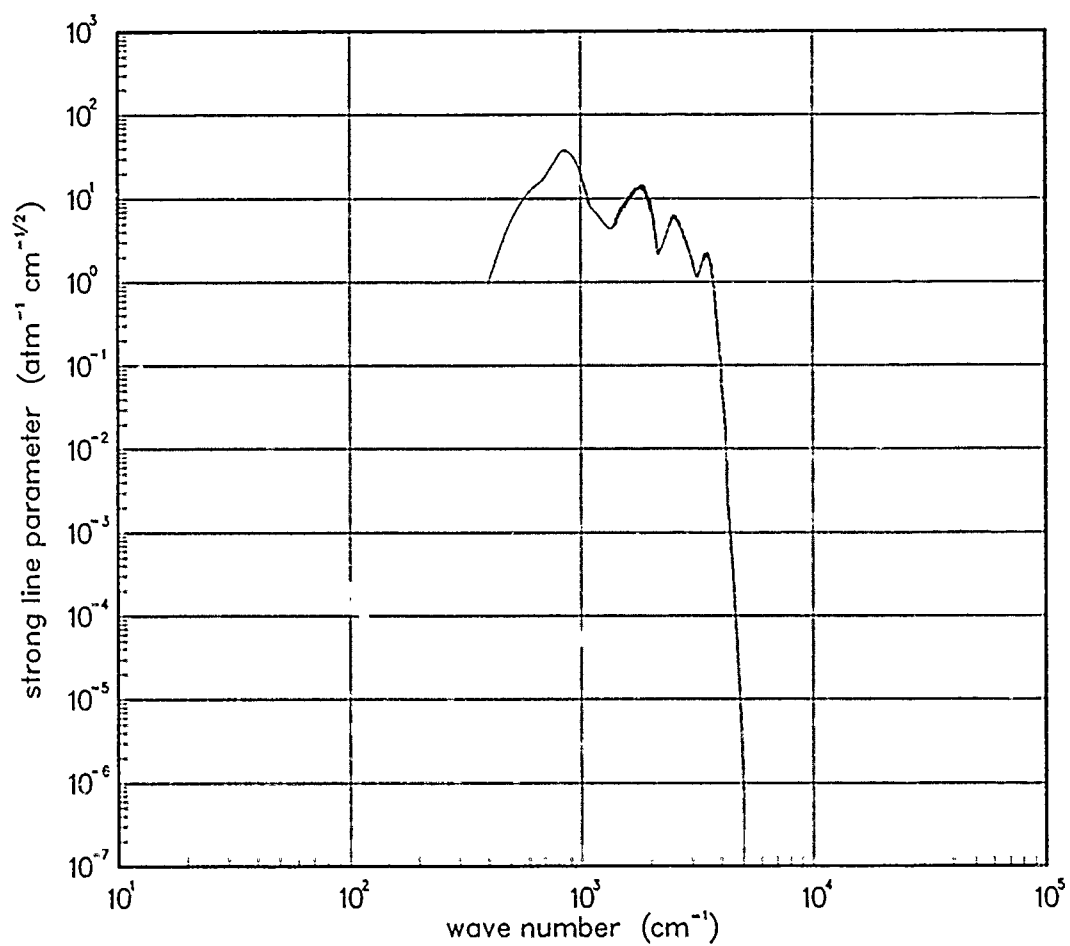


Figure 253. Strong-line parameter for O_3 at $2000^\circ K$.

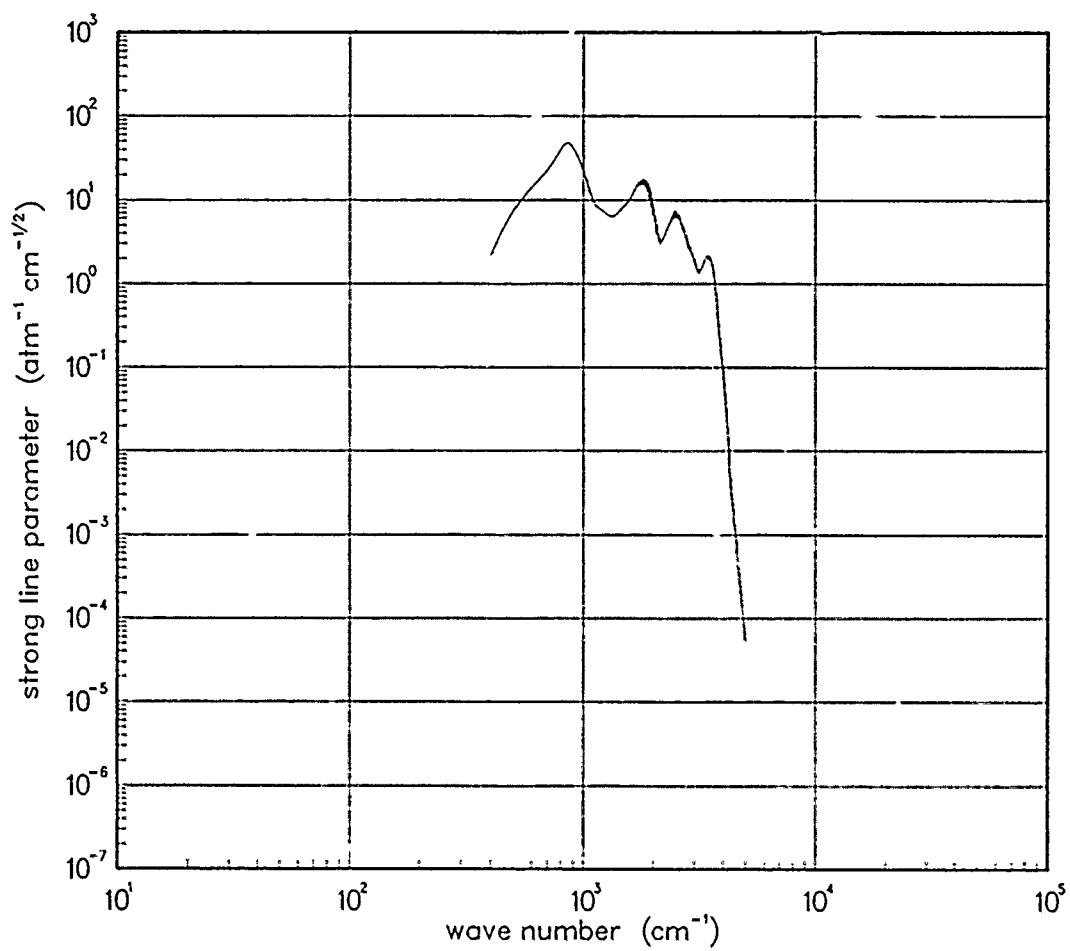


Figure 254. Strong-line parameter for O₃ at 3000°K.

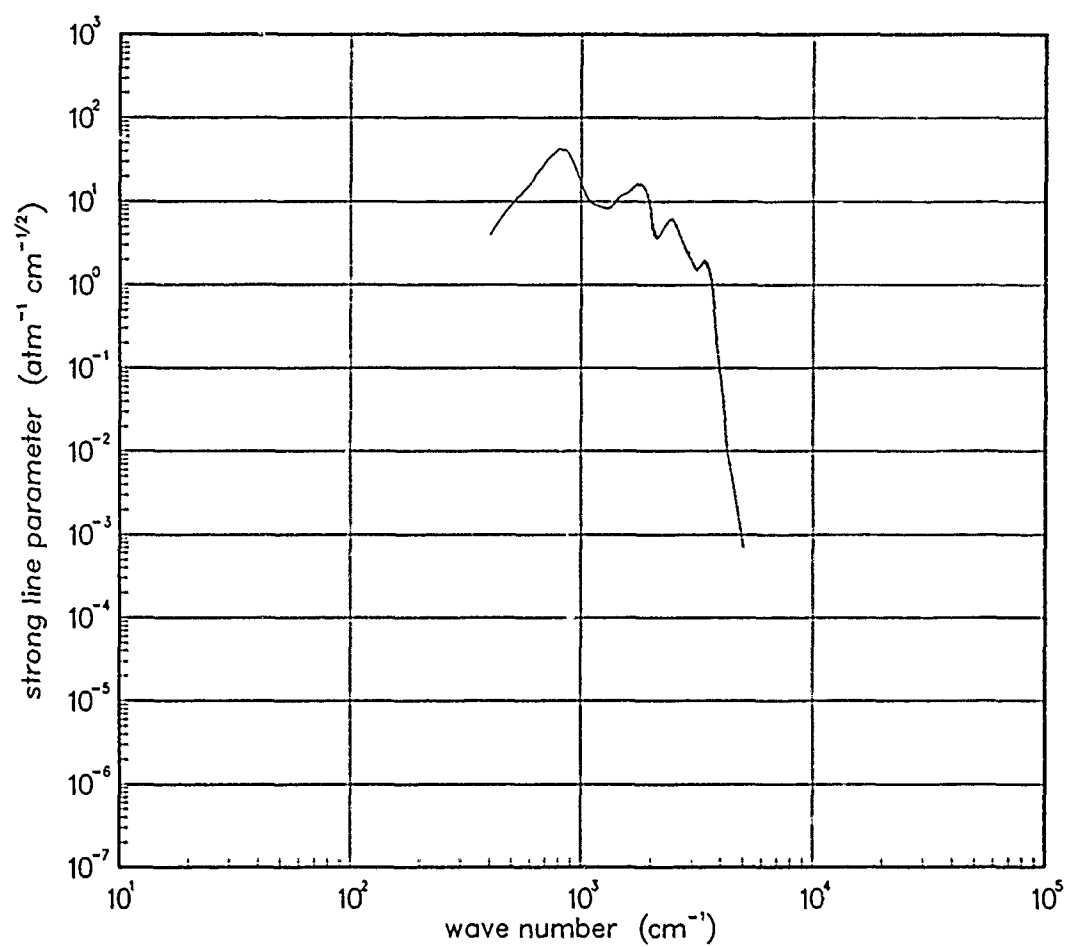


Figure 255. Strong-line parameter for O_3 at $5000^\circ K$.

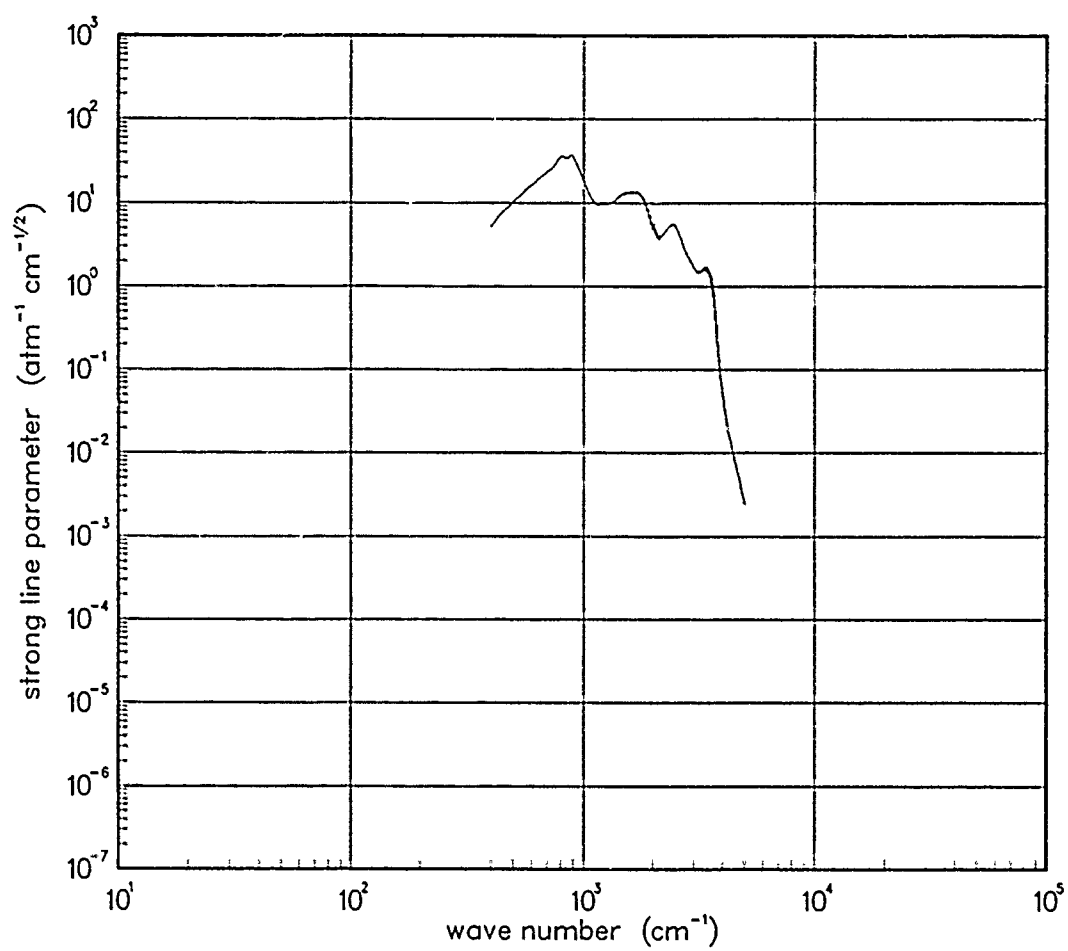


Figure 256. Strong-line parameter for O₃ at 7000°K.

5.8 SULFUR DIOXIDE (SO₂).

The local thermal equilibrium emission spectra for Sulfur Dioxide has been developed from the Air Force Geophysical Laboratory line atlas for 200, 300, 500, 750, 1000 °K.

The SO₂ molecule has been included within the NORSE LTE data base because of its contribution to ambient atmospheric absorption. The inclusion of accurate parameters for this species above 1000 °K is felt to be of low priority.

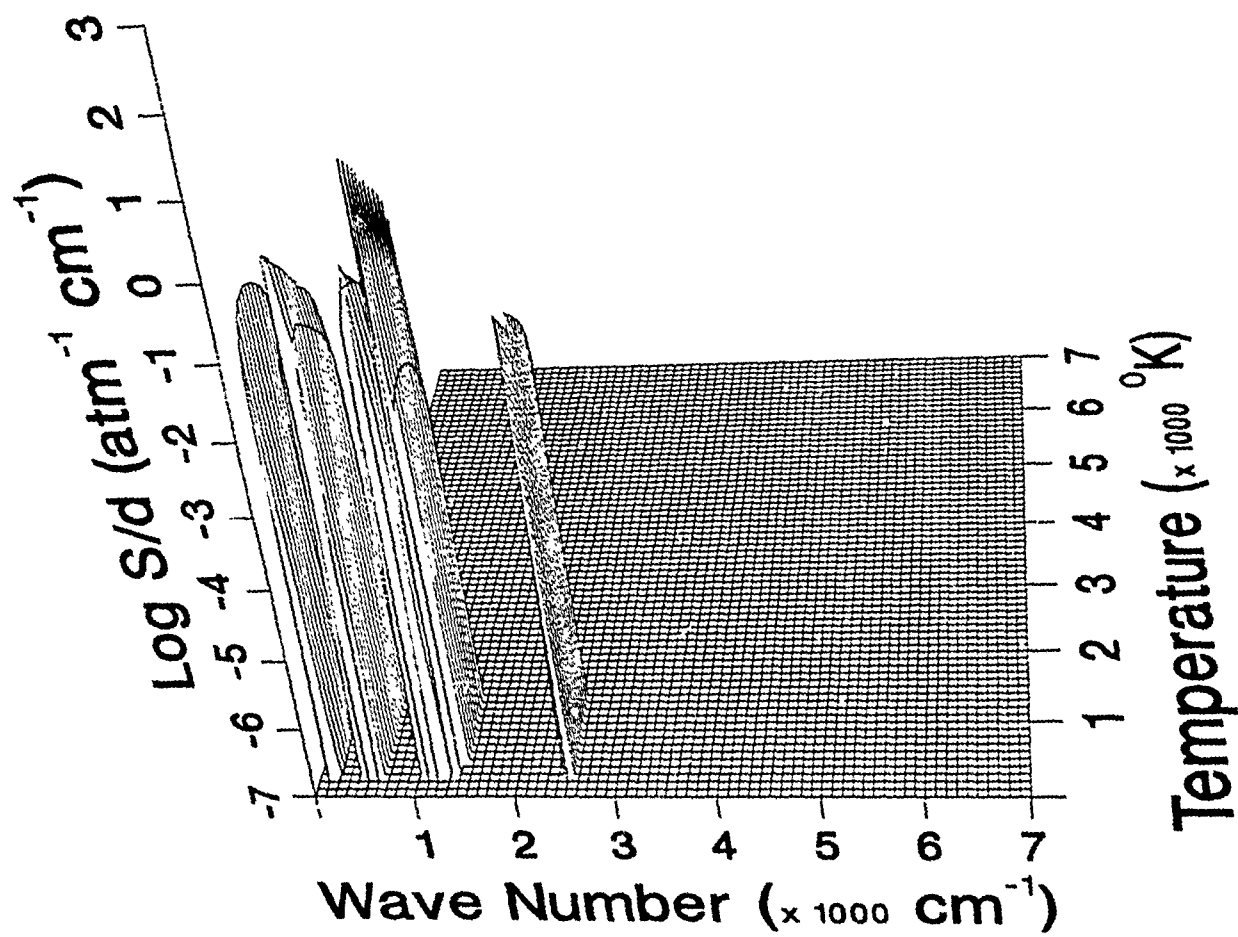


Figure 257. Weak-line parameter for SO_2 .

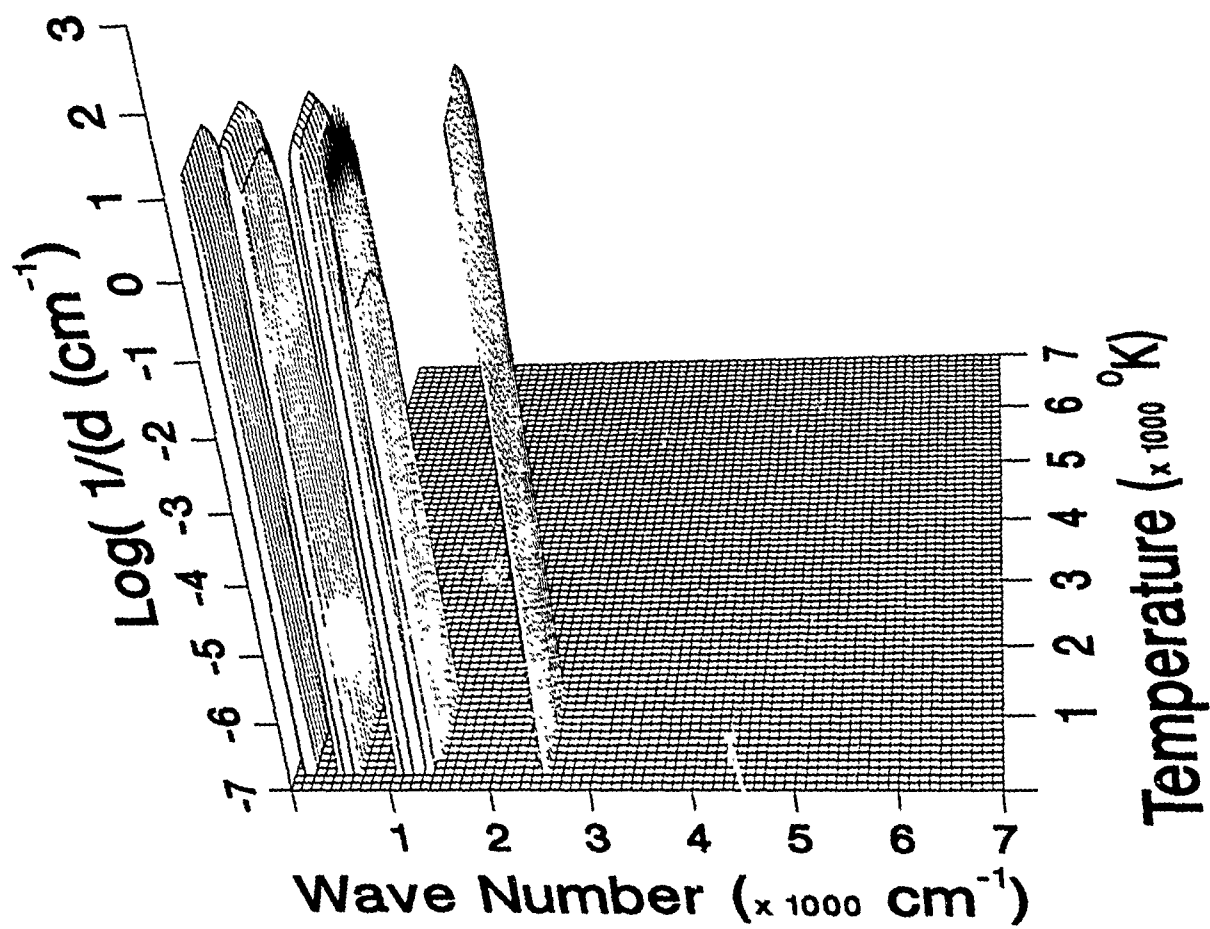


Figure 258. Inverse line spacing for SO_2 .

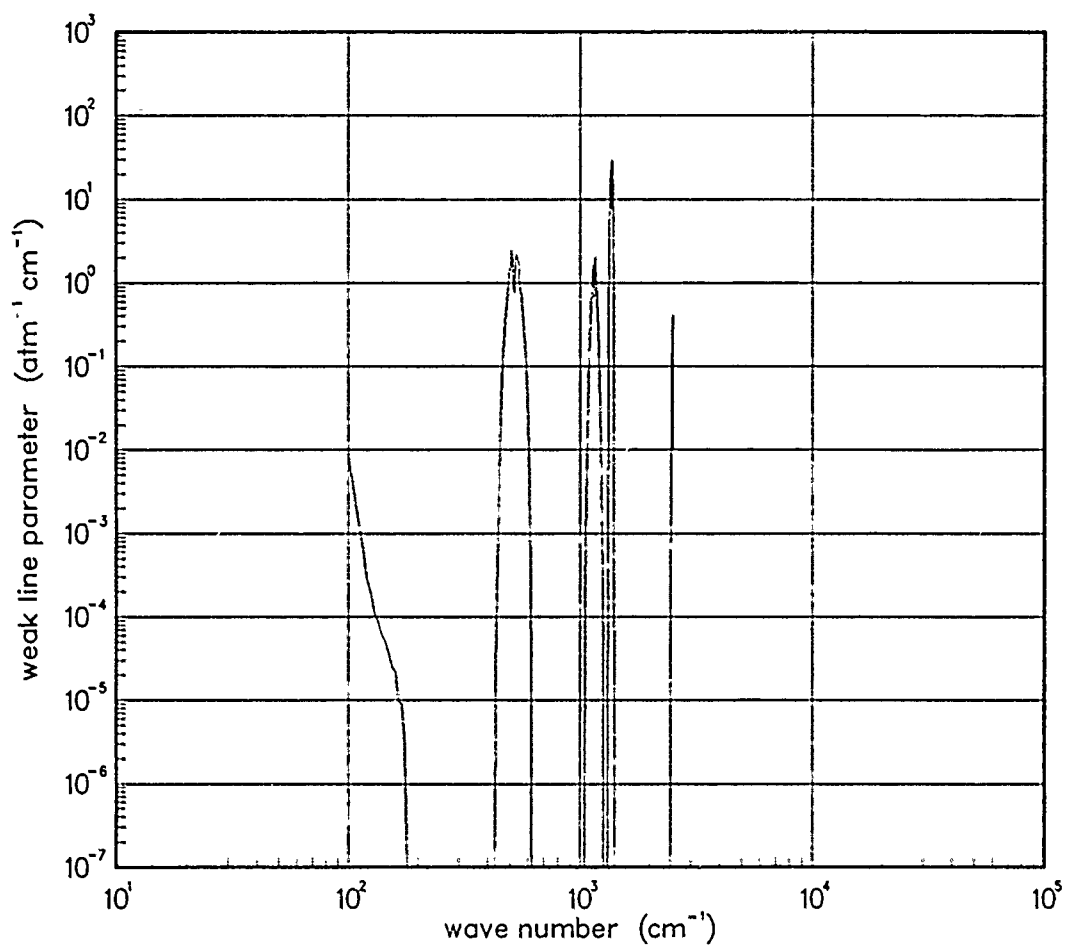


Figure 259. Weak-line parameter for SO₂ at 200°K.

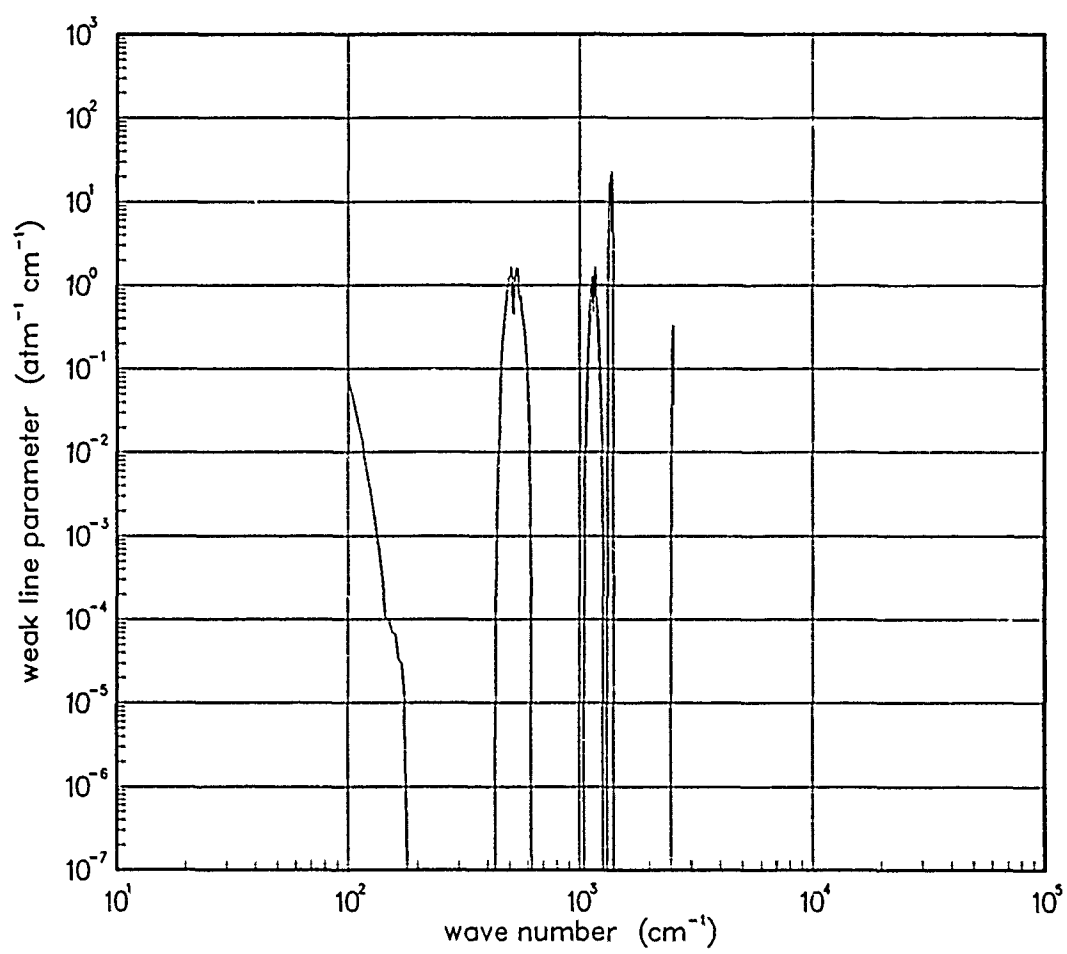


Figure 260. Weak-line parameter for SO₂ at 300°K.

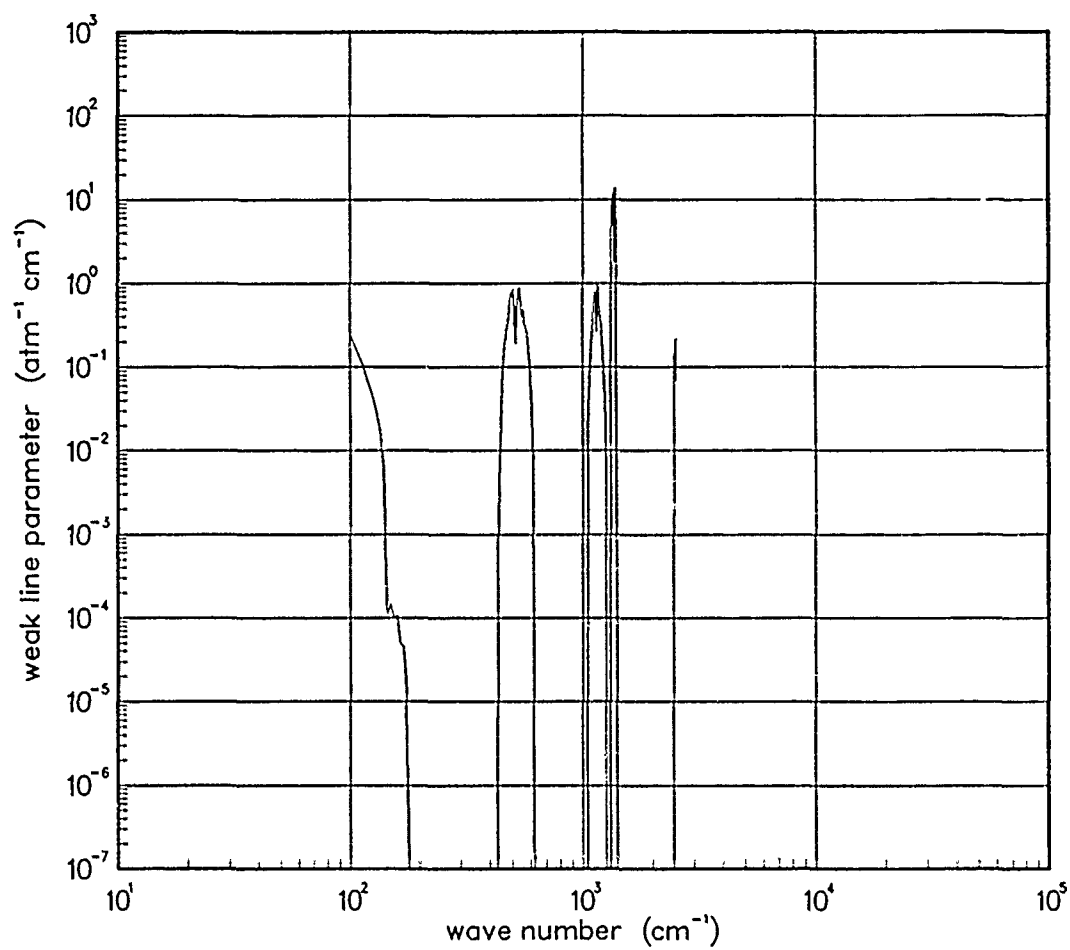


Figure 261. Weak-line parameter for SO₂ at 500°K.

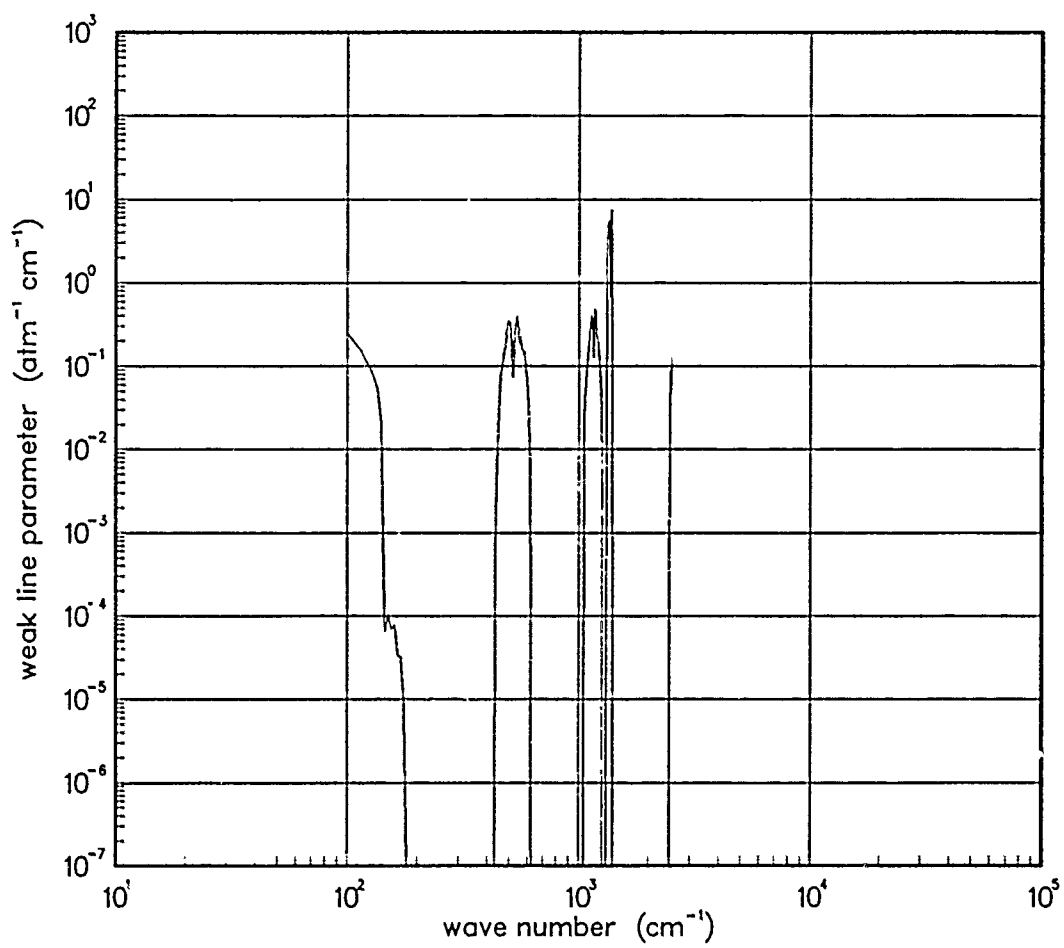


Figure 262. Weak-line parameter for SO₂ at 750°K.

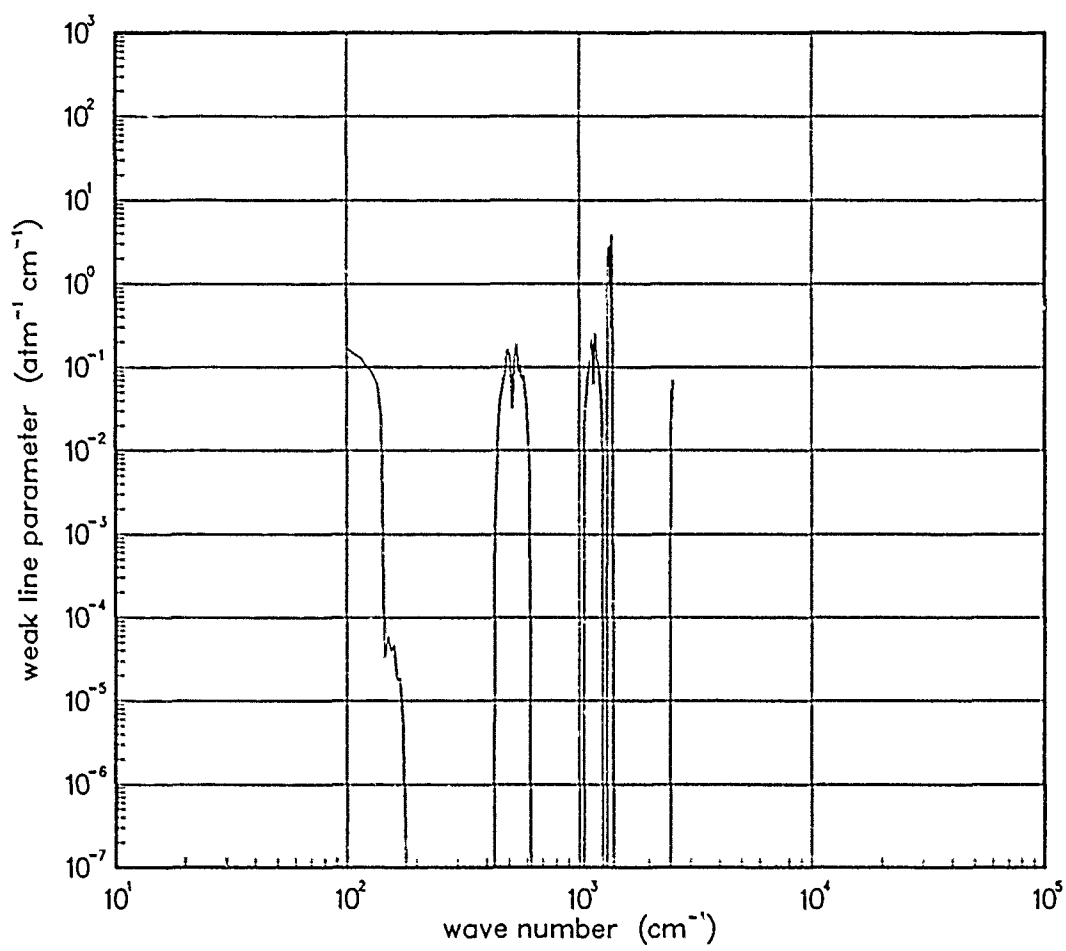


Figure 263. Weak-line parameter for SO₂ at 1000°K.

5.9 WATER (H₂O).

The local thermal equilibrium emission spectra for H₂O was taken from the ROSCOE LTE data base.

Low temperature (200, 300, 500 °K) H₂O data was derived from the Air Force Geophysical Laboratory Line Atlas*. For temperatures above 500 °K the curves were extracted from the WOE fireball LTE parameters† except in the spectral region 2000 - 5000 cm⁻¹ where ROSCOE-IR results were used. Both the WOE high temperature data and the ROSCOE-IR data are based on measurements performed at Convair‡.

Data Source:

*R.A. McClatchey, et al, AFCRL Atmospheric Line Parameters Compilation , AFCRL-TR-73-0096, Air Force Cambridge Research Laboratories, (January 1973) 1982 version of the data tape.

†J.G. DeVore, and T.L. Stephens, Band Model Parameters for Thermal Emission (U) , 72TMP-20, General Electric - TEMPO, June 1972 (Secret).

‡C.C. Ferriso, C.B. Ludwig, and A.L. Thomson, J. Quant. Spectrosc. Radiat. Transfer 6, 241 (1966). C.B. Ludwig, Appl. Opt. 10 (1971).

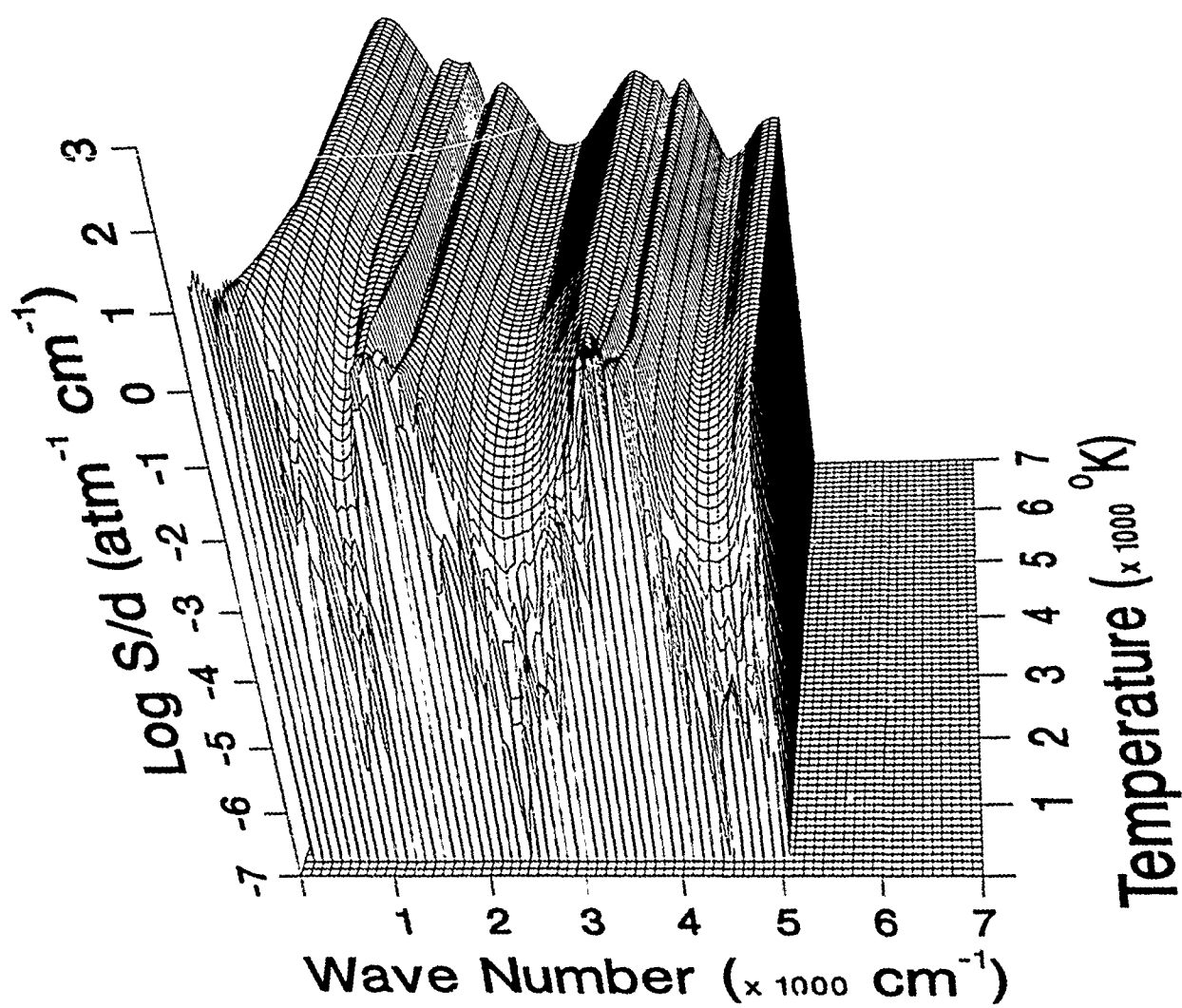


Figure 264. Weak-line parameter for H_2O .

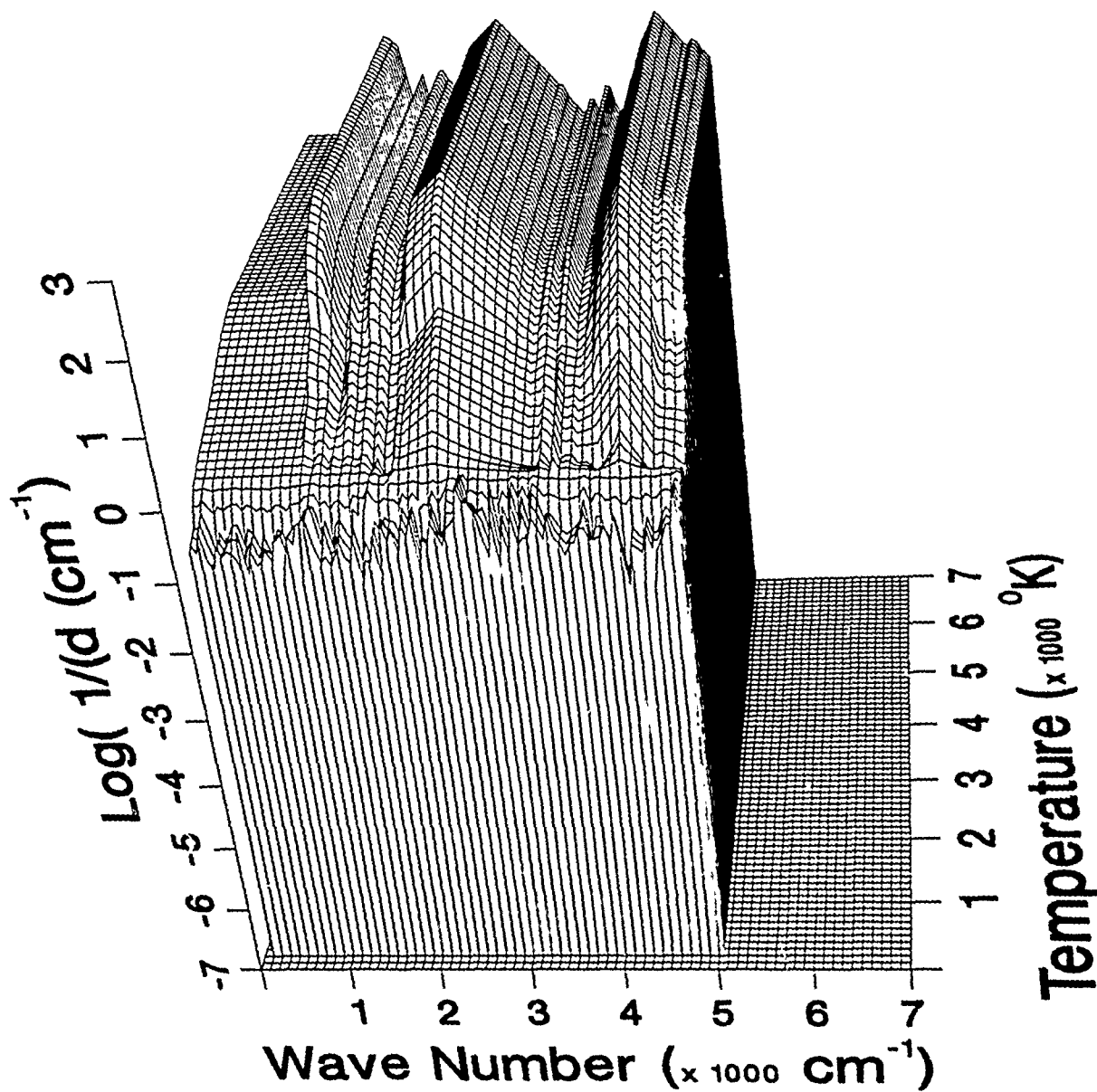


Figure 265. Inverse line spacing for H_2O .

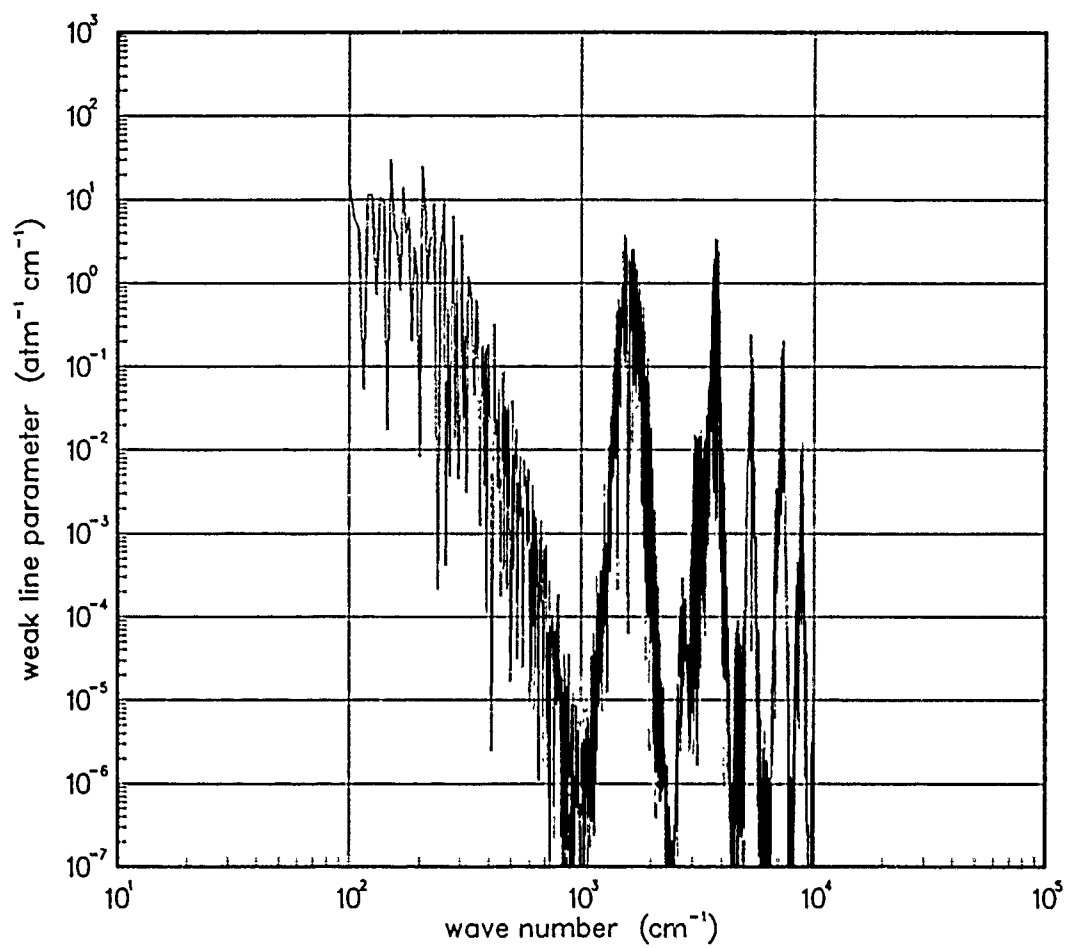


Figure 266. Weak-line parameter for H₂O at 200°K.

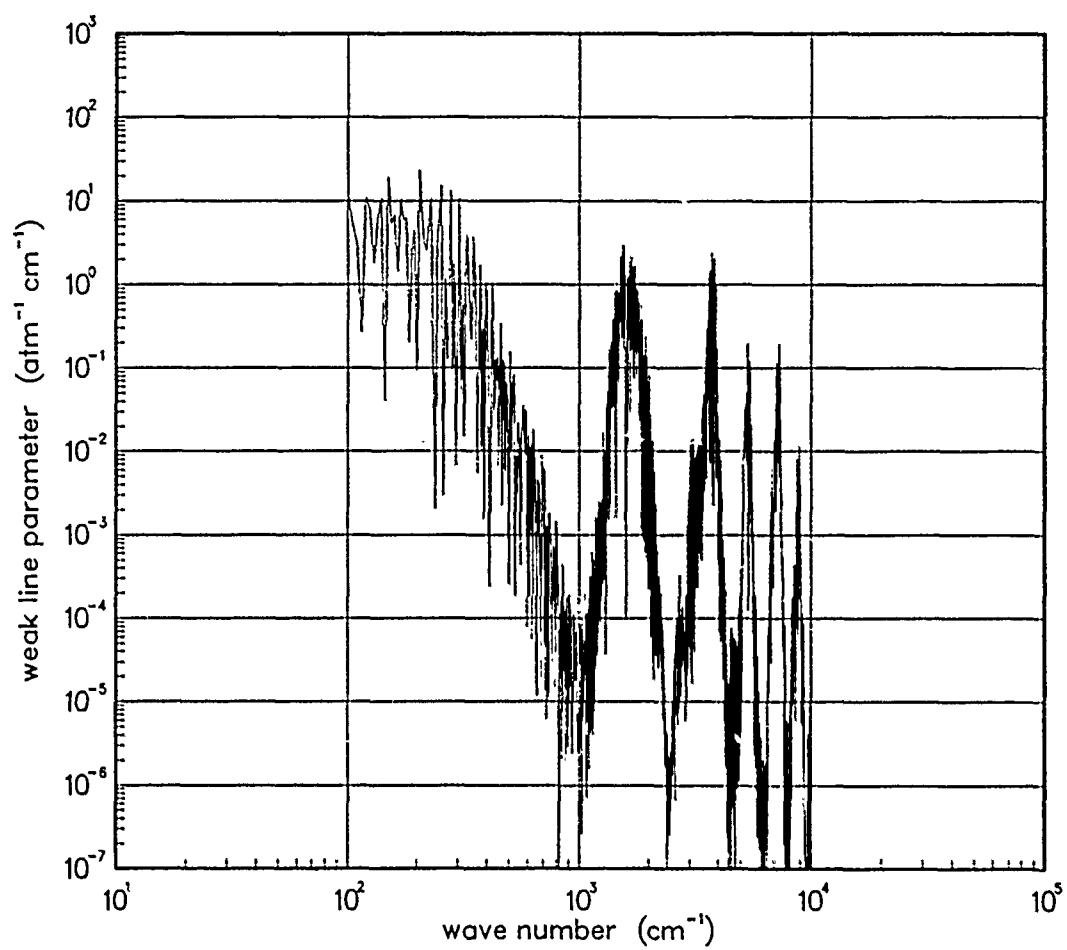


Figure 267. Weak-line parameter for H_2O at 300°K .

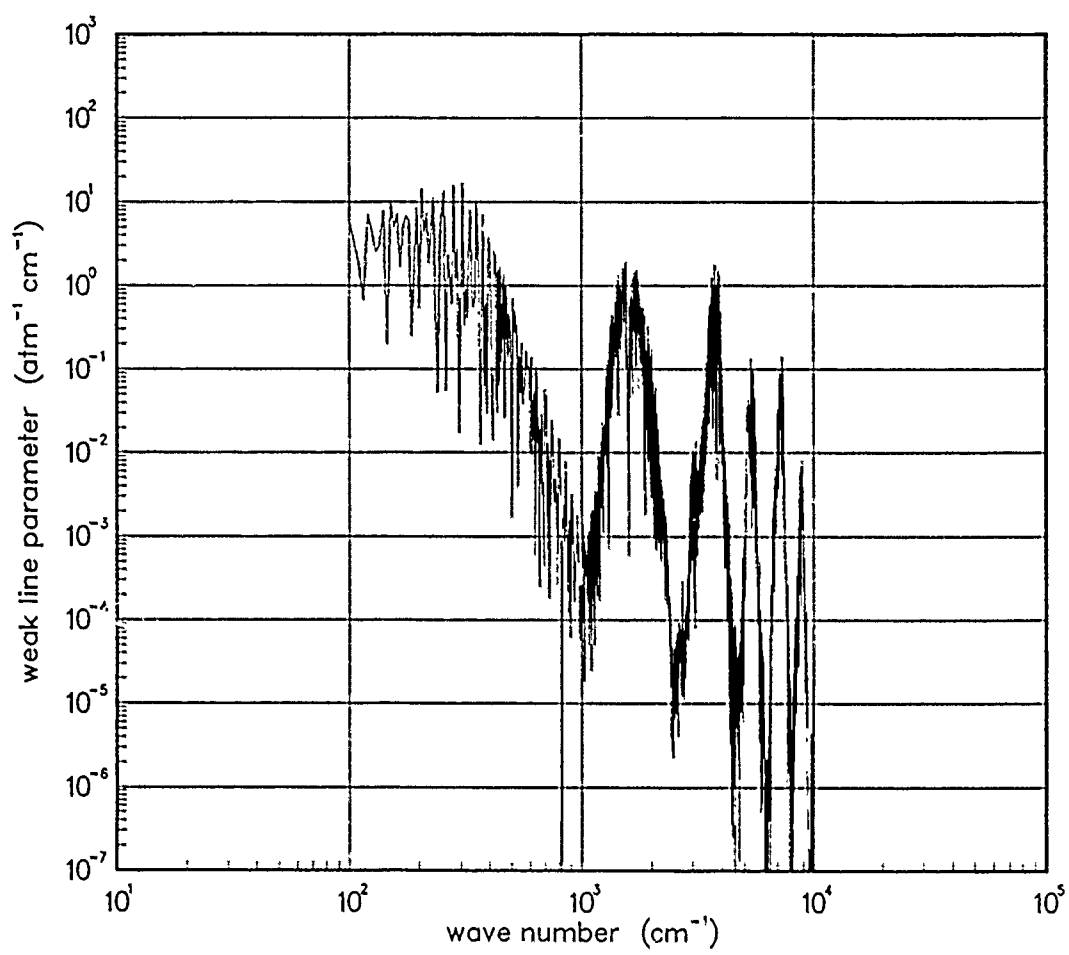


Figure 268. Weak-line parameter for H₂O at 500°K.

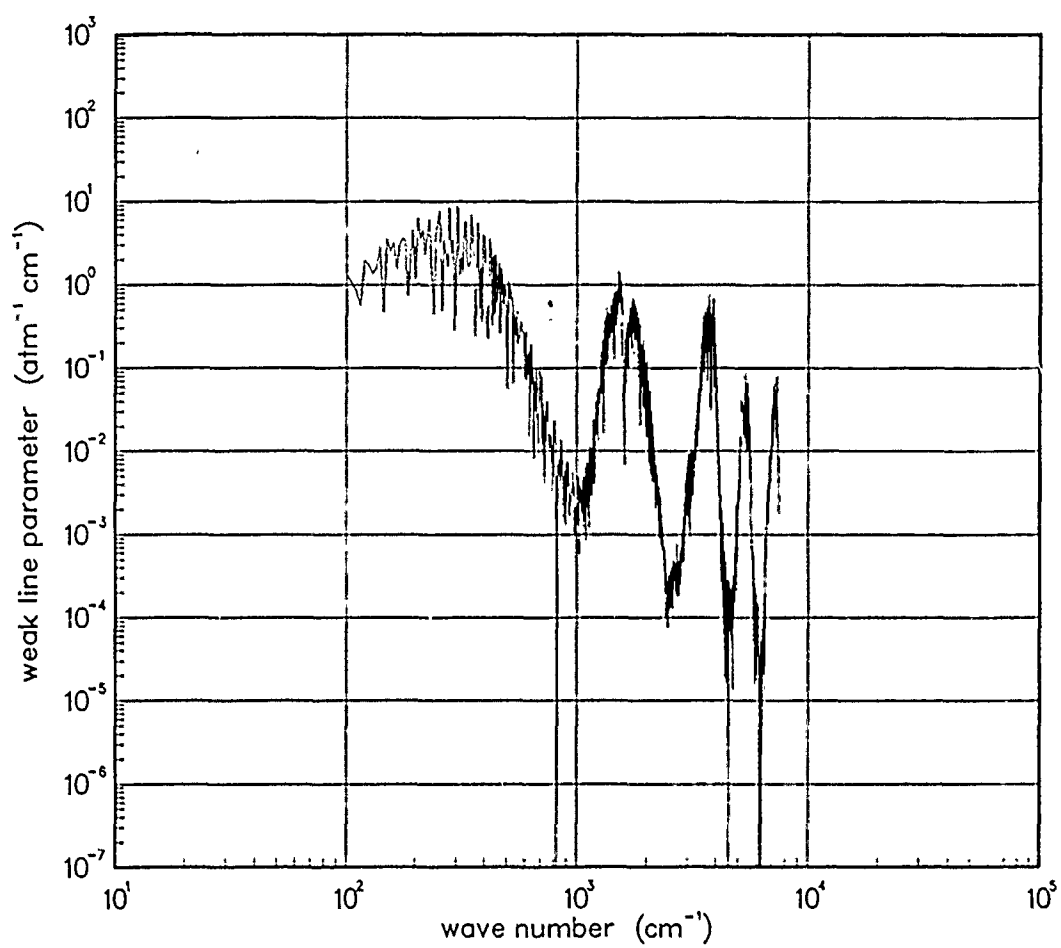


Figure 269. Weak-line parameter for H₂O at 750°K.

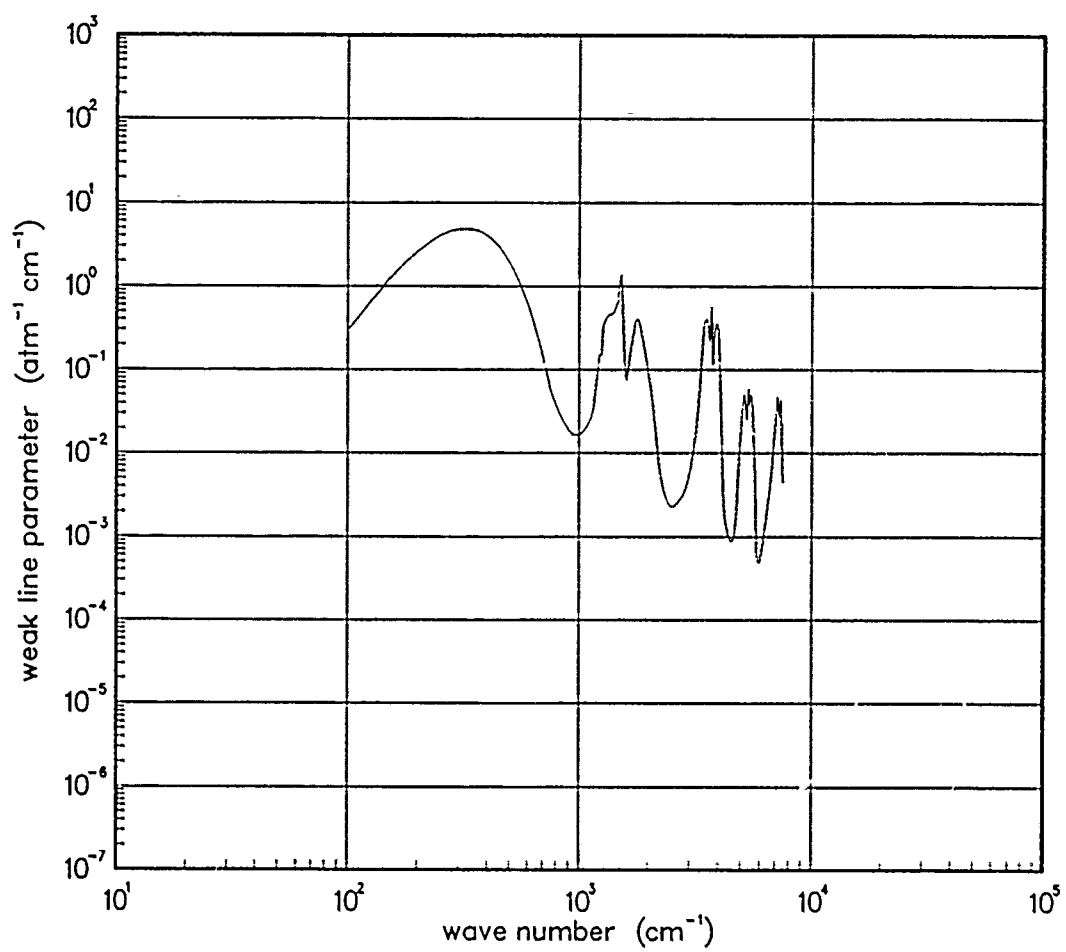


Figure 270. Weak-line parameter for H₂O at 1000°K.

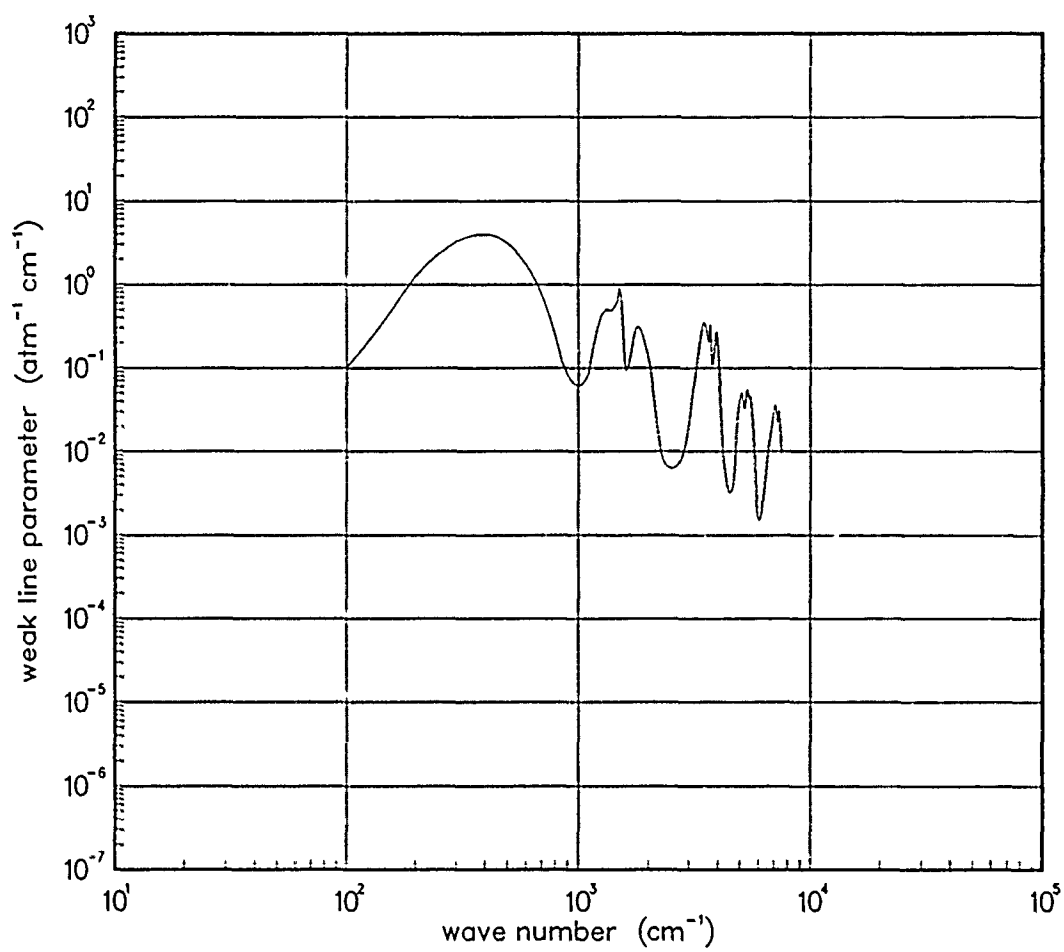


Figure 271. Weak-line parameter for H₂O at 1500°K.

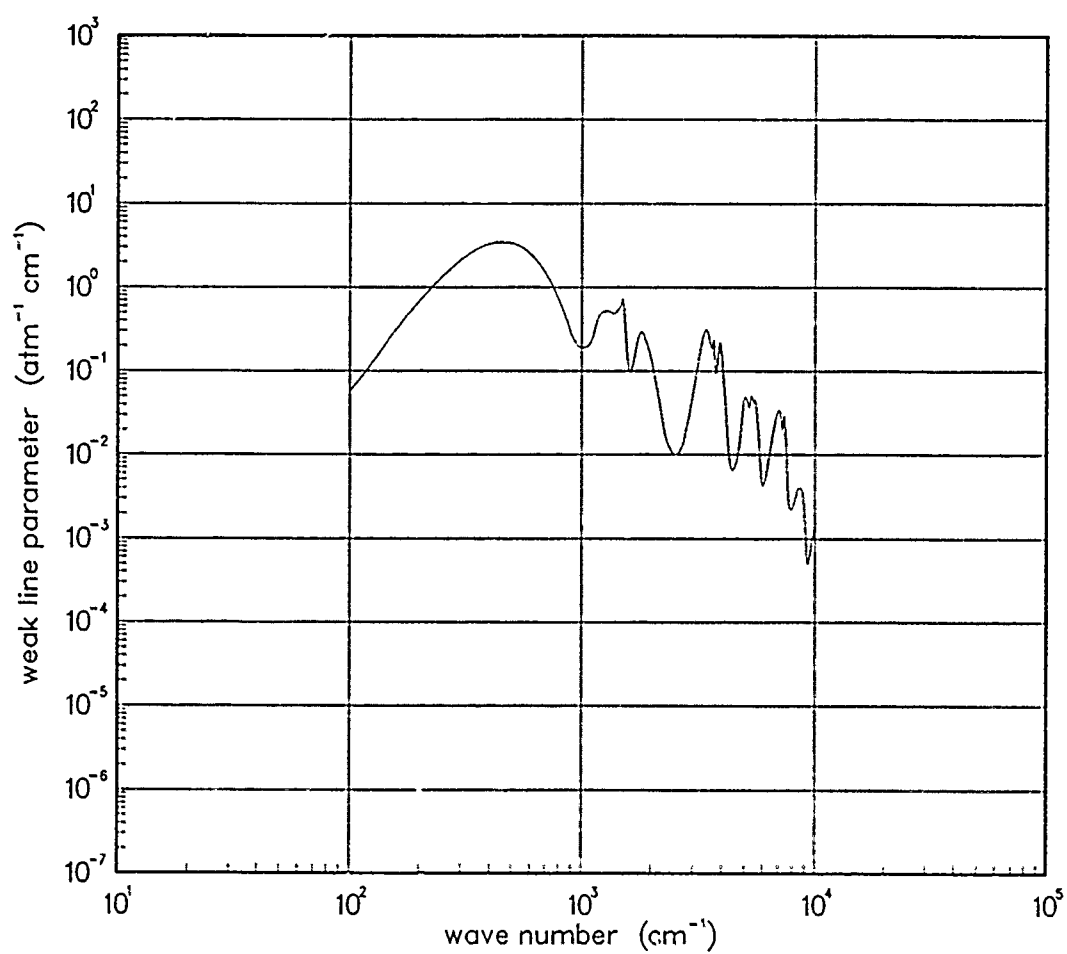


Figure 272. Weak-line parameter for H₂O at 2000°K.

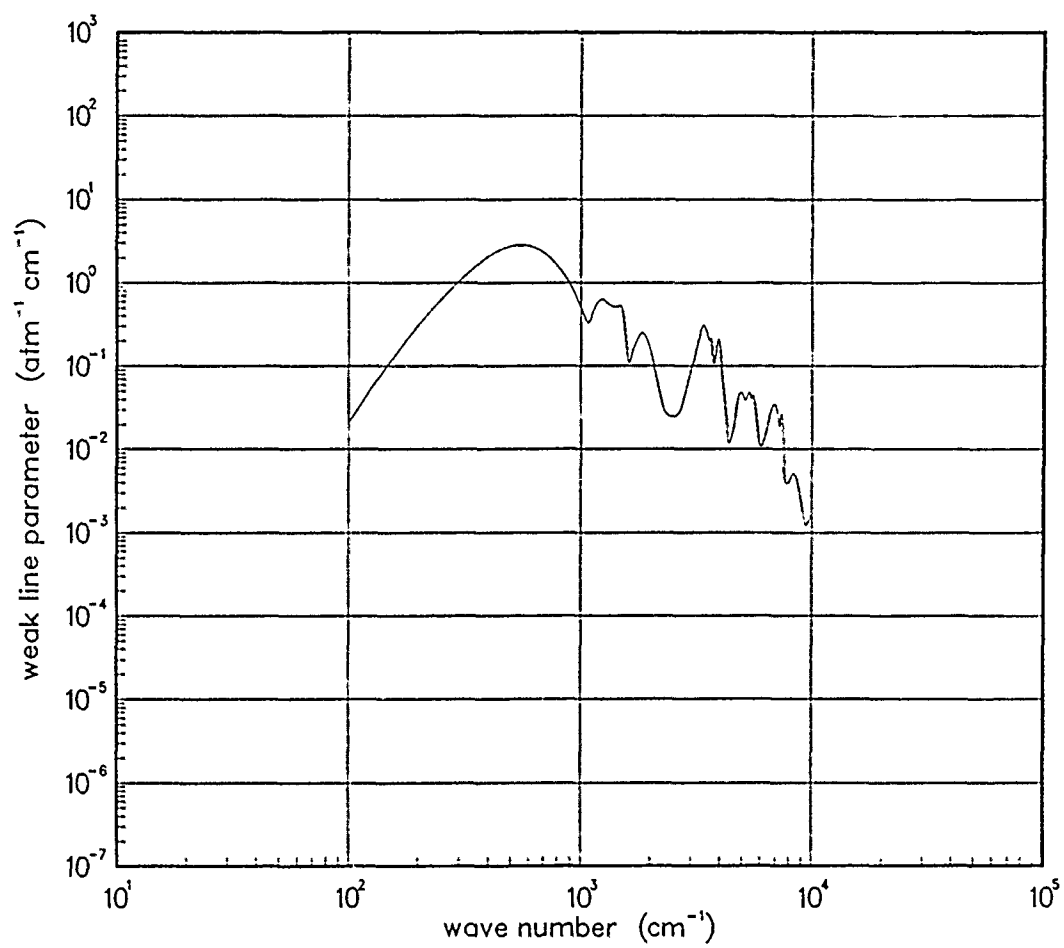


Figure 273. Weak-line parameter for H₂O at 3000°K.

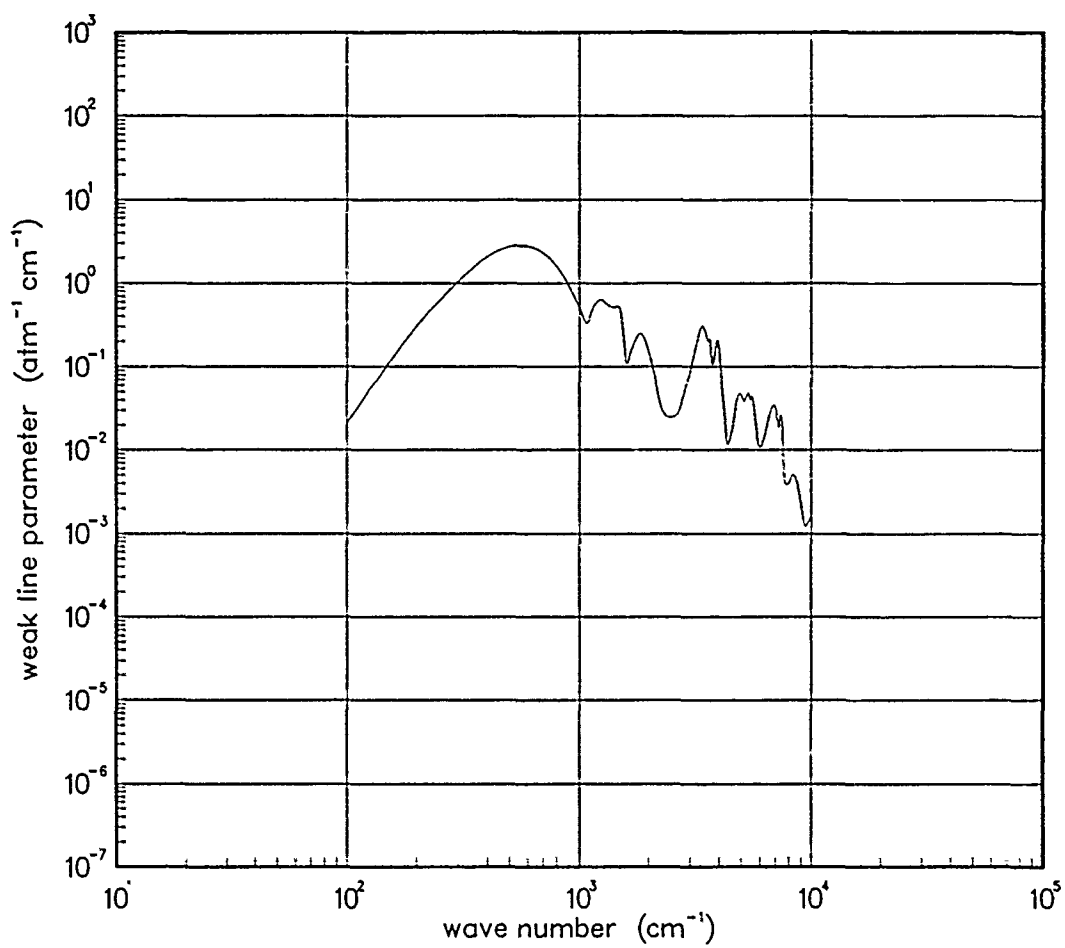


Figure 274. Weak-line parameter for H₂O at 5000°K.

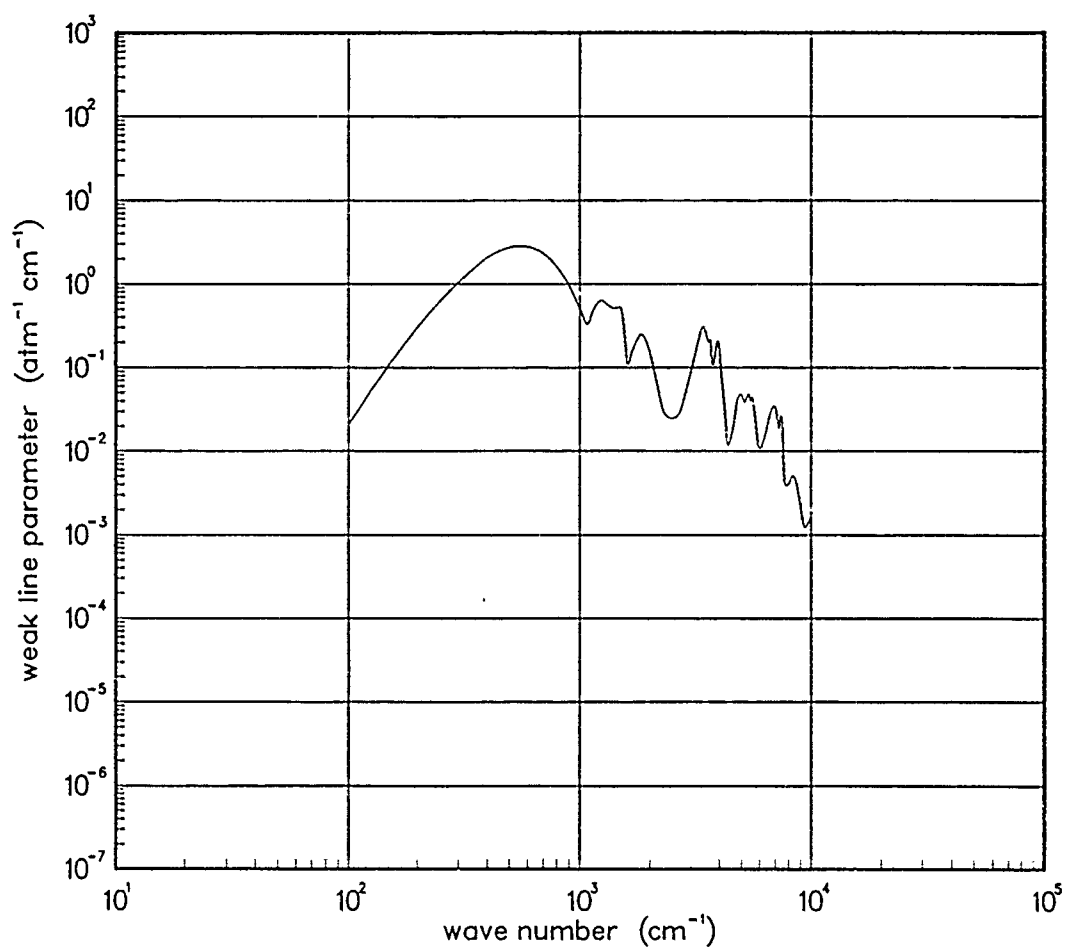


Figure 275. Weak-line parameter for H₂O at 7000°K.

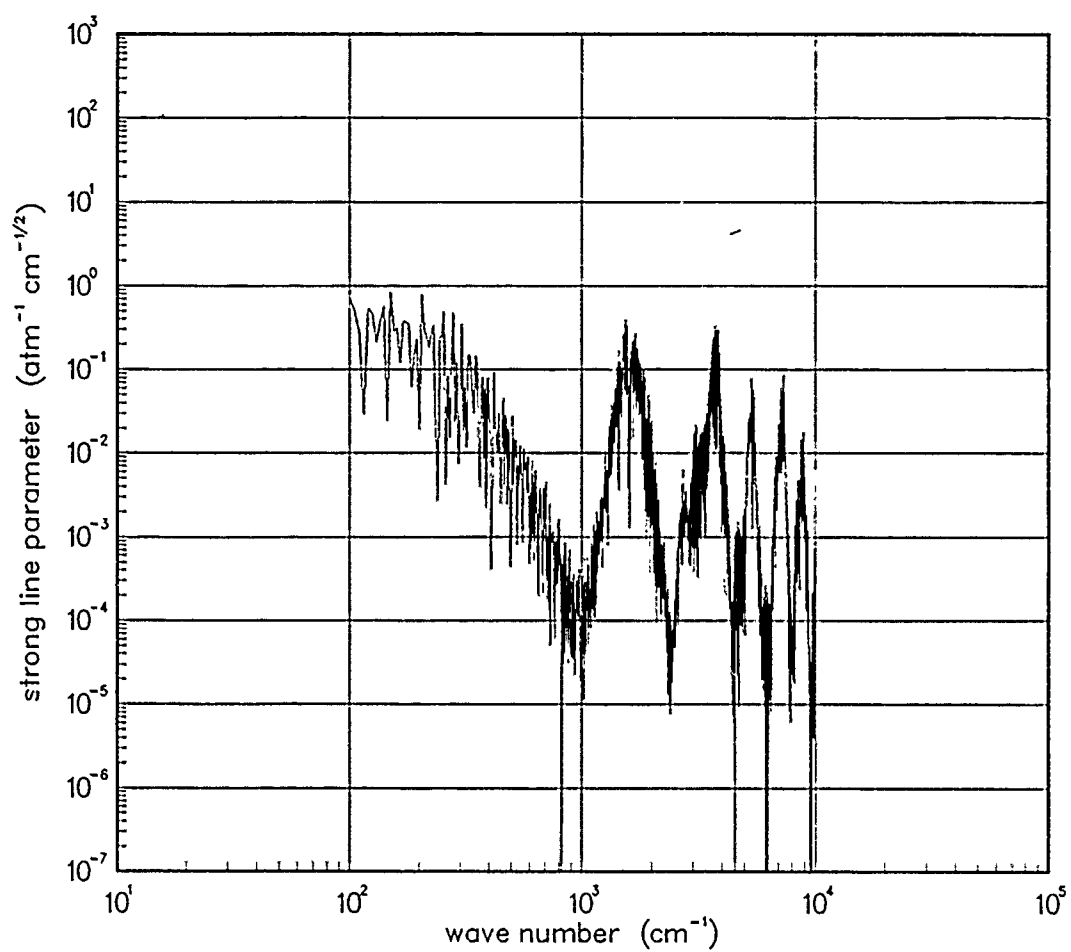


Figure 276. Strong-line parameter for H₂O at 200°K.

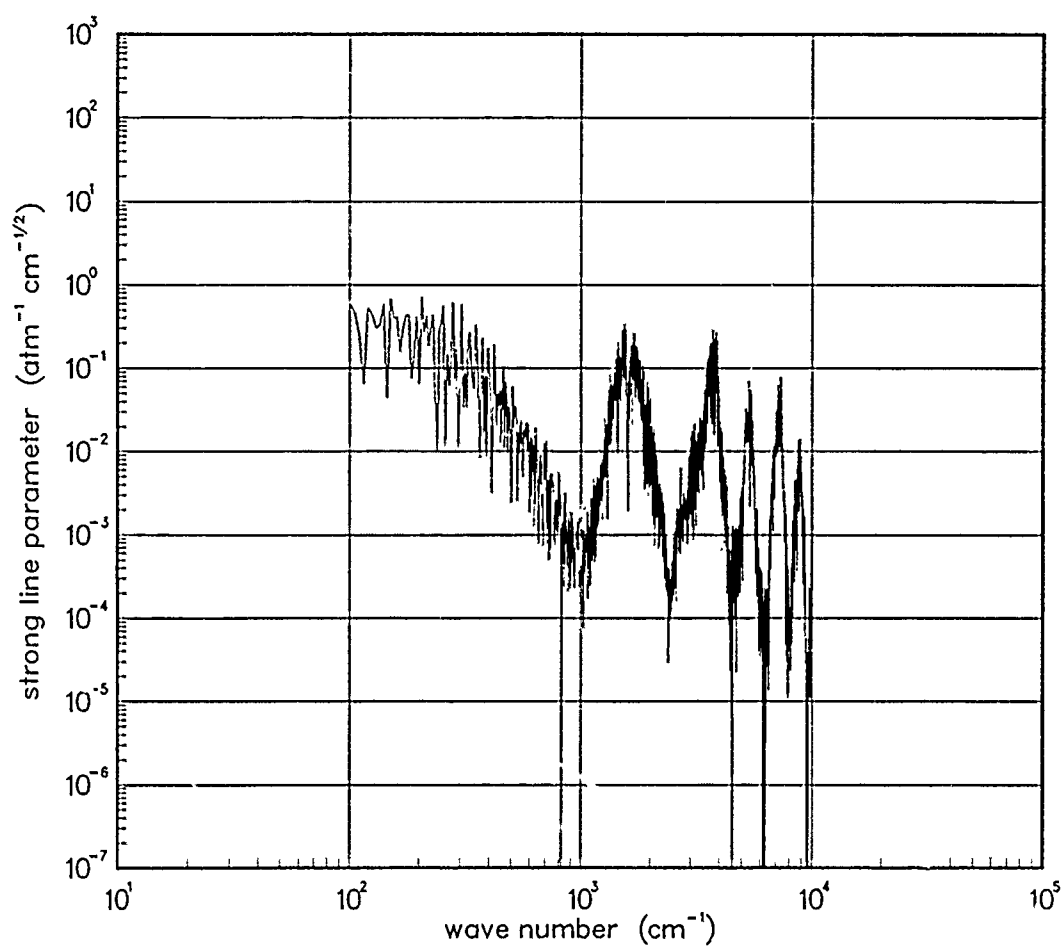


Figure 277. Strong-line parameter for H₂O at 300°K.

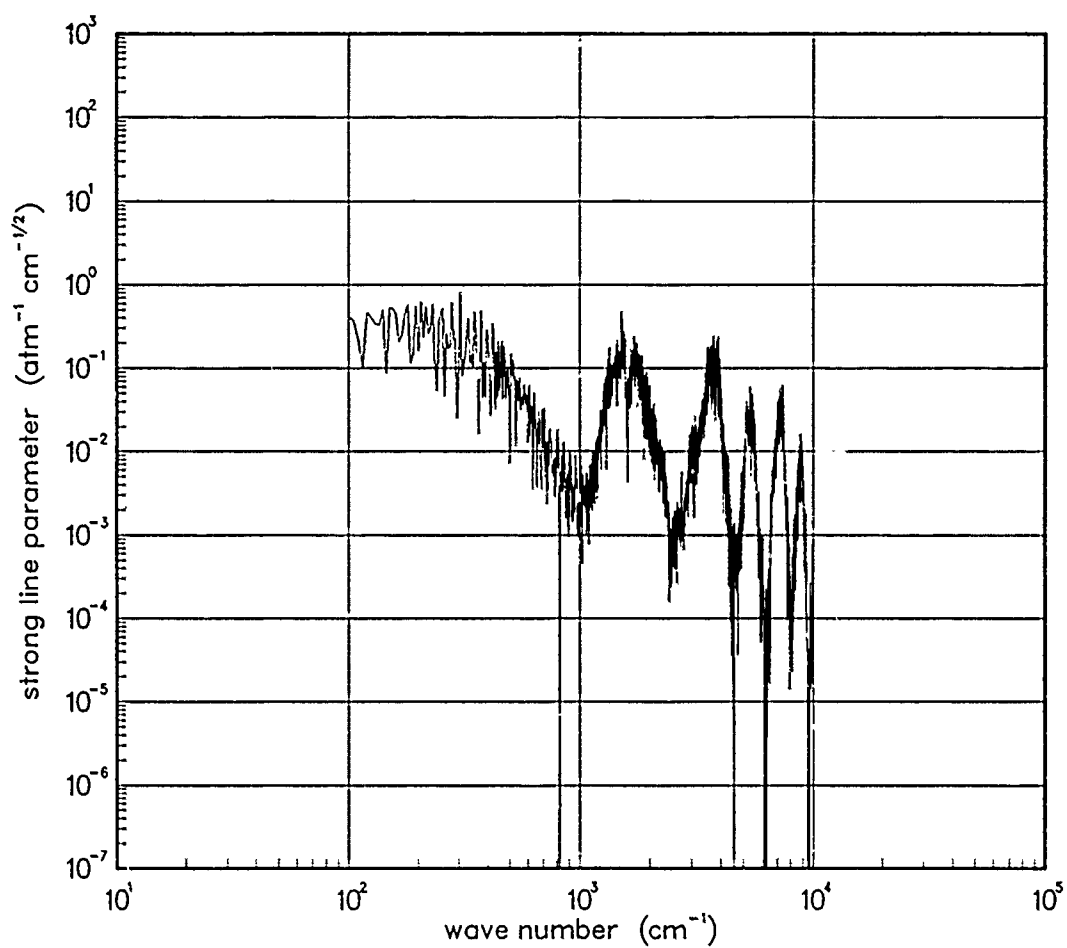


Figure 278. Strong-line parameter for H₂O at 500°K.

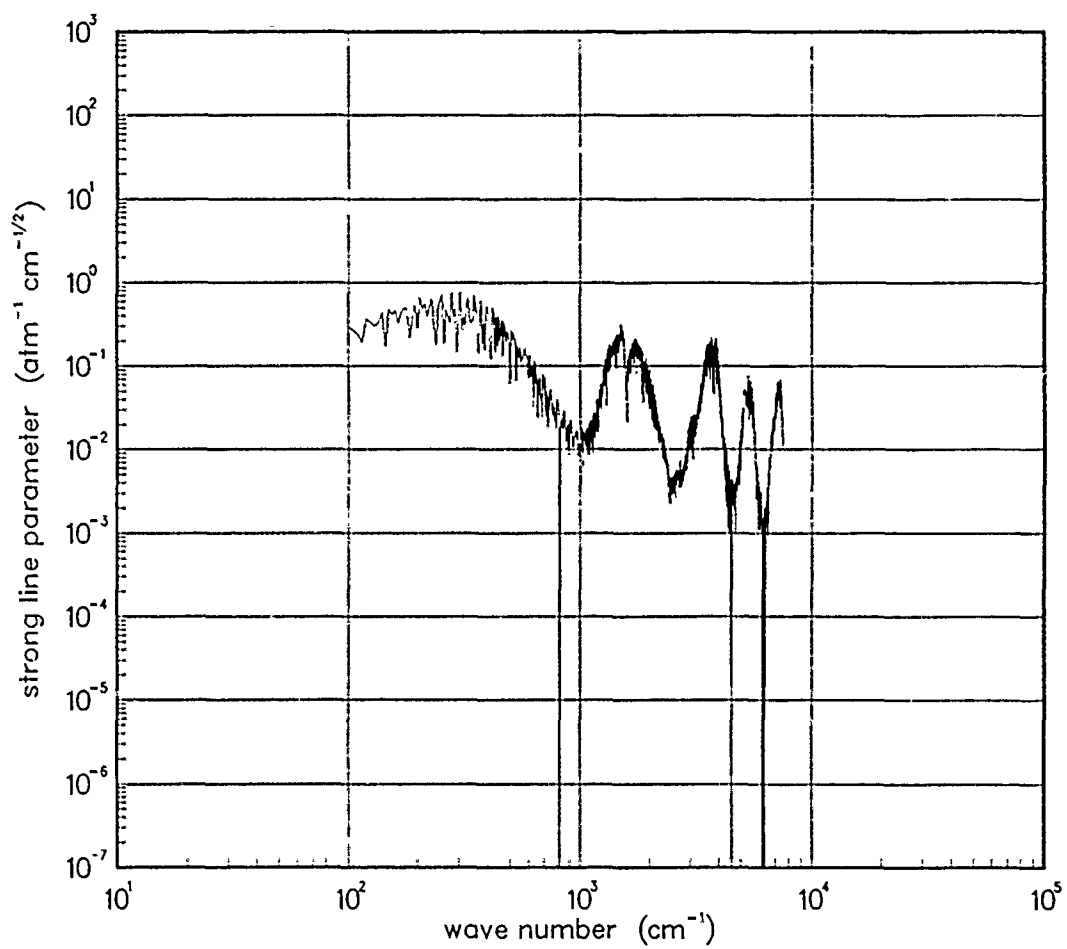


Figure 279. Strong-line parameter for H₂O at 750°K.

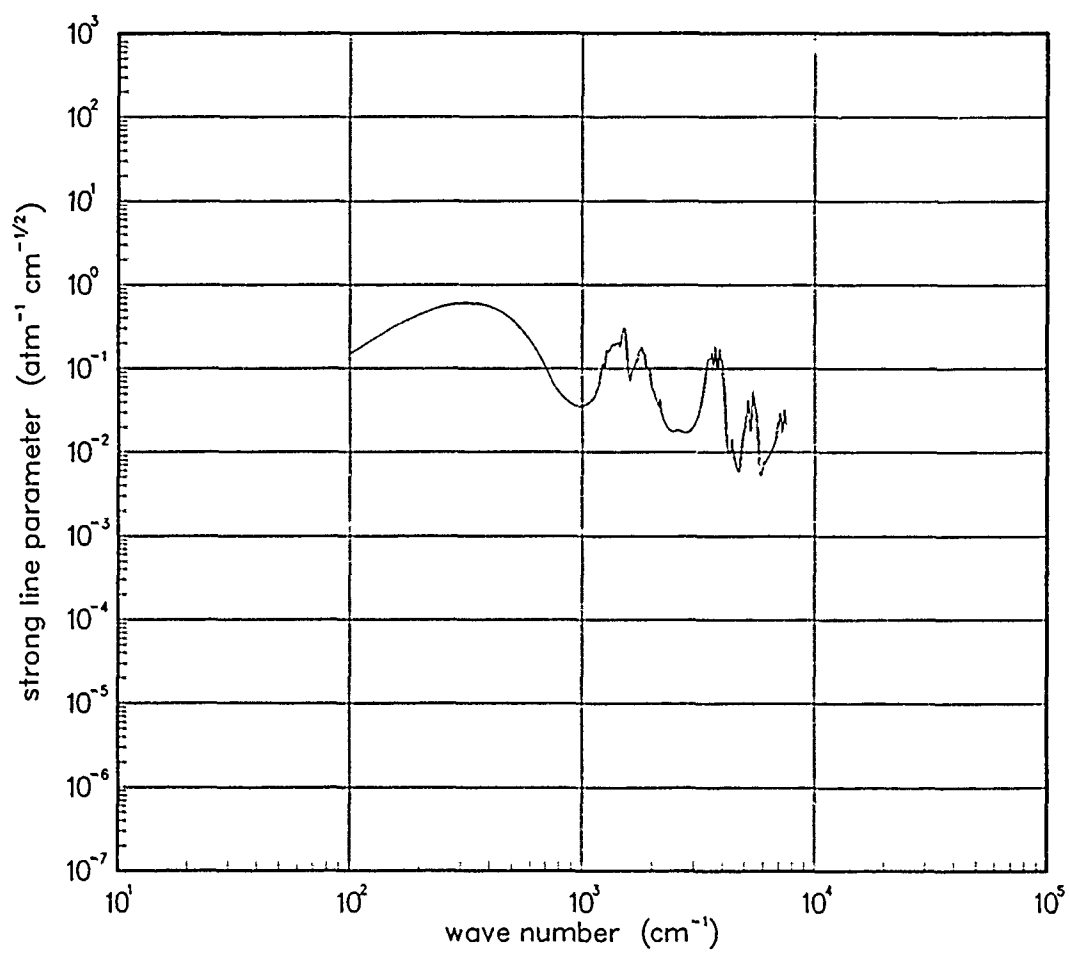


Figure 280. Strong-line parameter for H₂O at 1000°K.

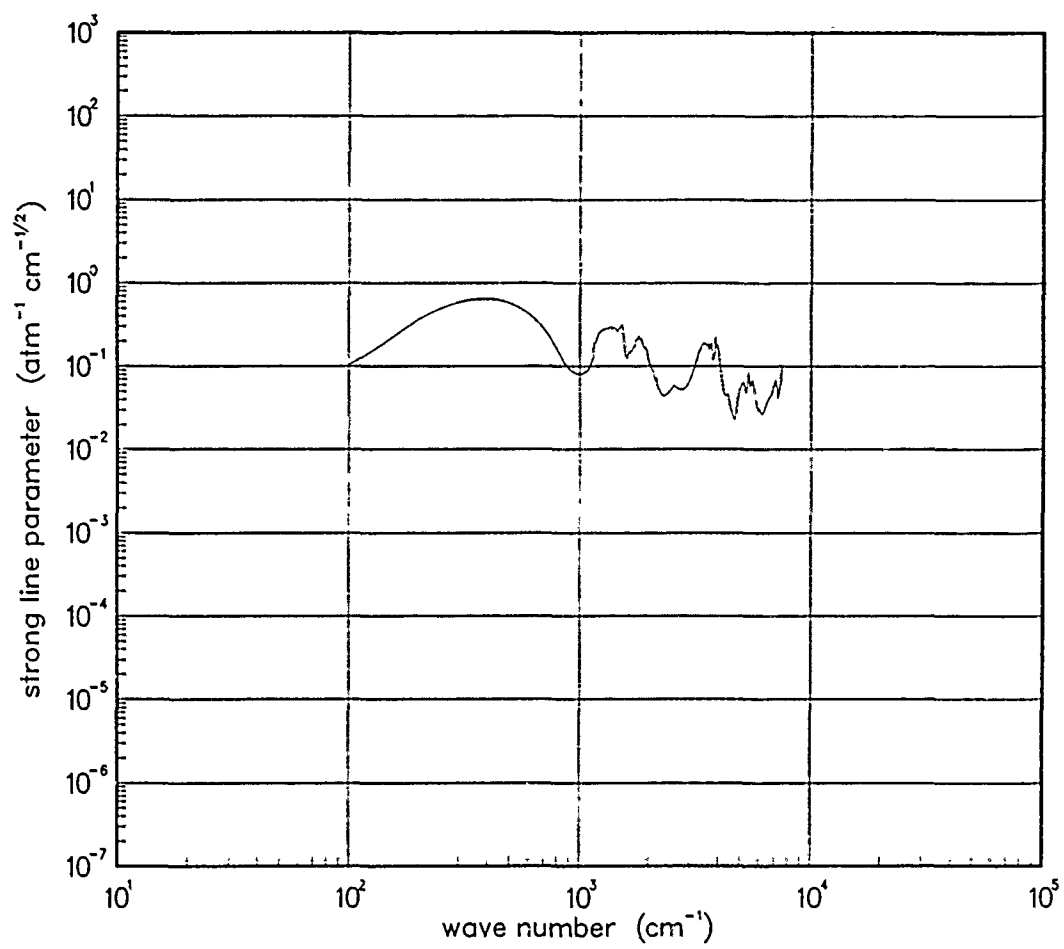


Figure 281. Strong-line parameter for H₂O at 1500°K.

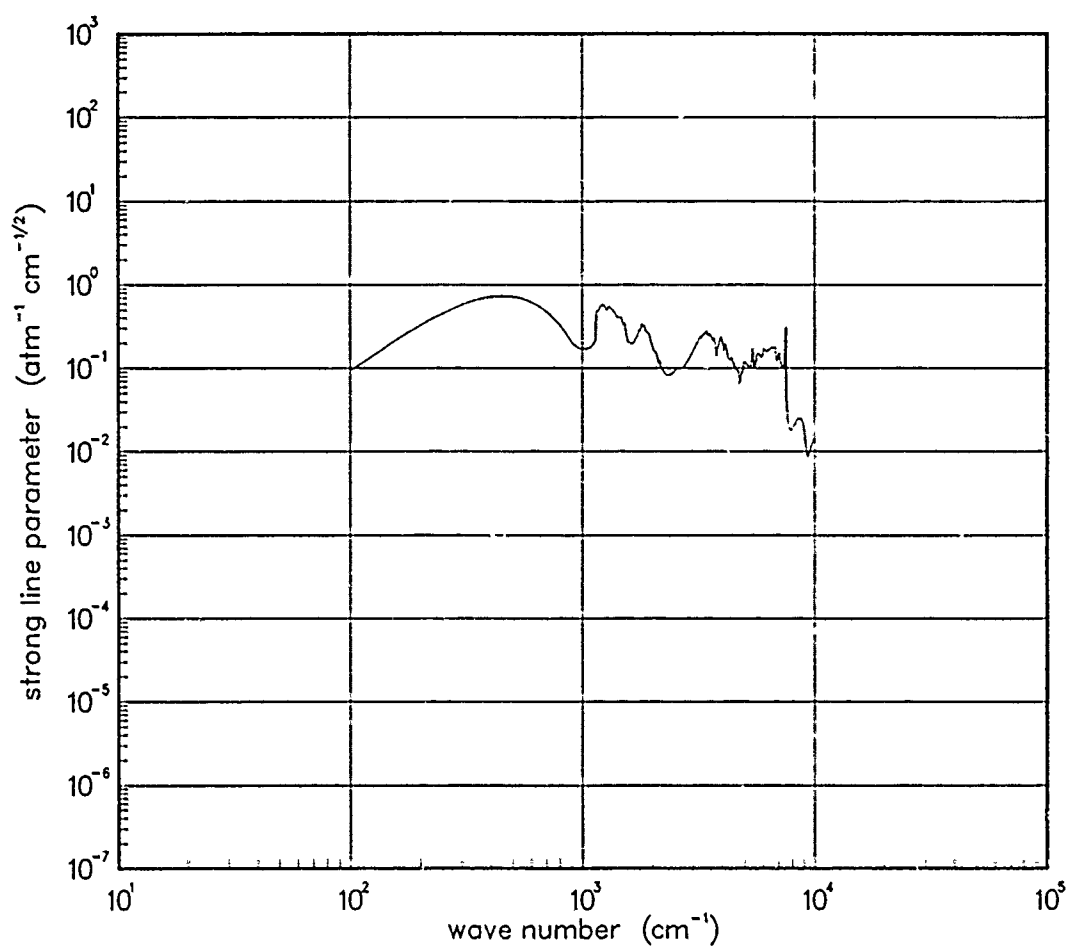


Figure 282. Strong-line parameter for H₂O at 2000°K.

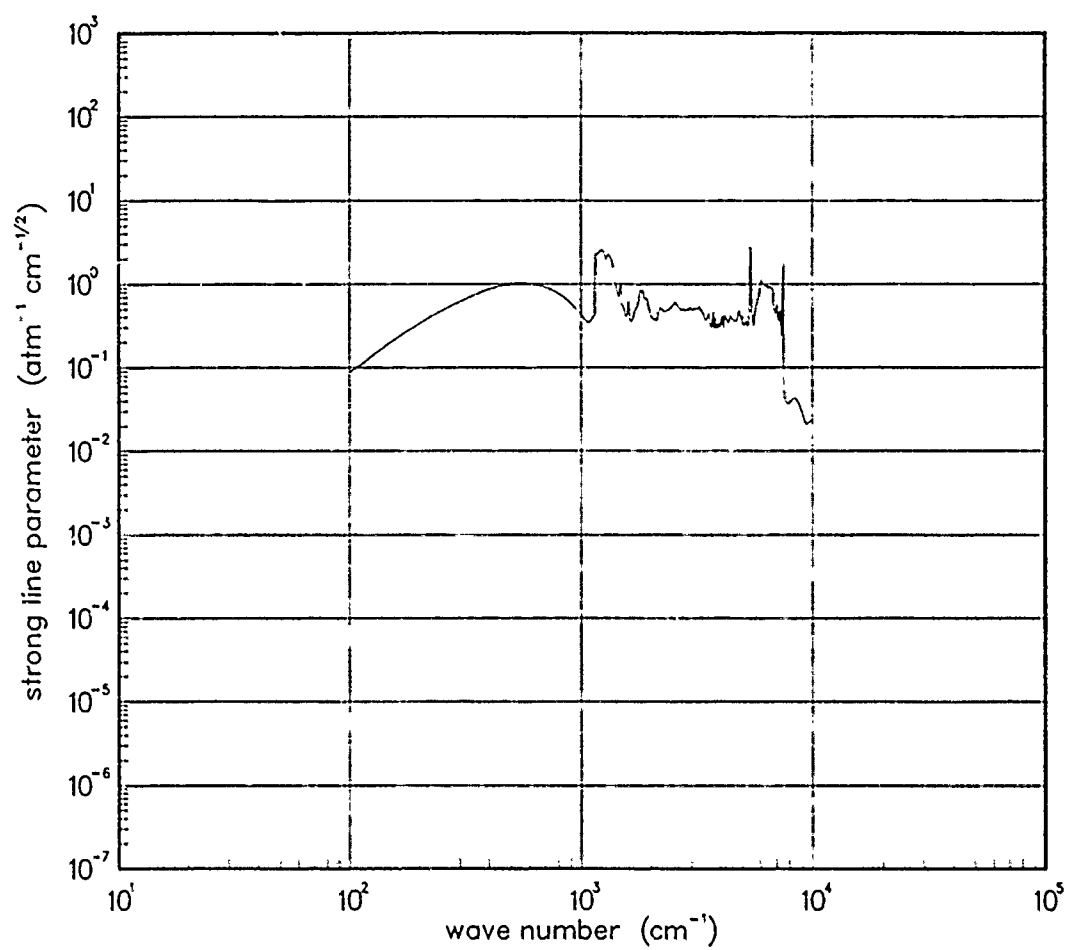


Figure 283. Strong-line parameter for H₂O at 3000°K.

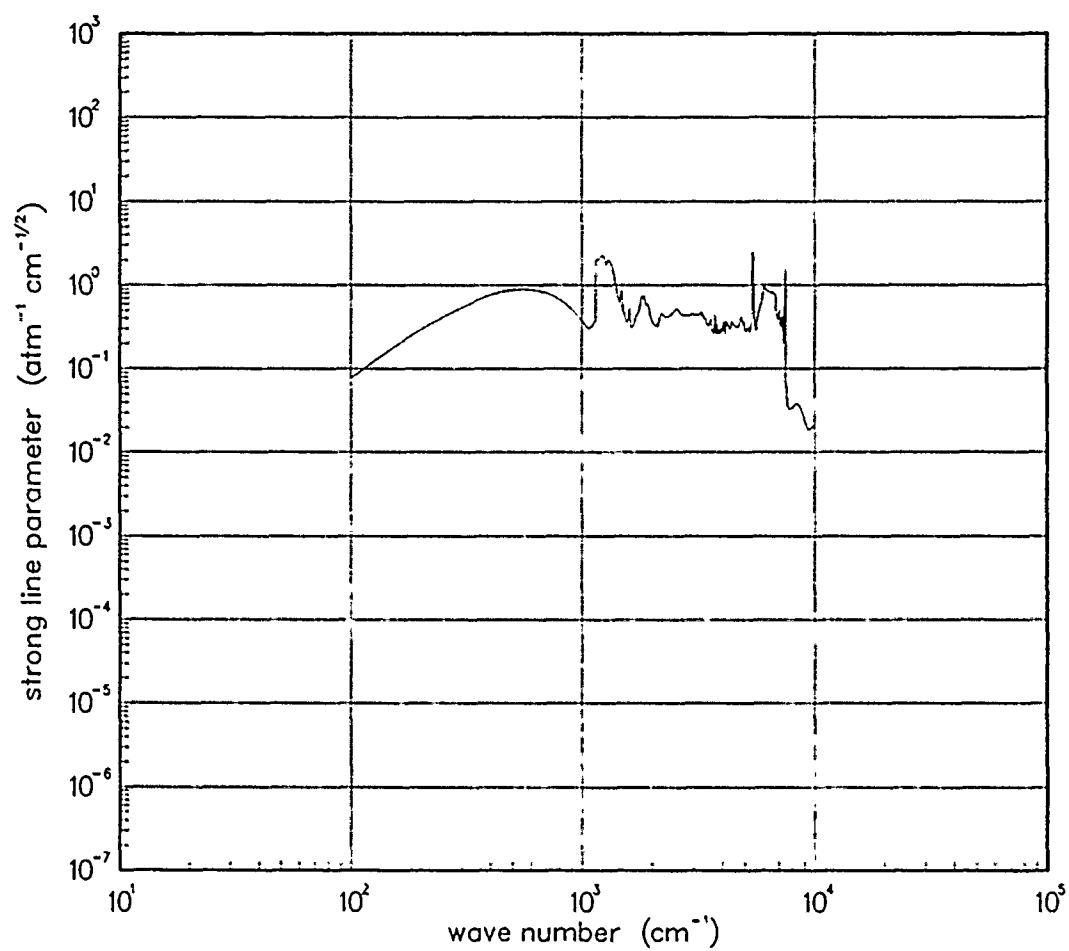


Figure 284. Strong-line parameter for H₂O at 5000°K.

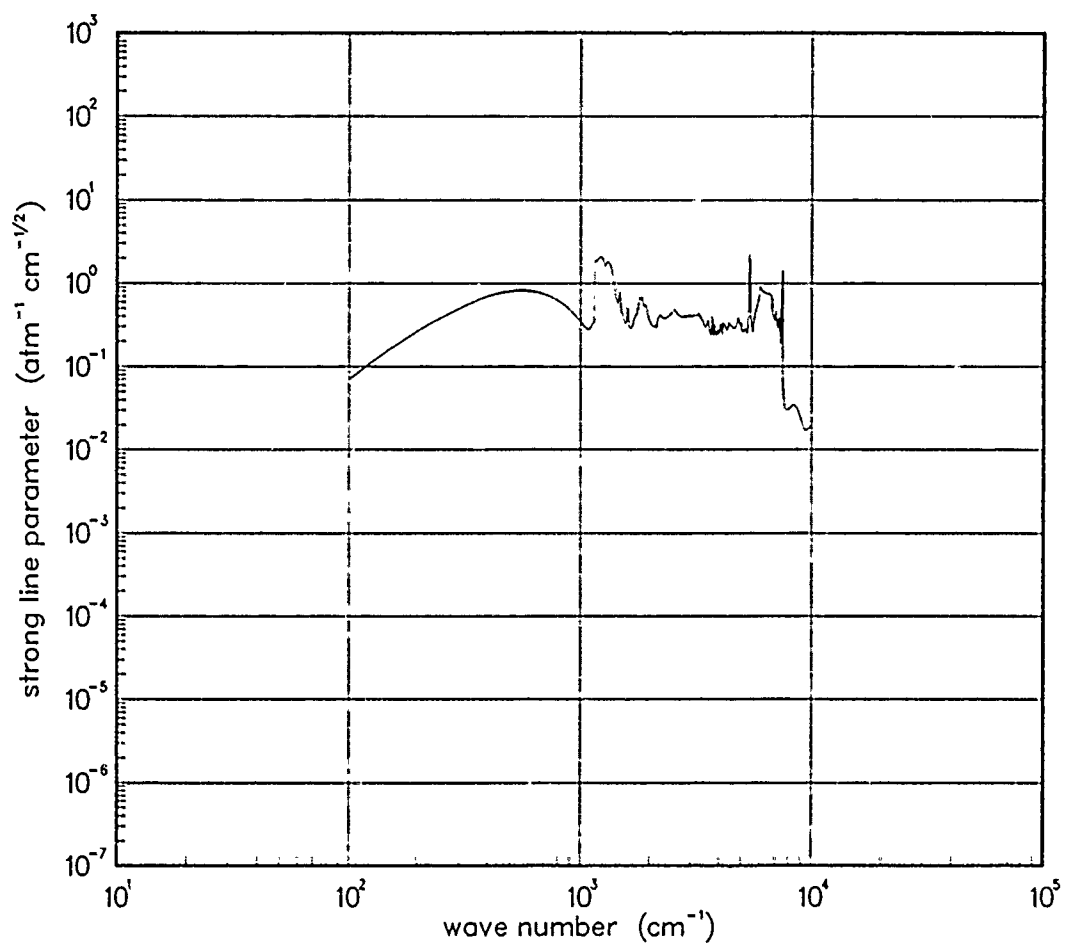


Figure 285. Strong-line parameter for H₂O at 7000°K.

SECTION 6

METAL OXIDES

LTE information for all of the metal oxides within the spectral range: 10 - 10,000 cm^{-1} have been computed using the DATE code. The DATE code has been discussed in detail in Reference 3.

6.1 ALUMINUM OXIDE (AlO).

Aluminum Oxide at temperatures from 200 - 18,000 $^{\circ}\text{K}$ was calculated using the DATE code.

Table 7. Spectroscopic data for AlO .

$\text{X } ^2\Sigma^+$

$$\begin{array}{lll} \omega_e = 979.23^* & \omega_e x_e = 6.97^* & A_e = 123.61 \\ \alpha_e = 0.0058^* & B_e = .64136^* & E_e = 0.0 \end{array}$$

$$S_{10} = 204.0^\dagger \quad S_{20} = 1.05^\dagger \quad S_{30} = 0.00381^\dagger$$

$$\gamma_t(300^\circ\text{K}) = 0.04^\S$$

Data Source:

*B. Rosen, ed., Spectroscopic Data Relative to Diatomic Molecules, Pergamon Press, New York (1970).

†H.H. Michels, Diatomic Oxide Vibrational Band Intensities, United Aircraft Research Laboratories, K921094-4 (May 1971).

‡J.K. McDonald, and K.K. Innes, A Low-Lying Excited Electronic State of the AlO Molecule and the Ground-State Dissociation Energy, Journal of Molecular Spectroscopy, **32**, pp 501-510 (1969).

§Estimate

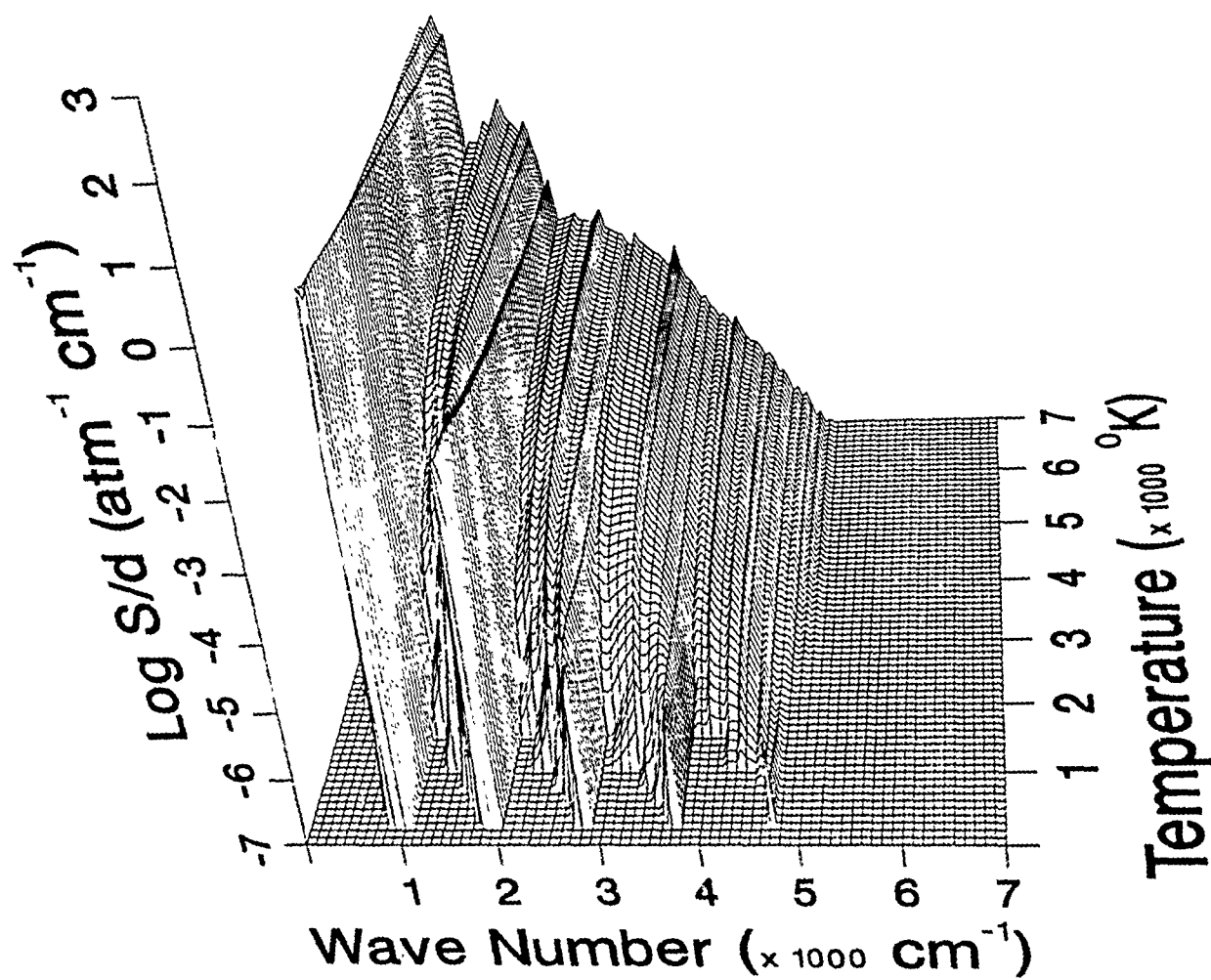


Figure 286. Weak-line parameter for Al_2O_3 .

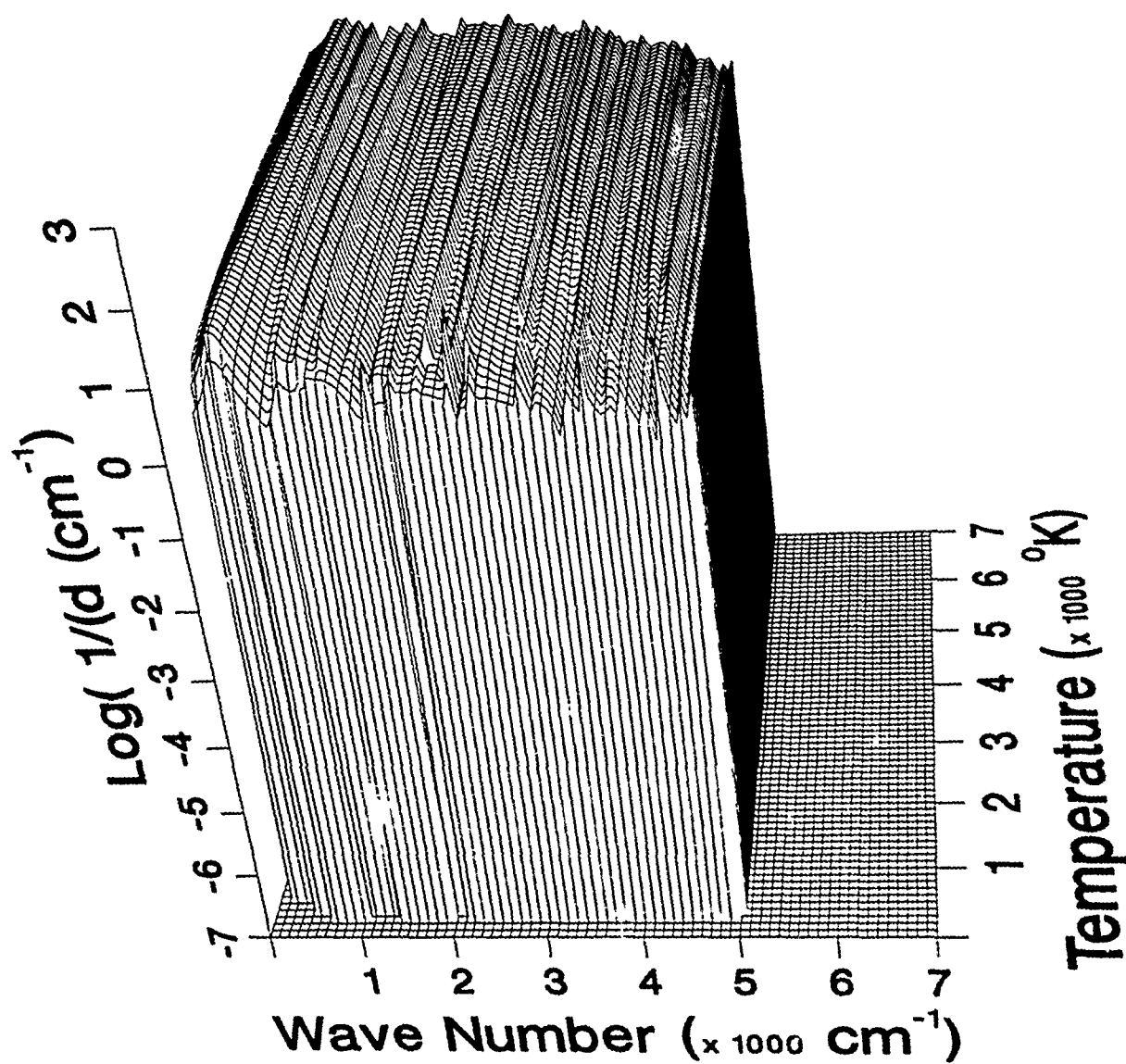


Figure 287. Inverse line spacing for Al_2O_3 .

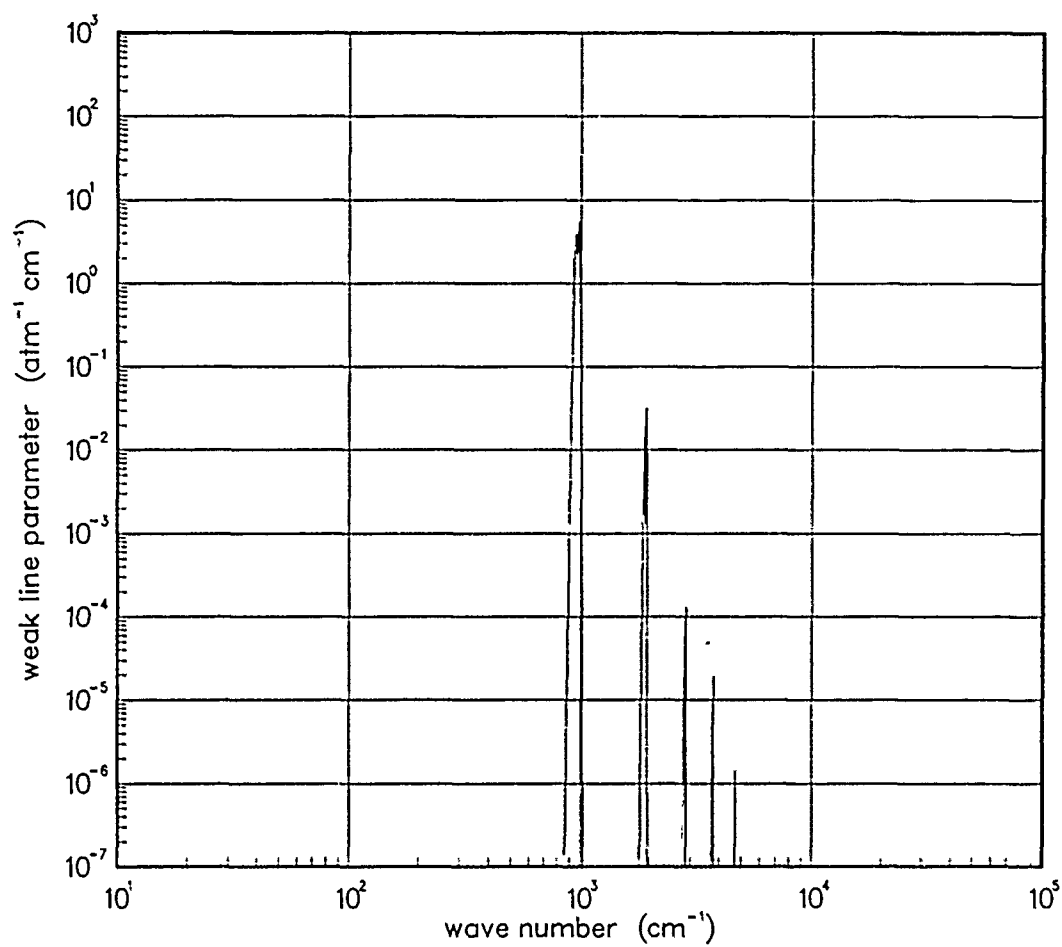


Figure 288. Weak-line parameter for AlO at 200°K.

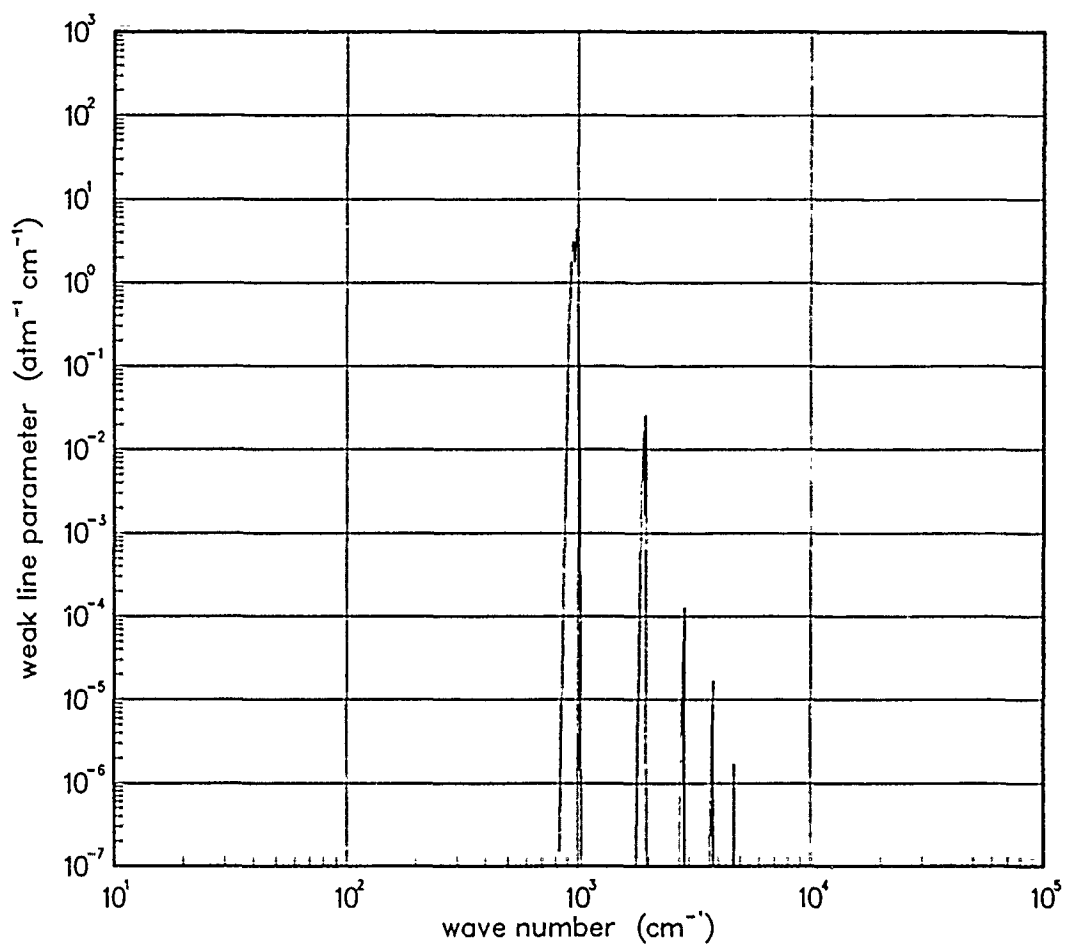


Figure 289. Weak-line parameter for AlO at 300°K.

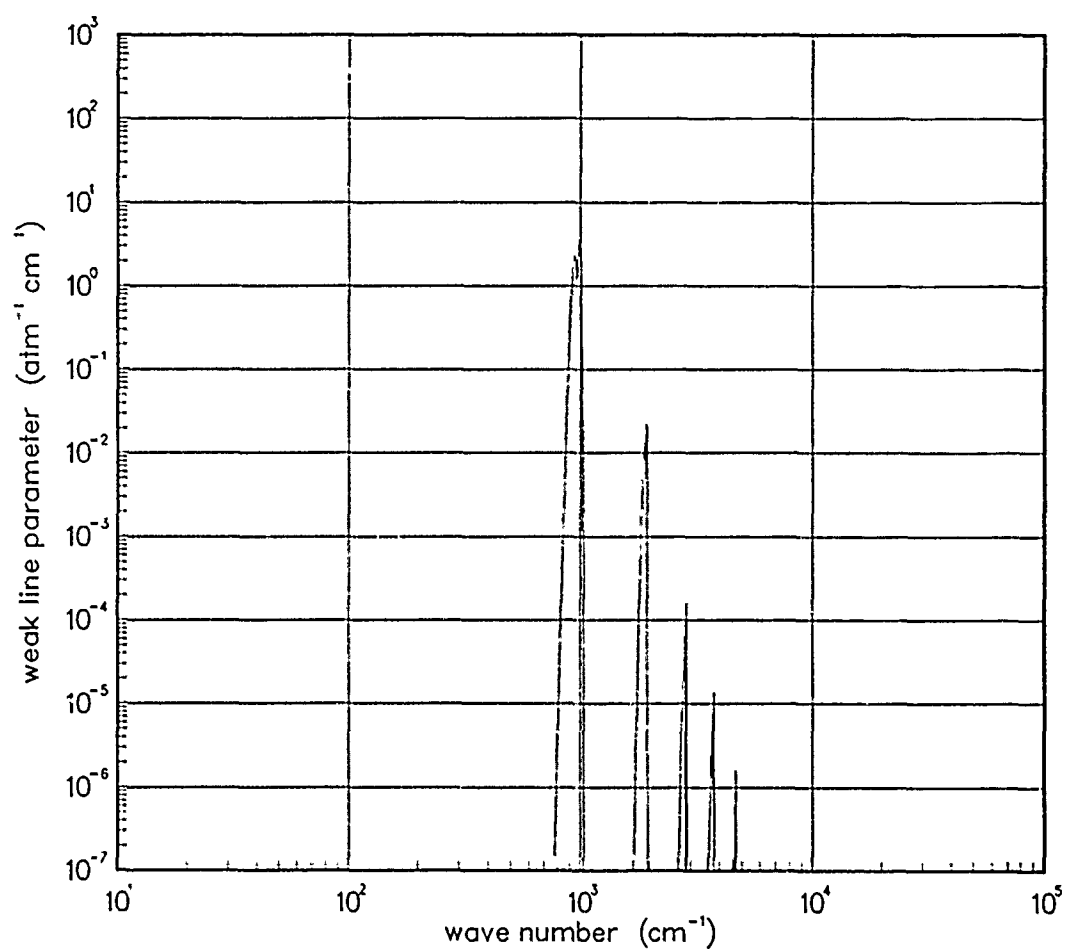


Figure 290. Weak-line parameter for AlO at 500°K.

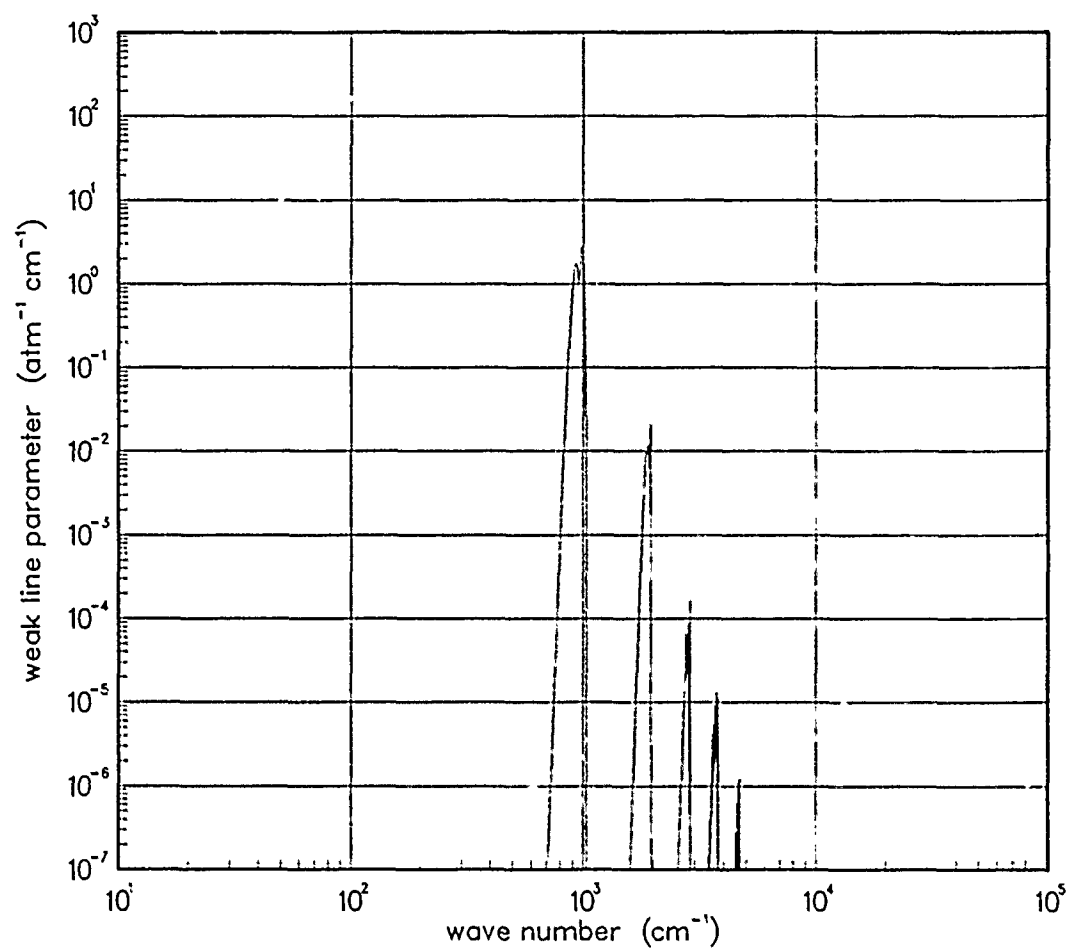


Figure 291. Weak-line parameter for AlO at 750°K.

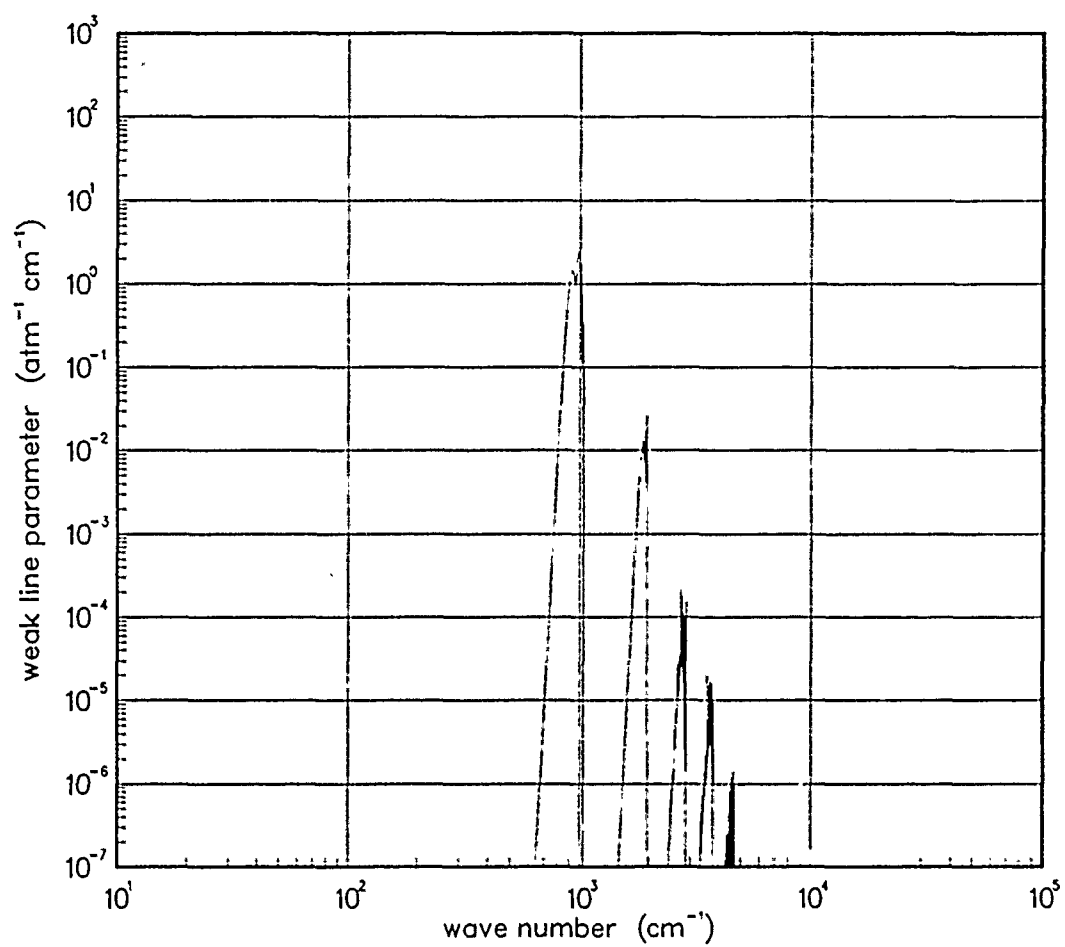


Figure 292. Weak-line parameter for AlO at 1000°K.

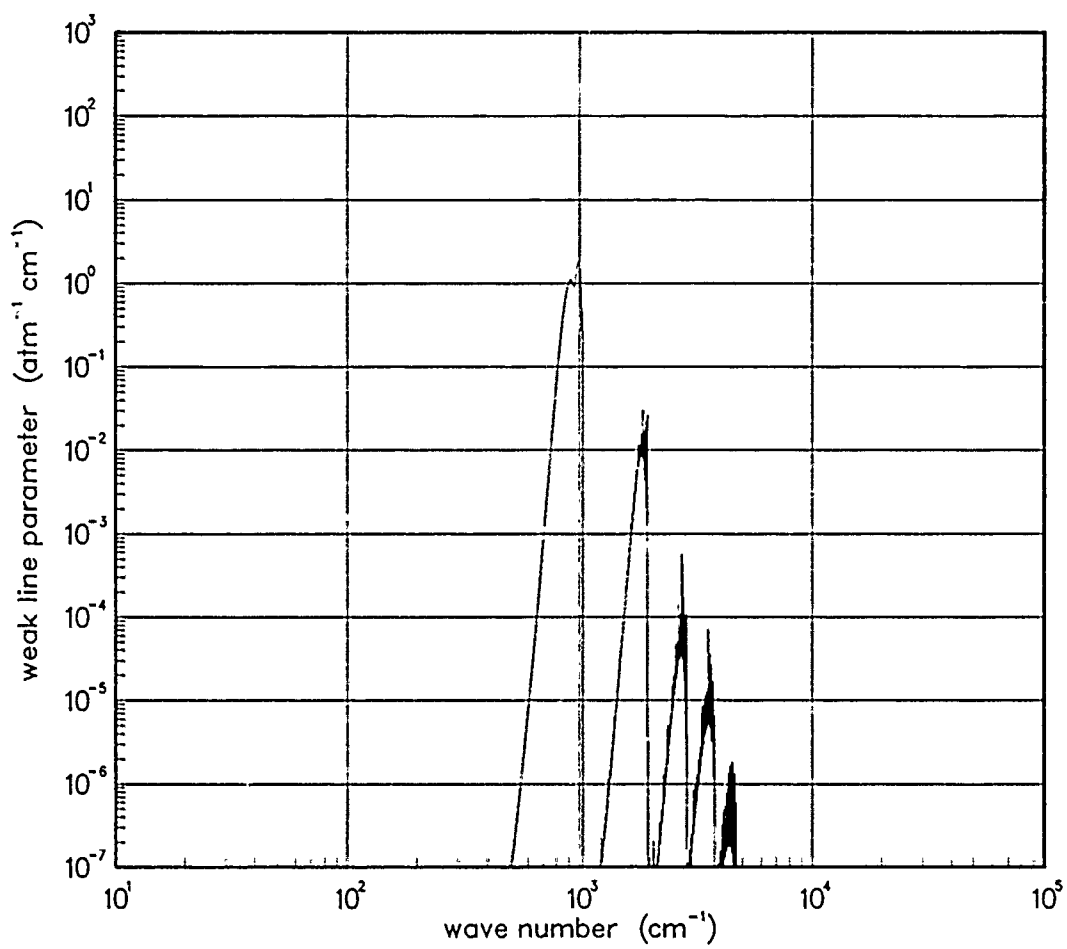


Figure 293. Weak-line parameter for AlO at 1500°K.

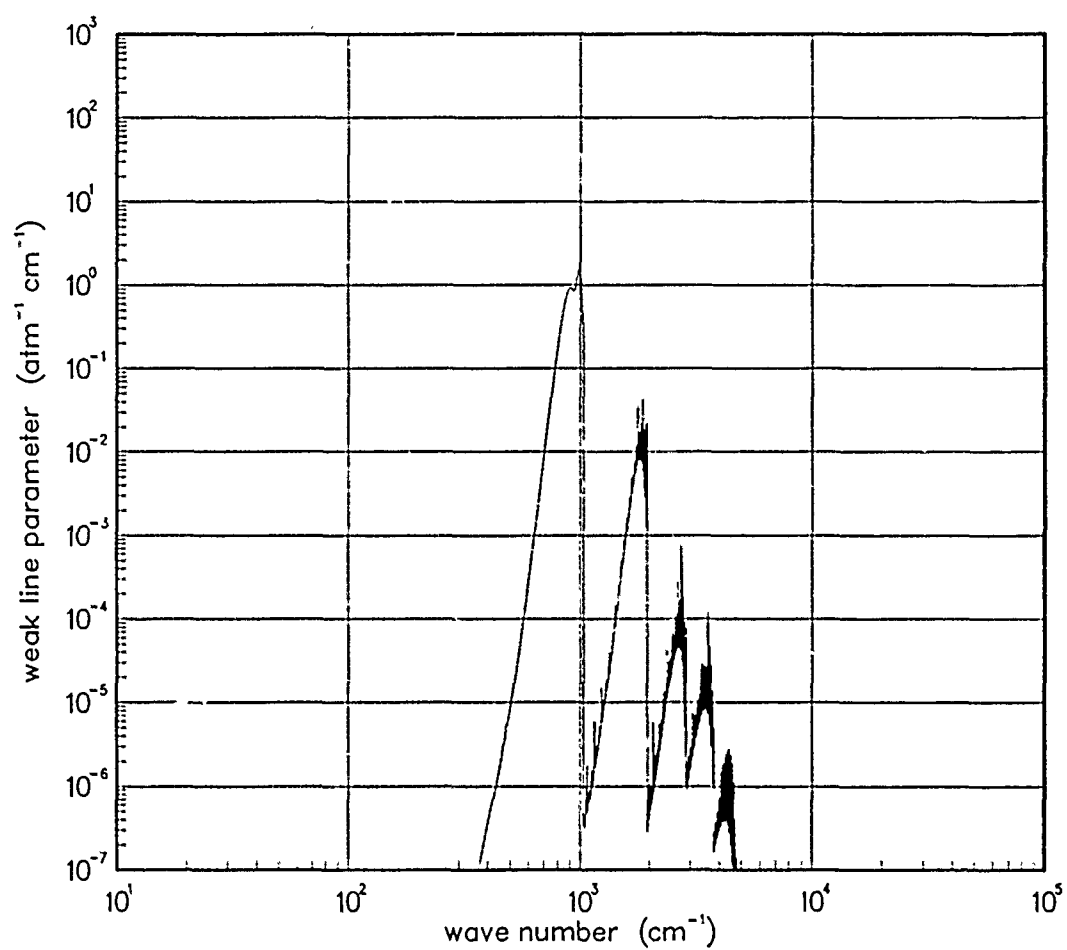


Figure 294. Weak-line parameter for AlO at 2000°K.

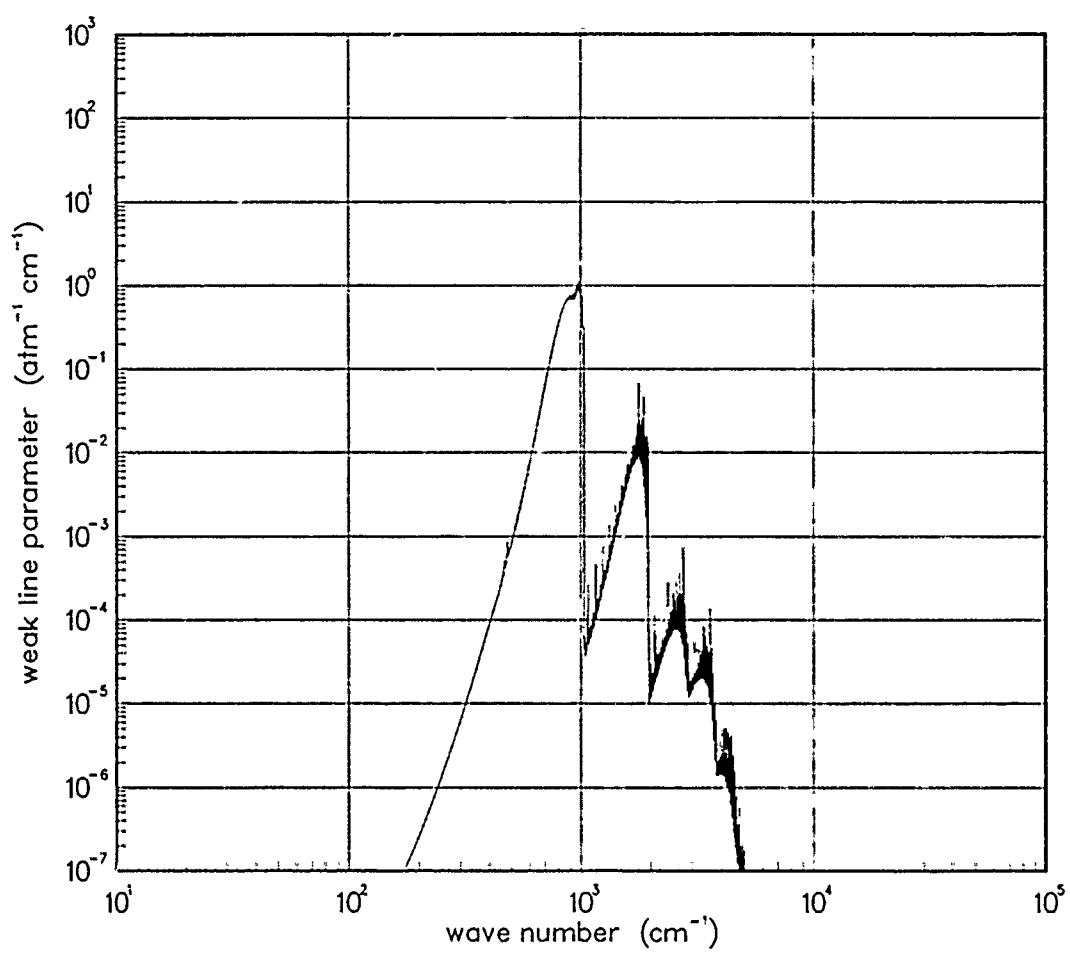


Figure 295. Weak-line parameter for AlO at 3000°K.

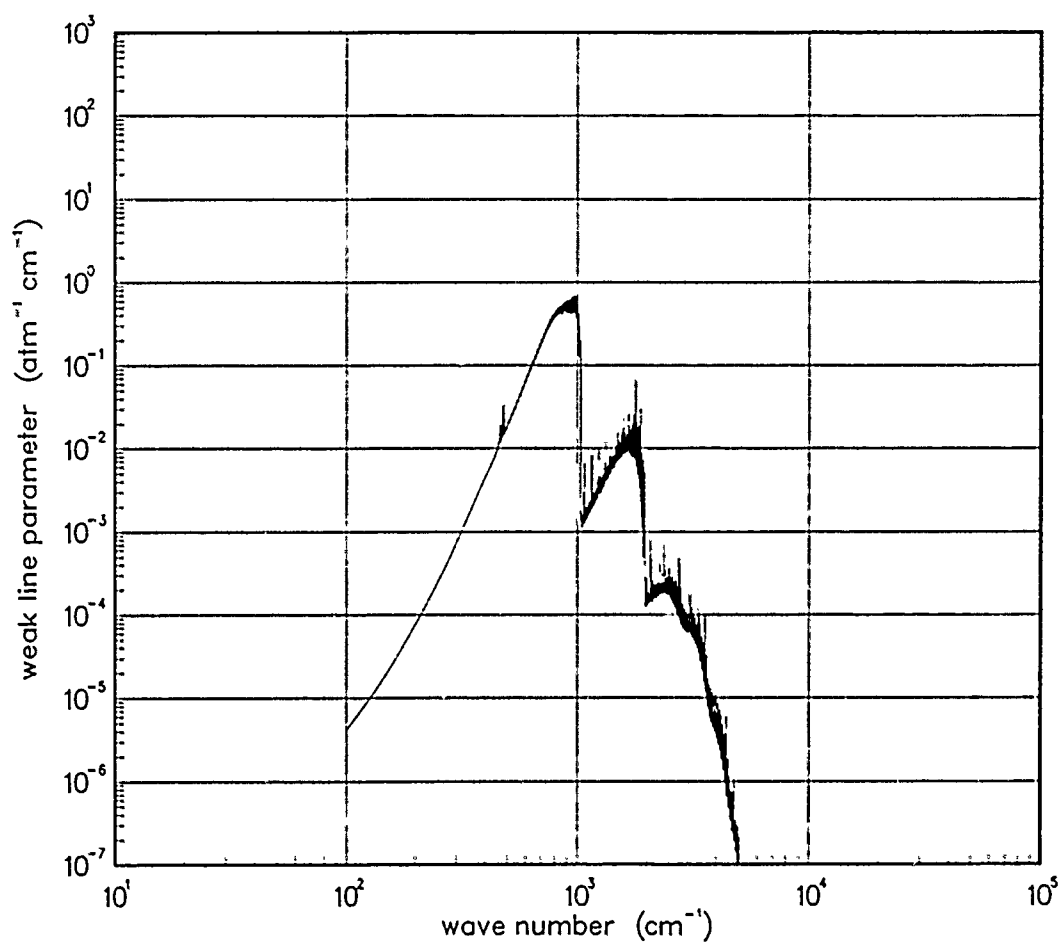


Figure 296. Weak-line parameter for Al_2O_3 at 5000°K .

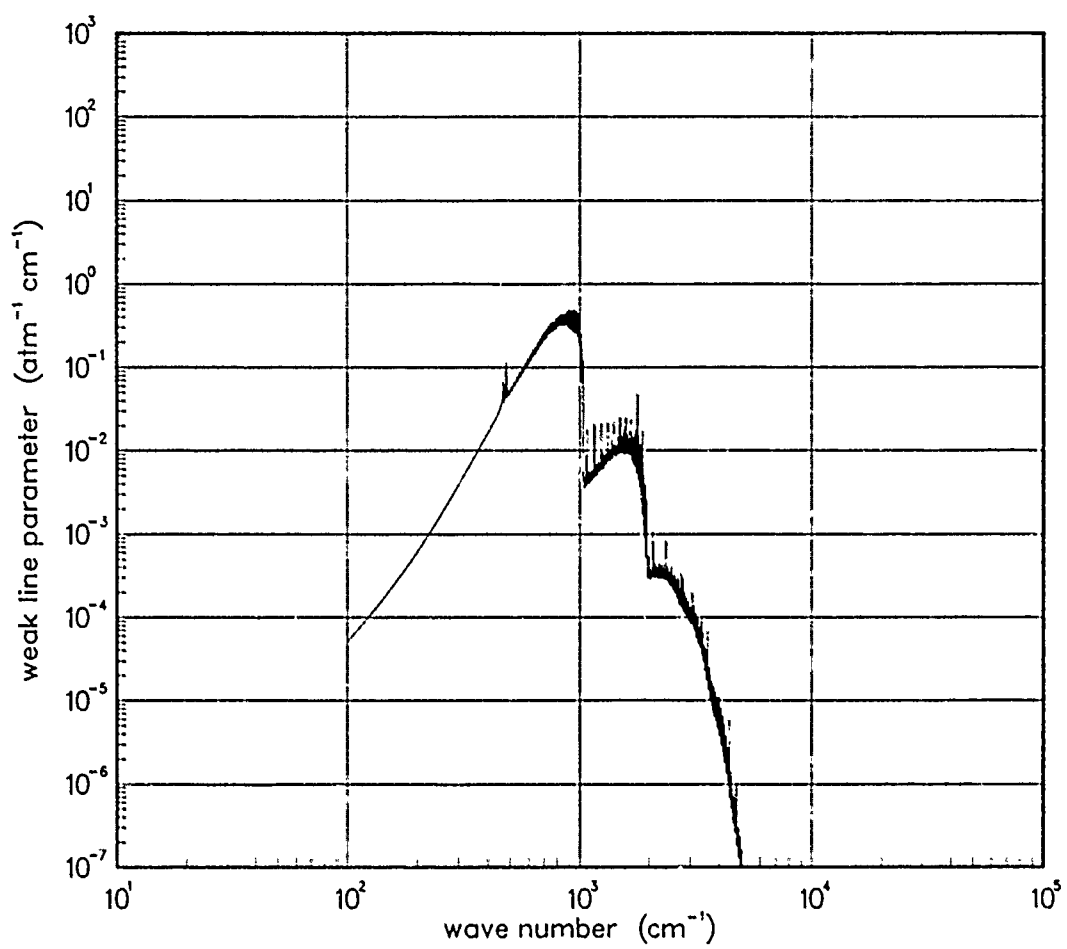


Figure 297. Weak-line parameter for AlO at 7000°K.

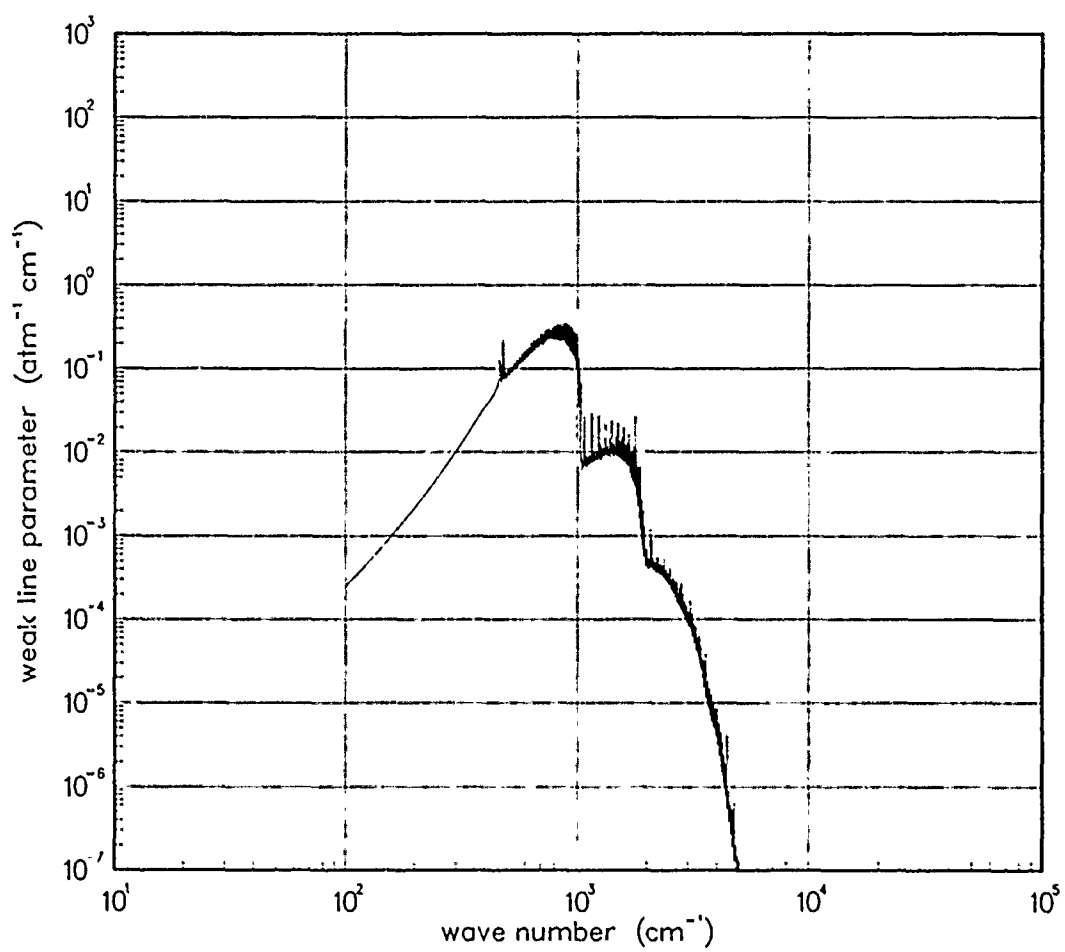


Figure 298. Weak-line parameter for AlO at 10000°K.

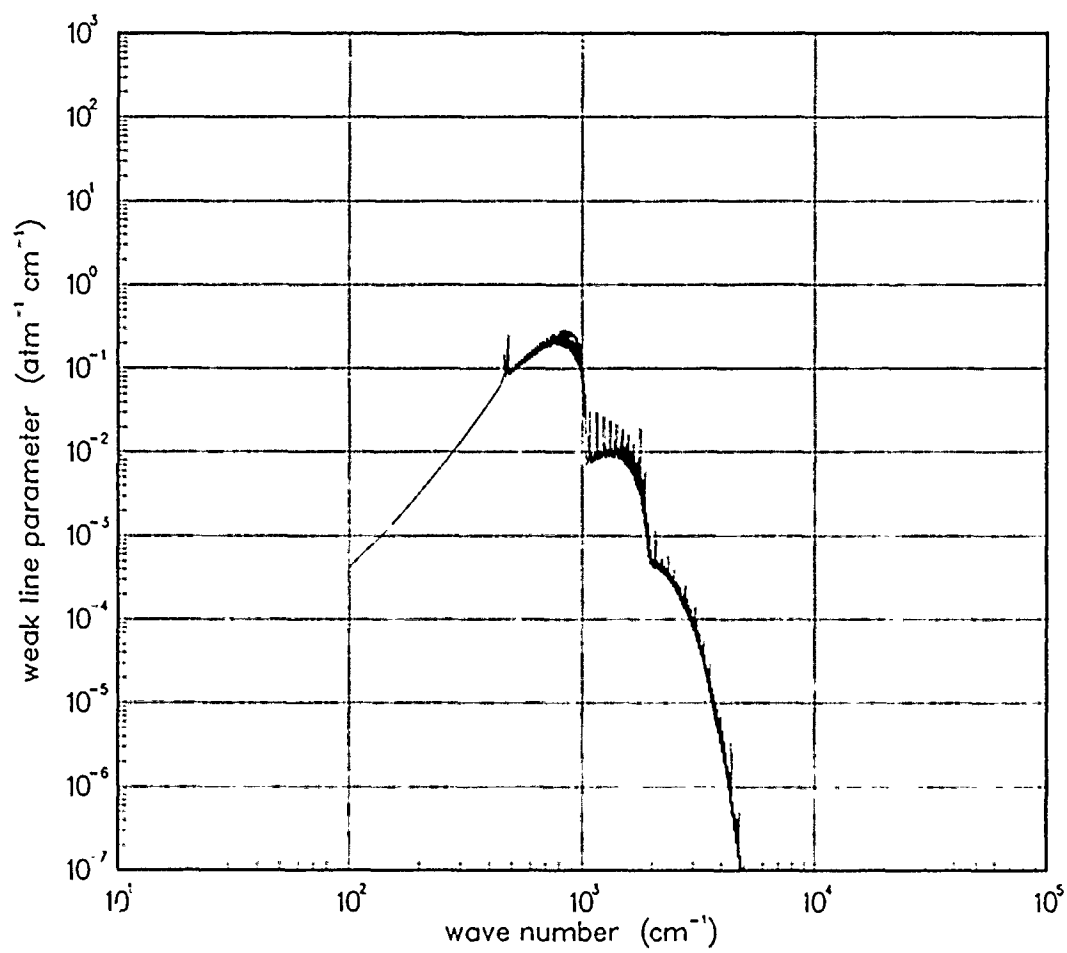


Figure 299. Weak-line parameter for AlO at 12000°K.

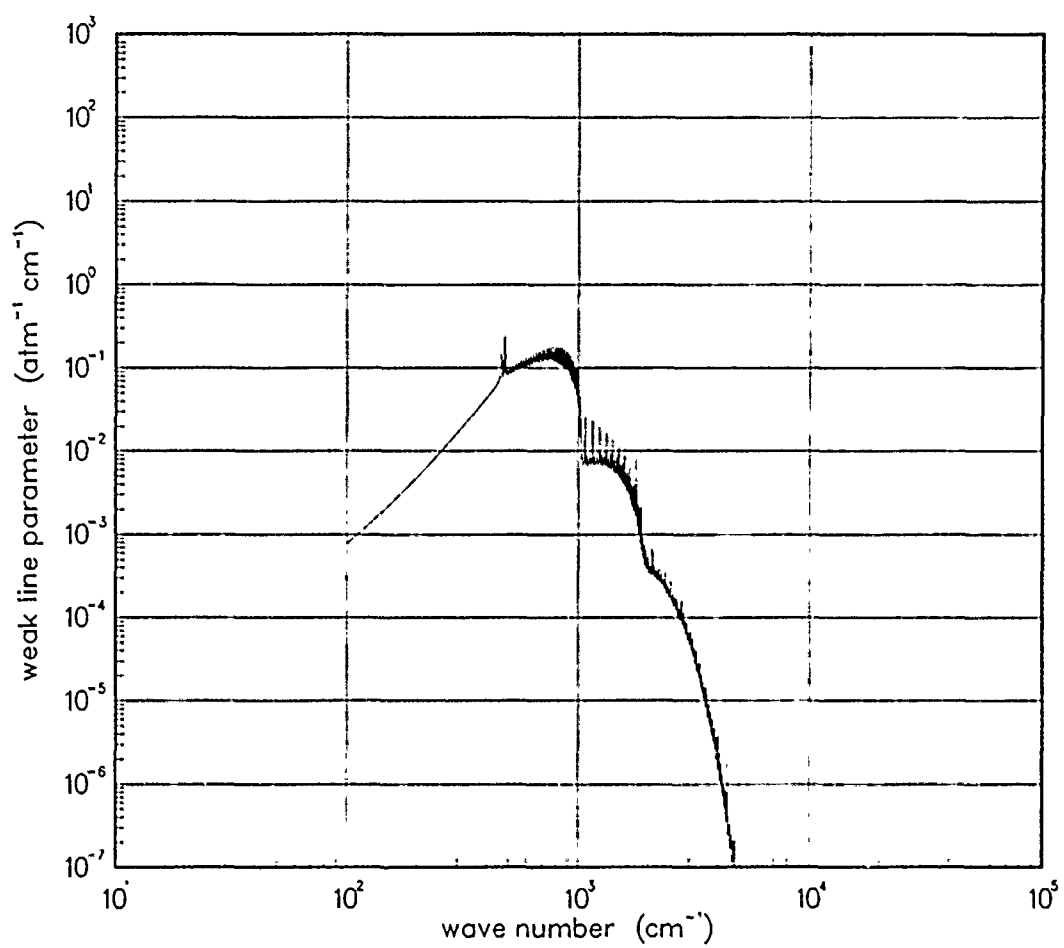


Figure 300. Weak-line parameter for Al_2O at 18000°K .

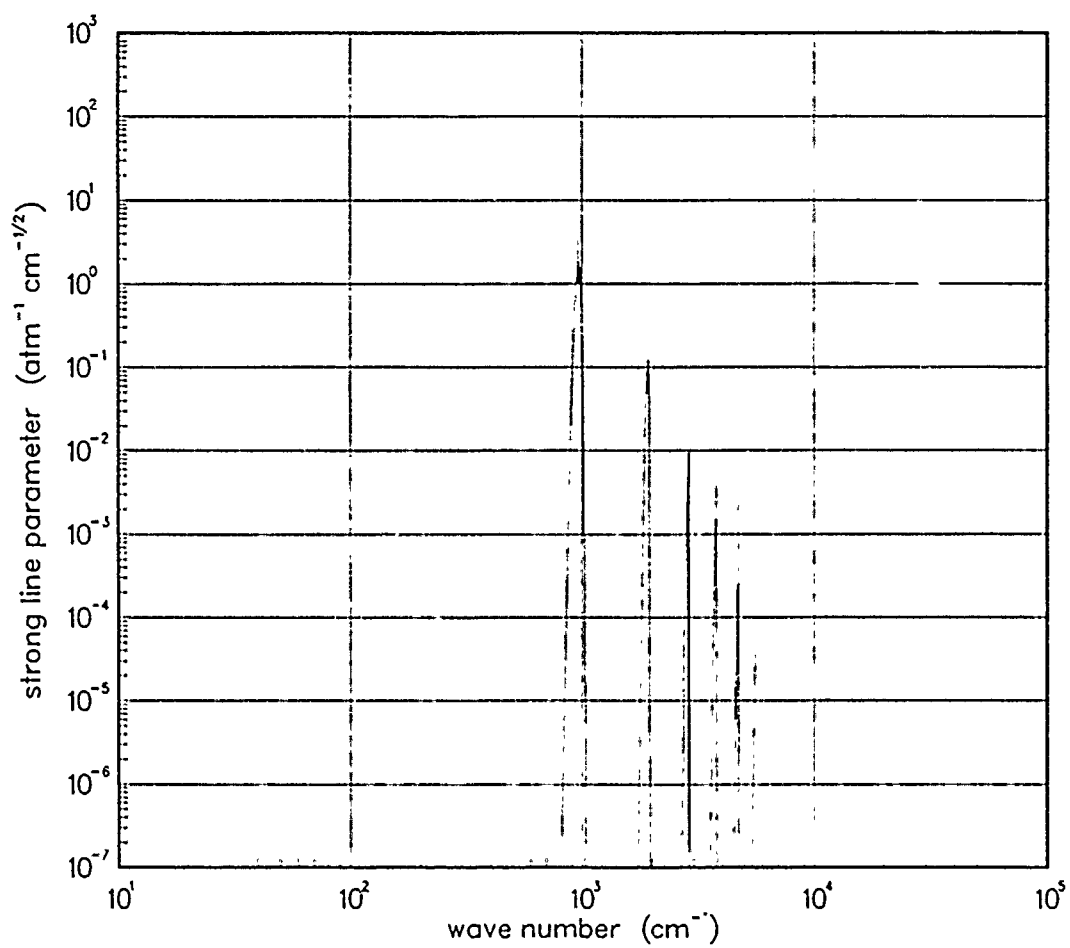


Figure 301. Strong-line parameter for Al₂O₃ at 200°K.

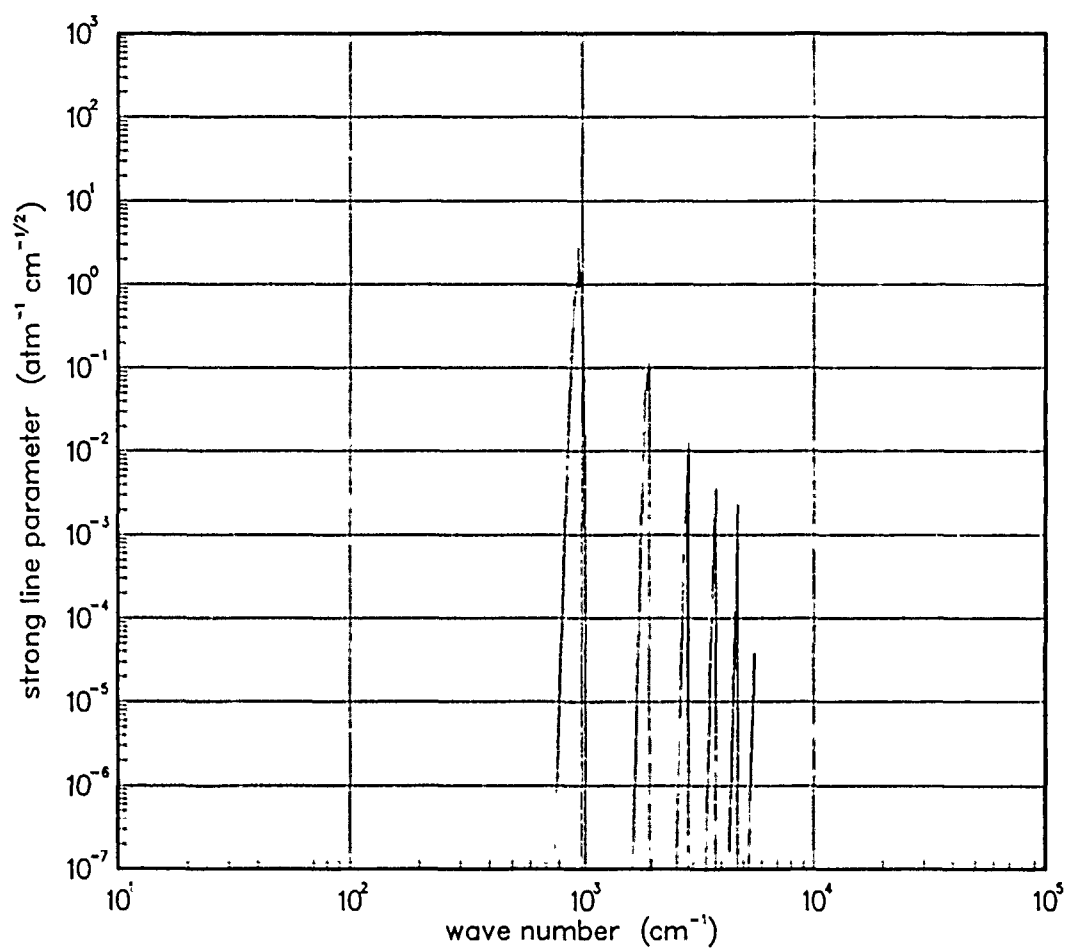


Figure 302. Strong-line parameter for AlO at 300°K.

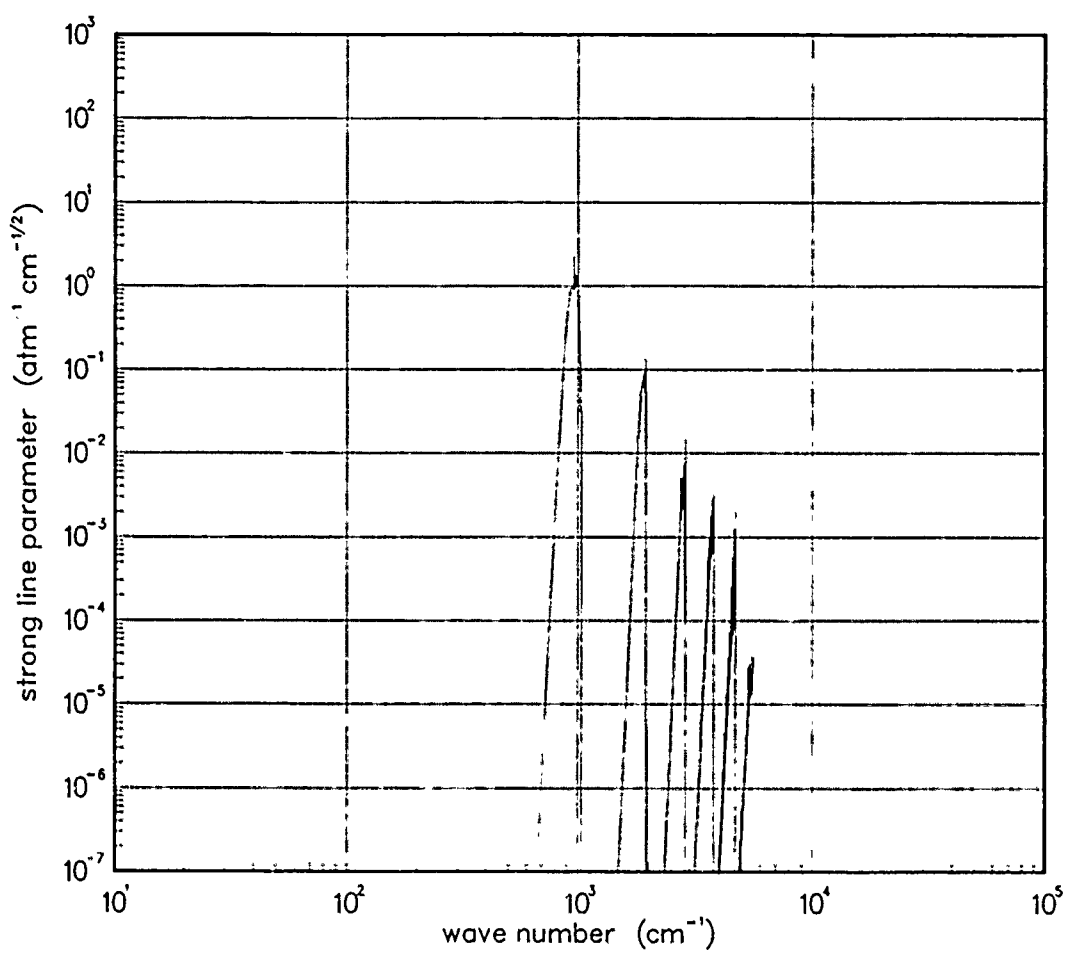


Figure 303. Strong-line parameter for Al_2O_3 at 500°K .

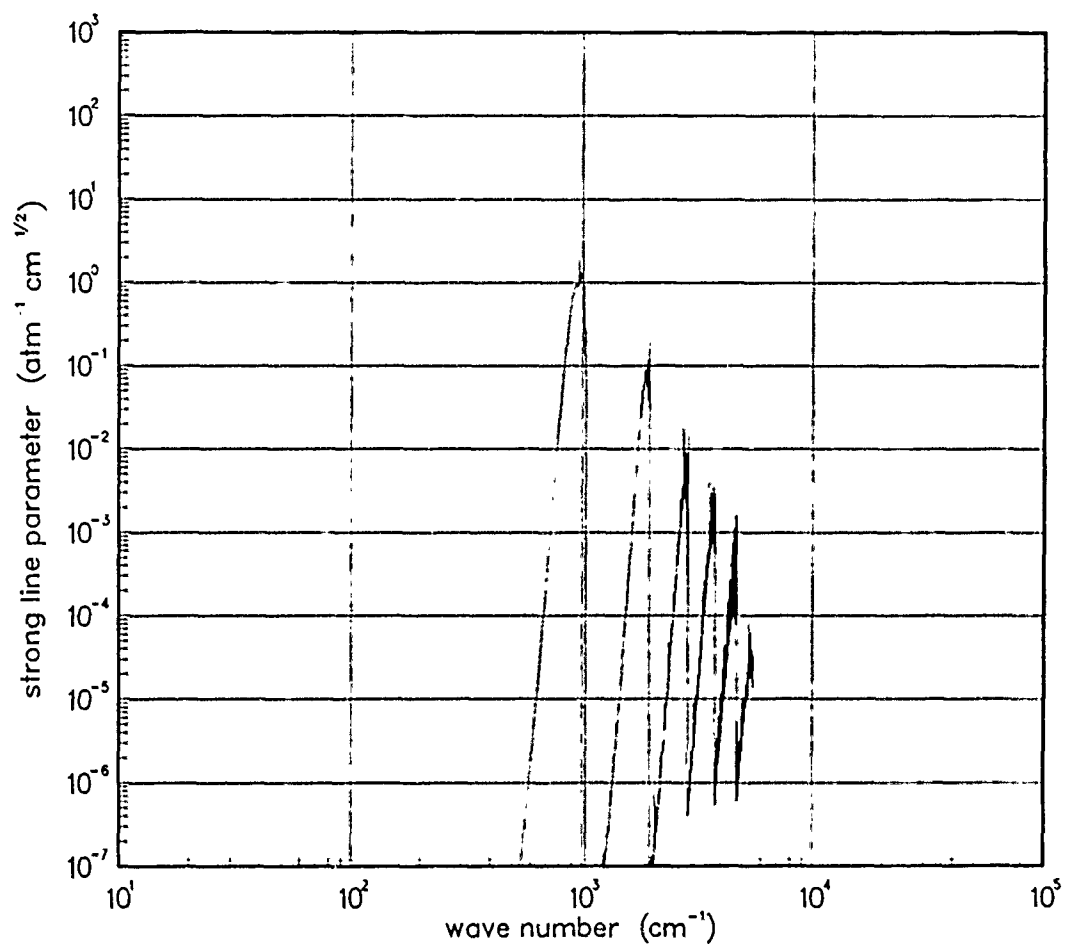


Figure 304. Strong-line parameter for Al₂O₃ at 750°K.

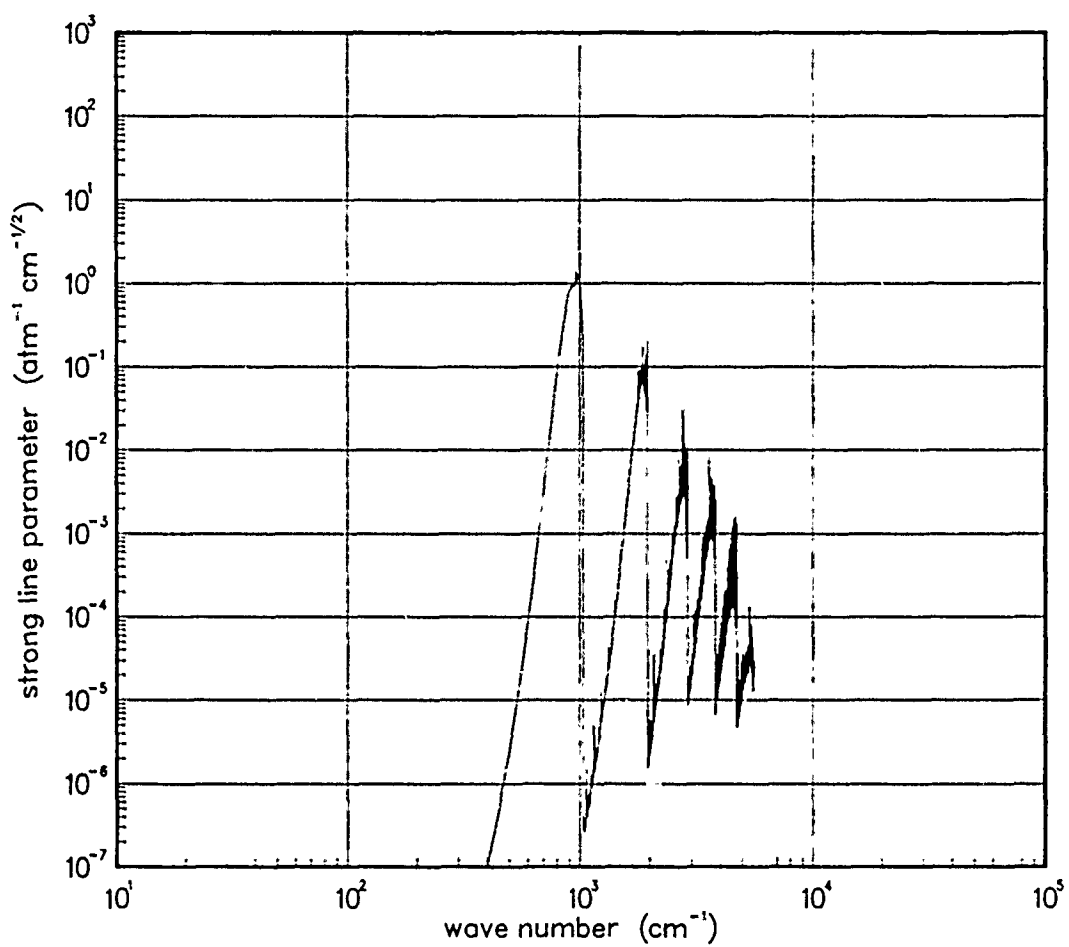


Figure 305. Strong-line parameter for AlO at 1000°K.

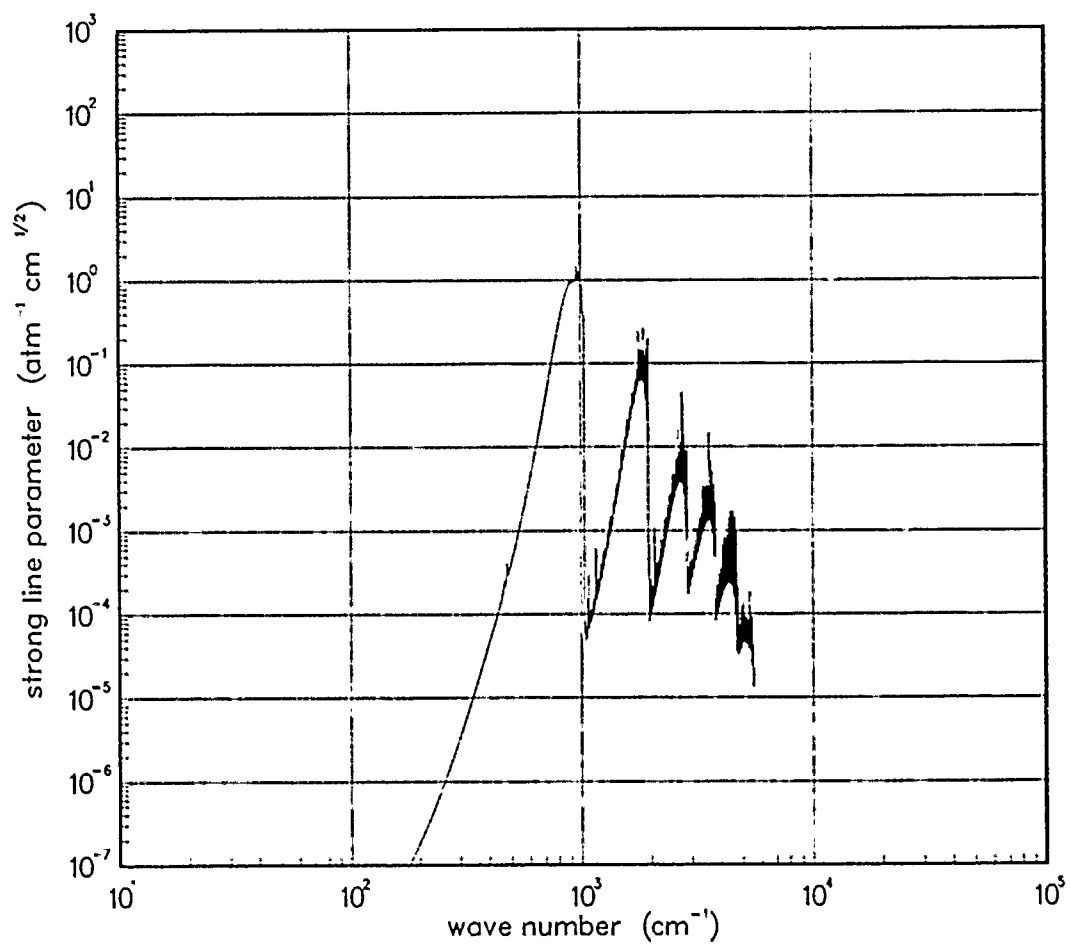


Figure 306. Strong-line parameter for Al_2O_3 at 1500°K .

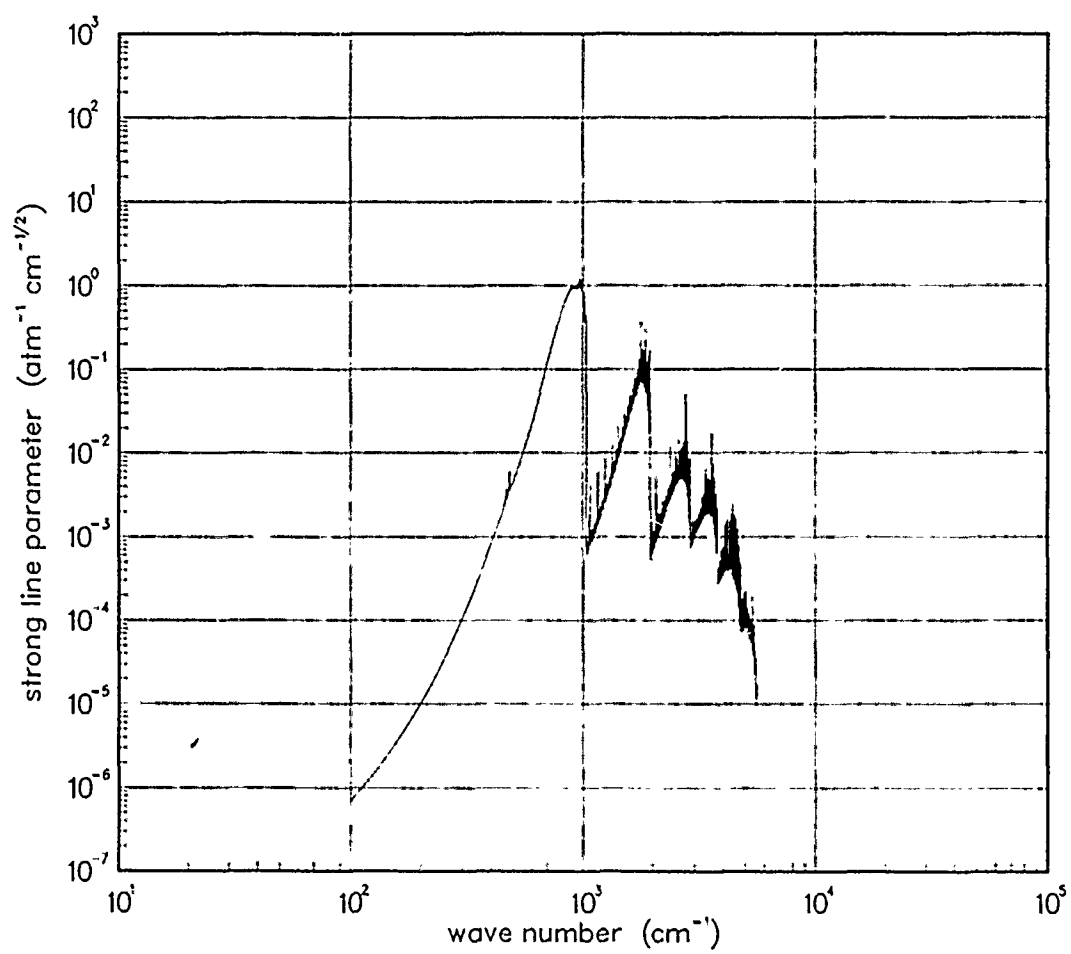


Figure 307. Strong-line parameter for AlO at 2000°K.

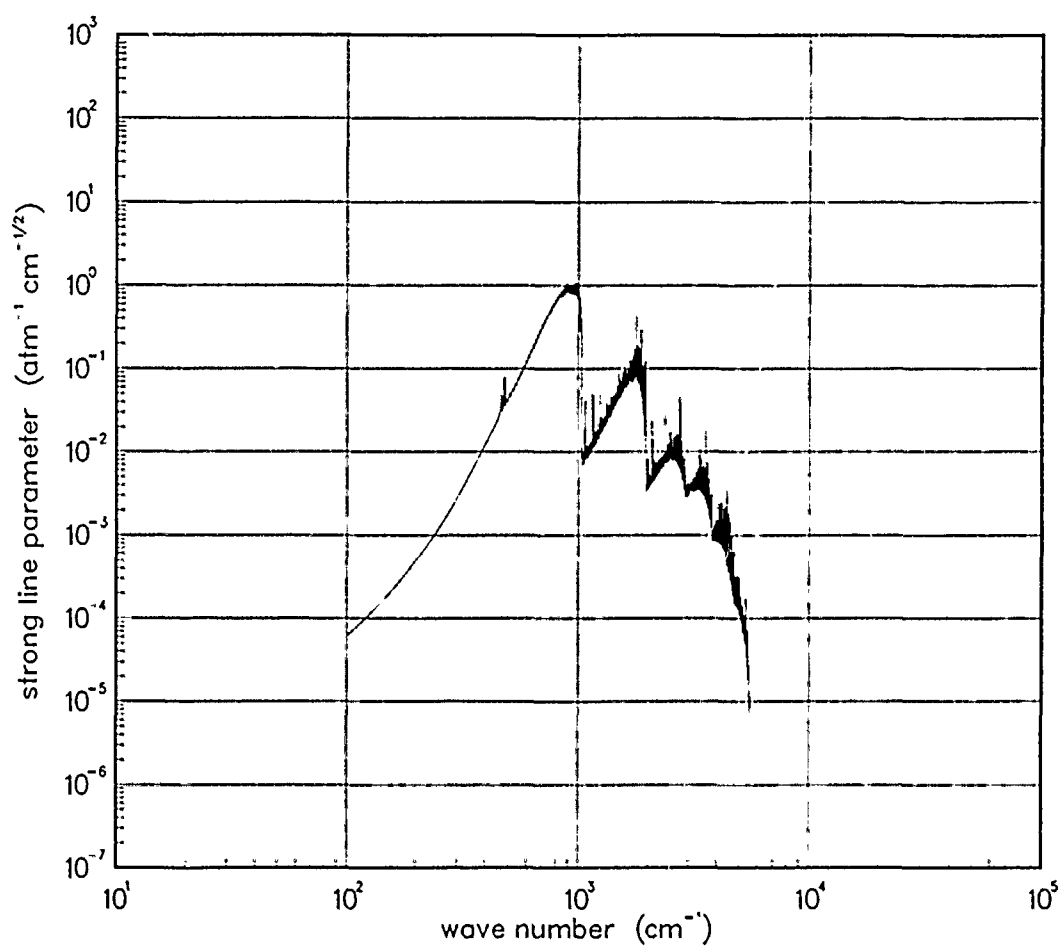


Figure 308. Strong-line parameter for AlO at 3000°K.

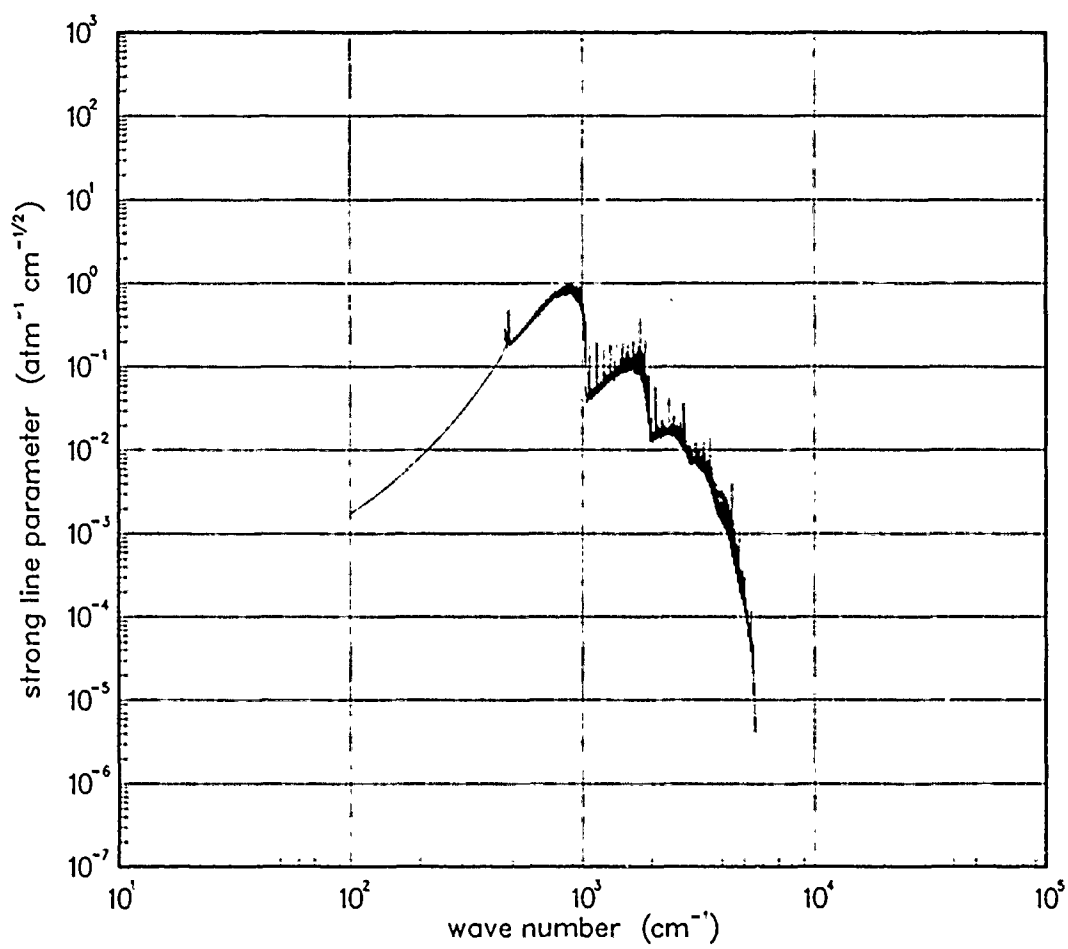


Figure 309. Strong-line parameter for AlO at 5000°K.

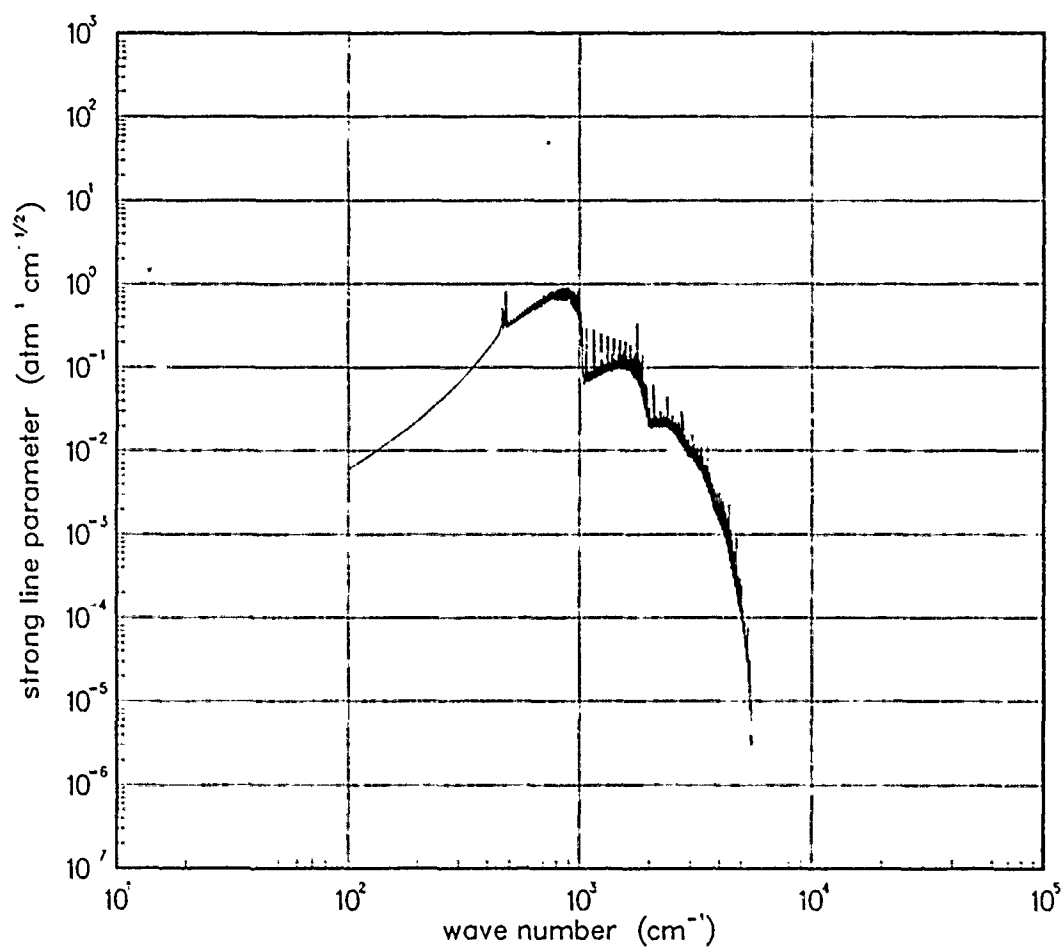


Figure 310. Strong-line parameter for Al_2O_3 at 7000°K .

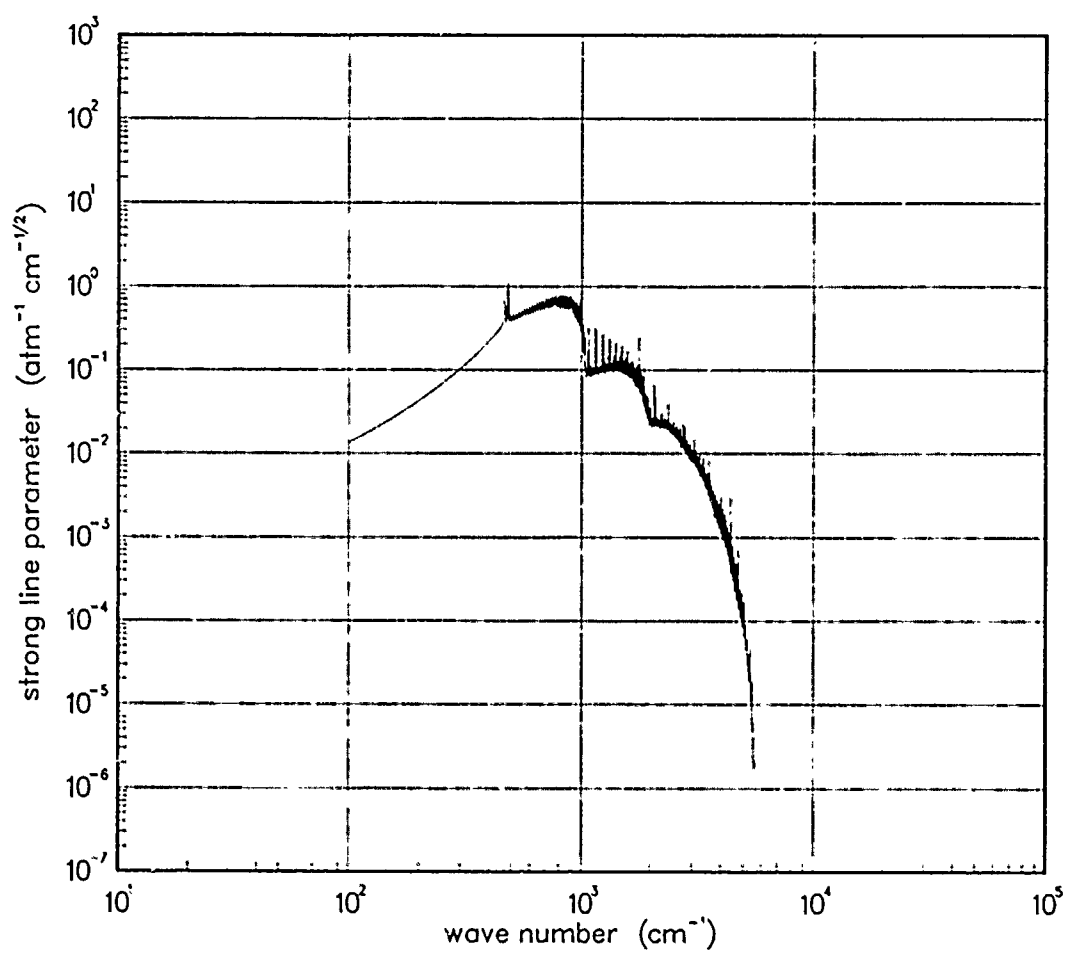


Figure 311. Strong-line parameter for AlO at 10000°K.

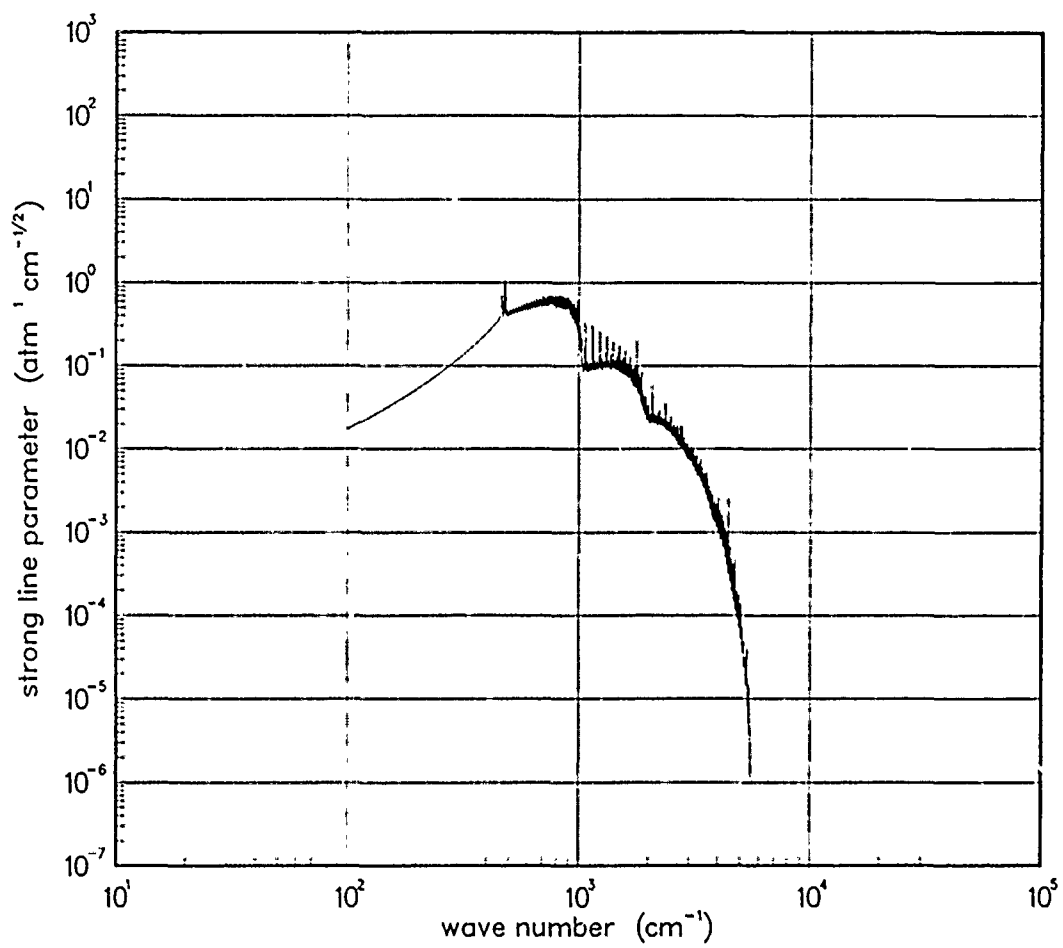


Figure.312. Strong-line parameter for AlO at 12000°K.

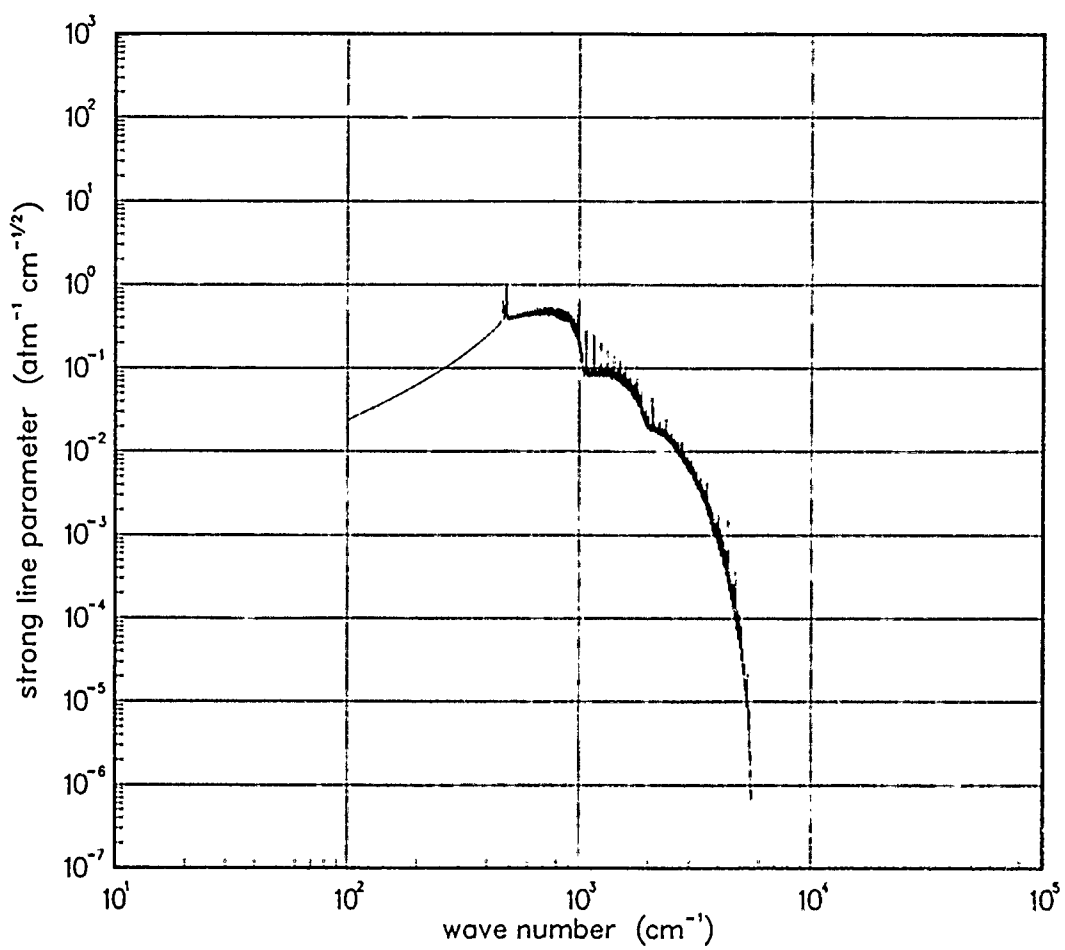


Figure 313. Strong-line parameter for AlO at 18000°K.

6.2 COPPER OXIDE (CuO).

Table 8. Spectroscopic data for CuO.

X $^2\Pi^*$

$$\begin{array}{llll} \omega_e = 633.^{\dagger} & \omega_e x_e = 4.5^{\dagger} & A_e = 275.00^{\dagger} \\ \alpha_e = .0058^{\ddagger} & A_e = 275.0^{\dagger} & B_e = 0.53530^{\ddagger} & E_e = 0.0 \end{array}$$

$$S_{10} = 450.^{\ddagger}$$

$$\gamma_t(300^{\circ}\text{K}) = 0.04^{\S}$$

Data Source:

*A. Antic-Jovanovic, D.S. Pesic, and A.G. Gaydon, Proc. Roy. 307 399 (1968).

† J.S. Shirk, and A.M. Bass, J. Chem. Phys. 52 (1970).

‡ T.L. Stephens, and J.G. DeVore, Band Models for Calculating Fireball Thermal Emission (U) , 71TMP-35, General Electric-TEMPO, Santa Barbara, California (May 1971).

§ Estimate.

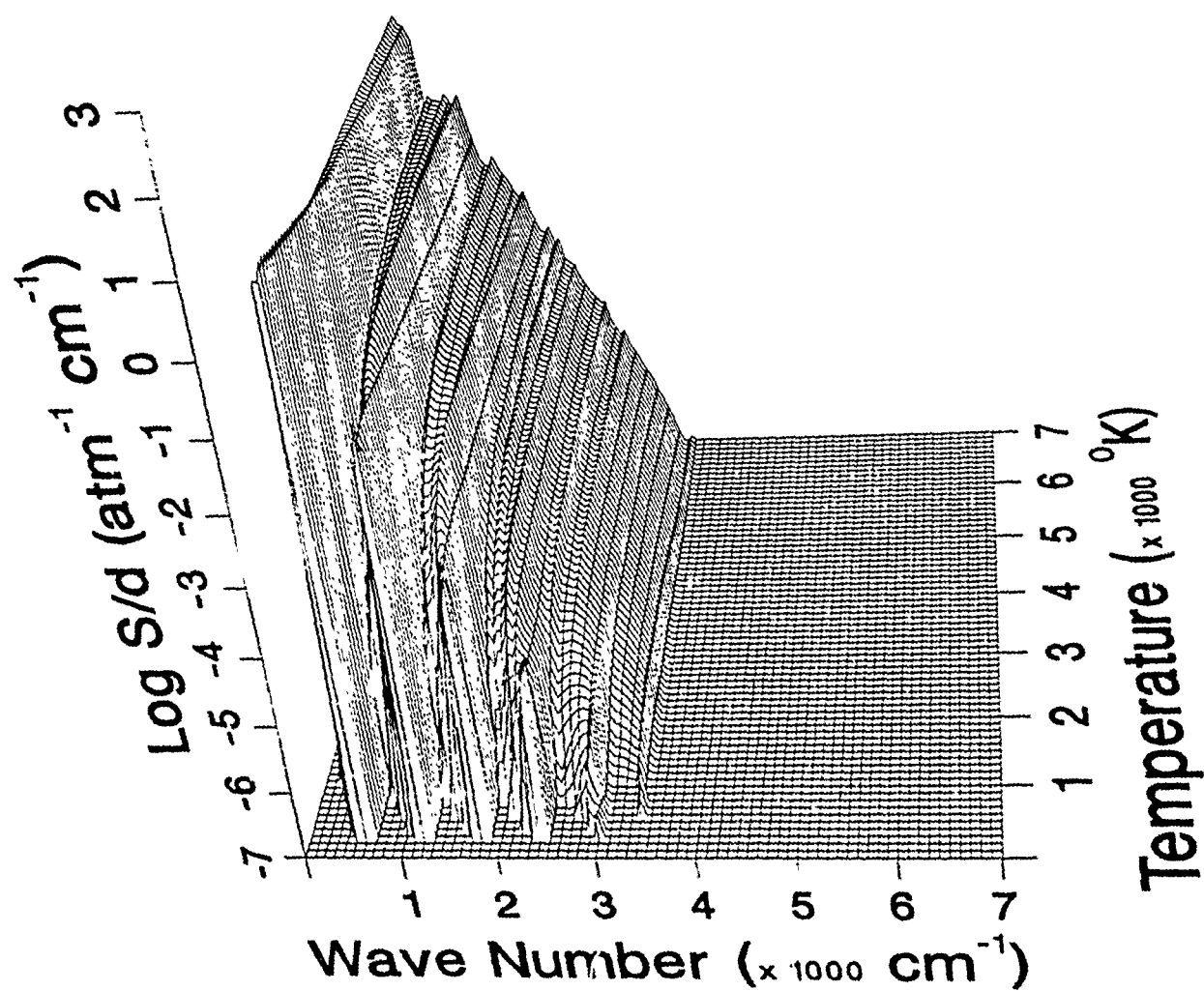


Figure 314. Weak-line parameter for CuO.

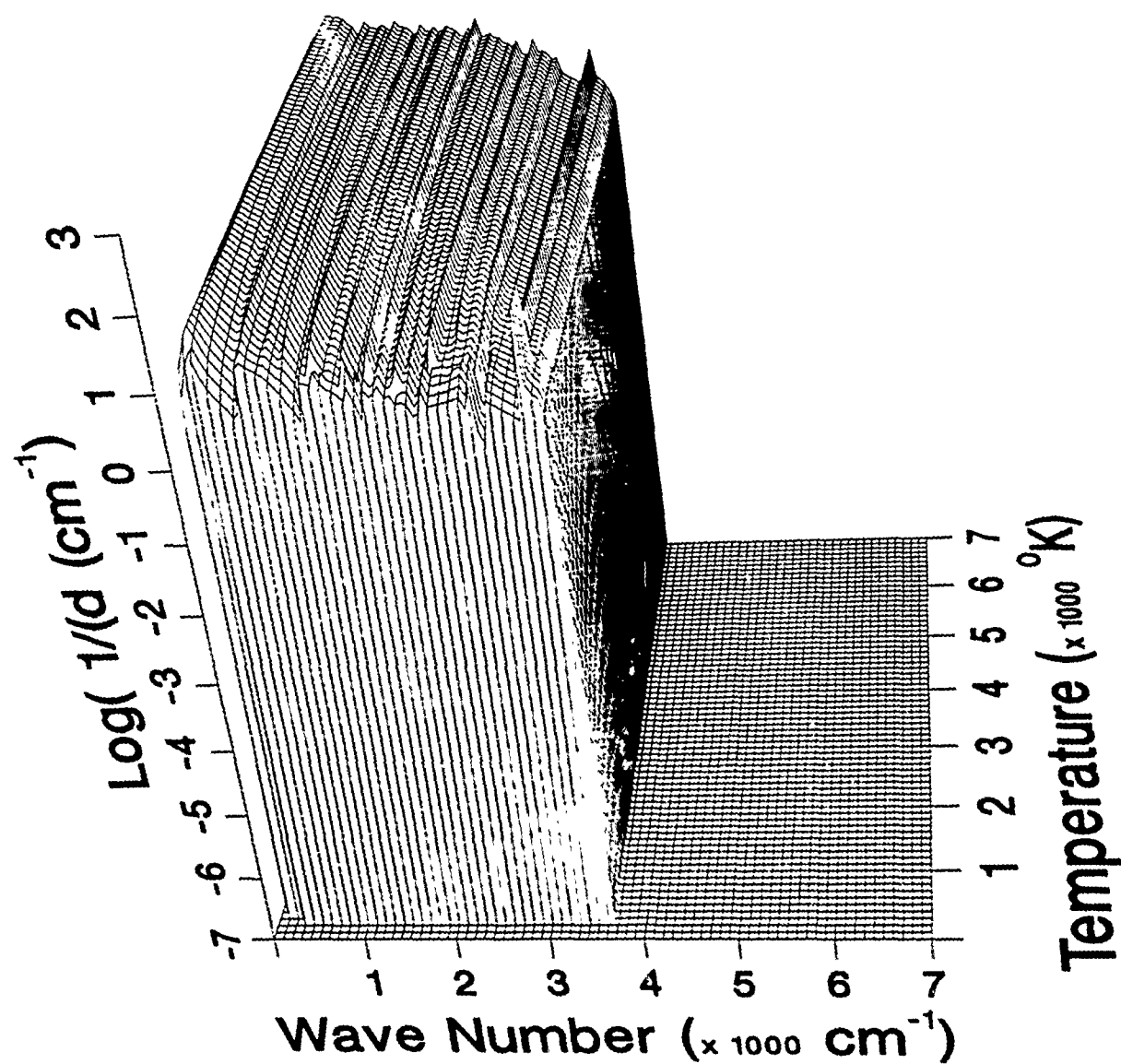


Figure 315. Inverse line spacing for CuO.

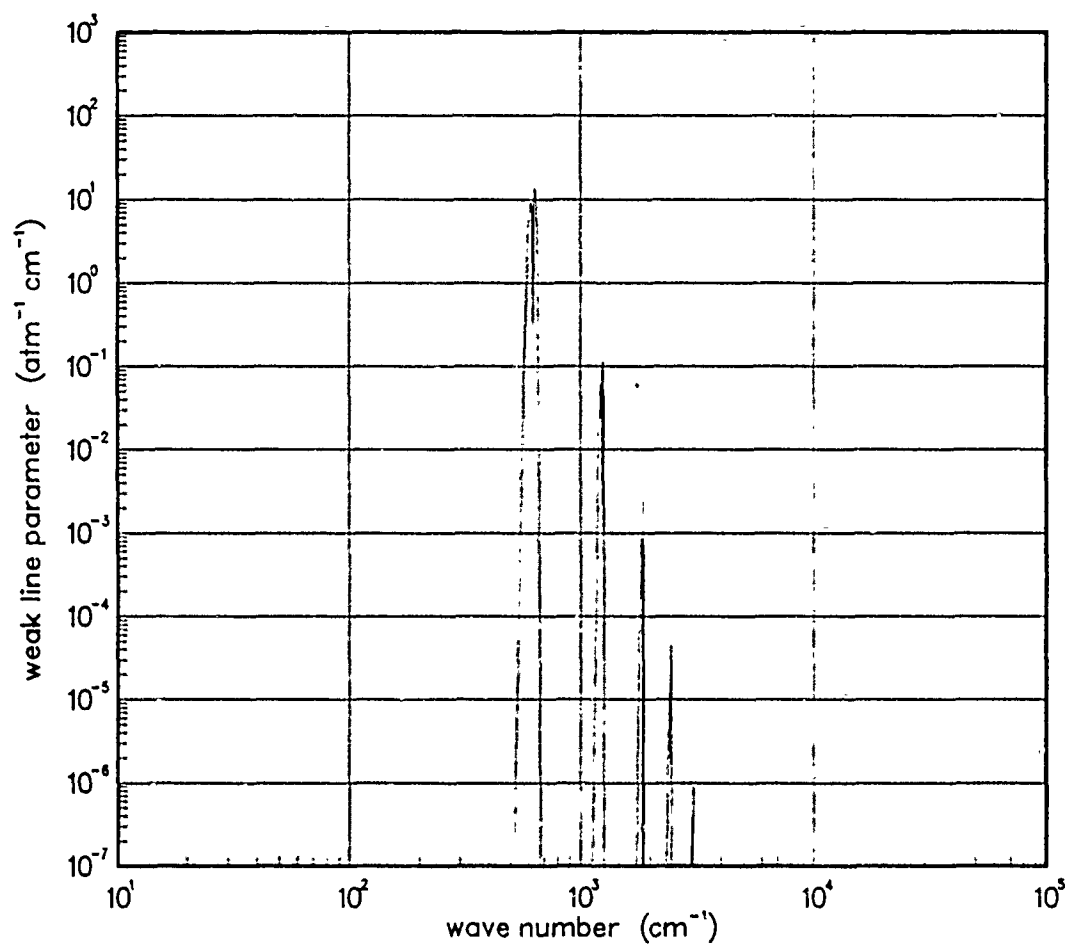


Figure 316. Weak-line parameter for CuO at 200°K.

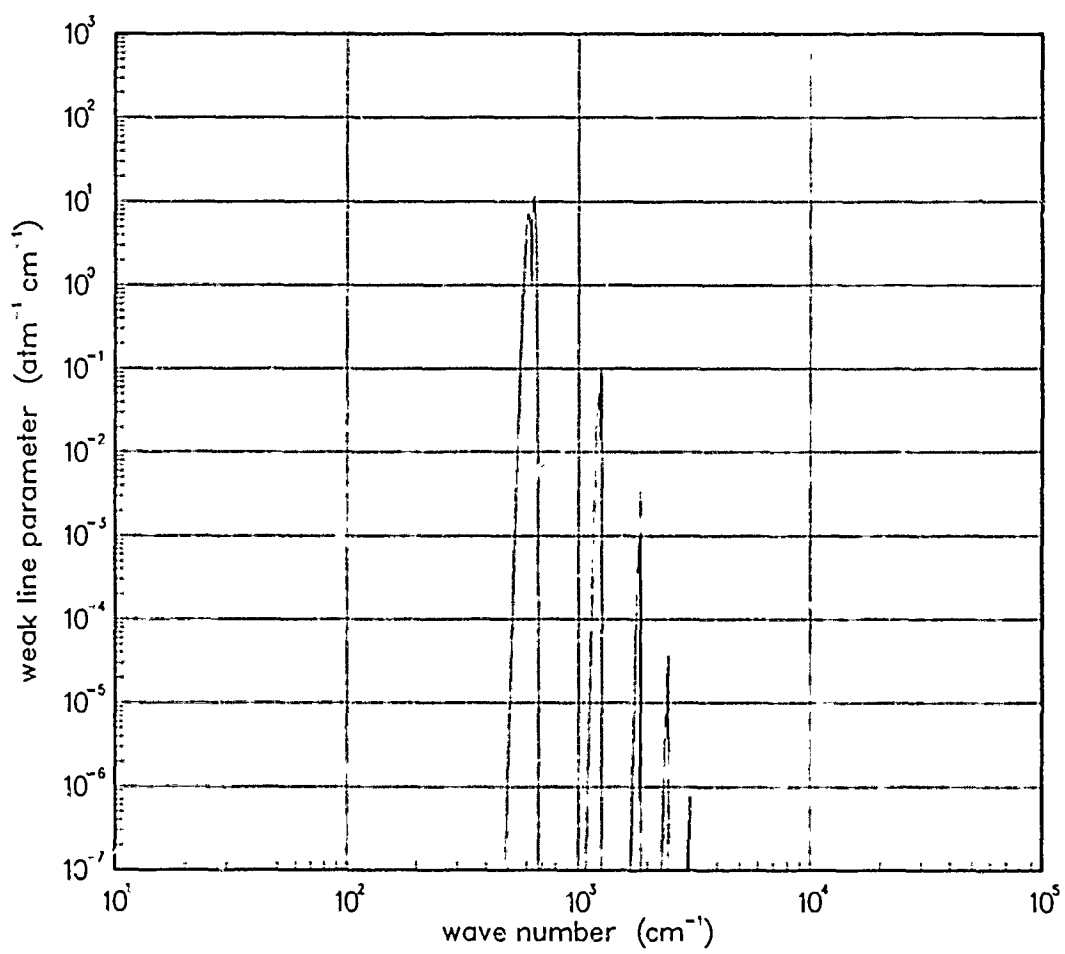


Figure 317. Weak-line parameter for CuO at 300°K.

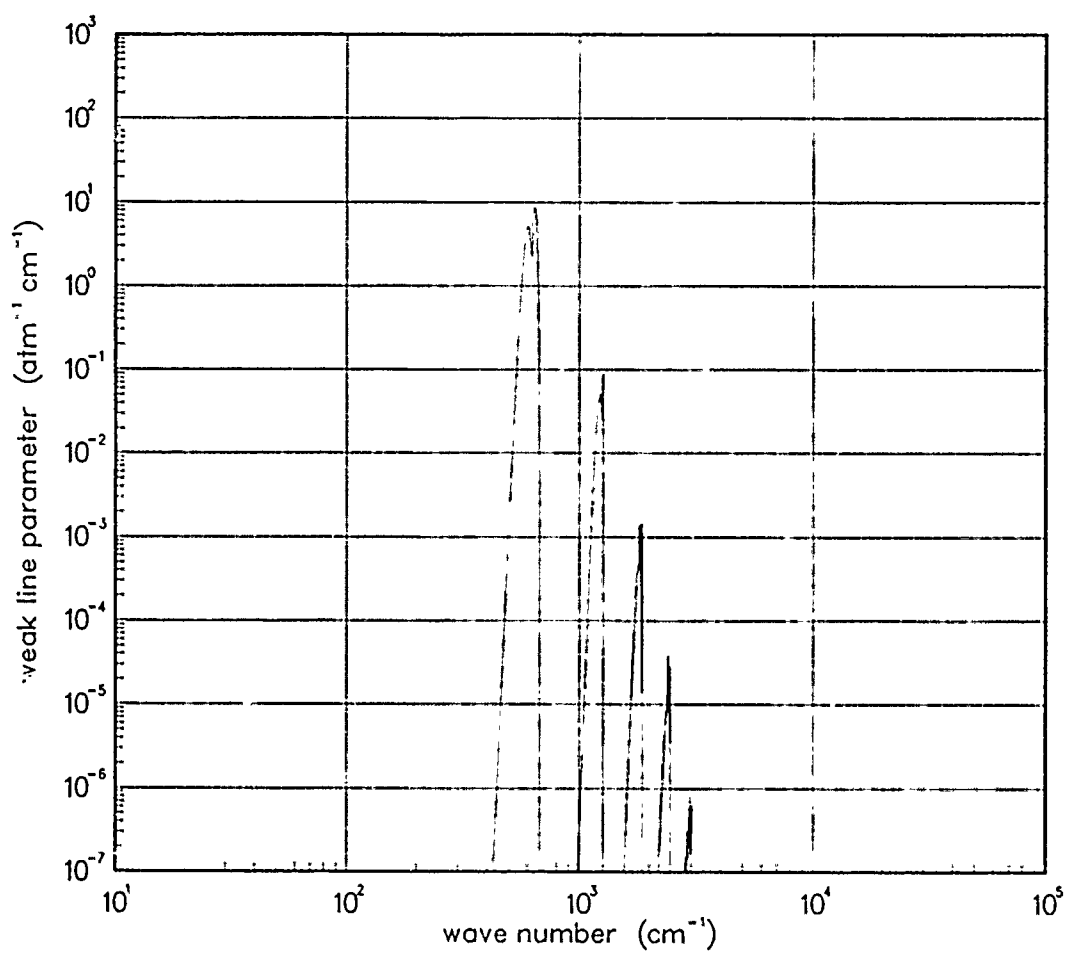


Figure 318. Weak-line parameter for CuO at 500°K.

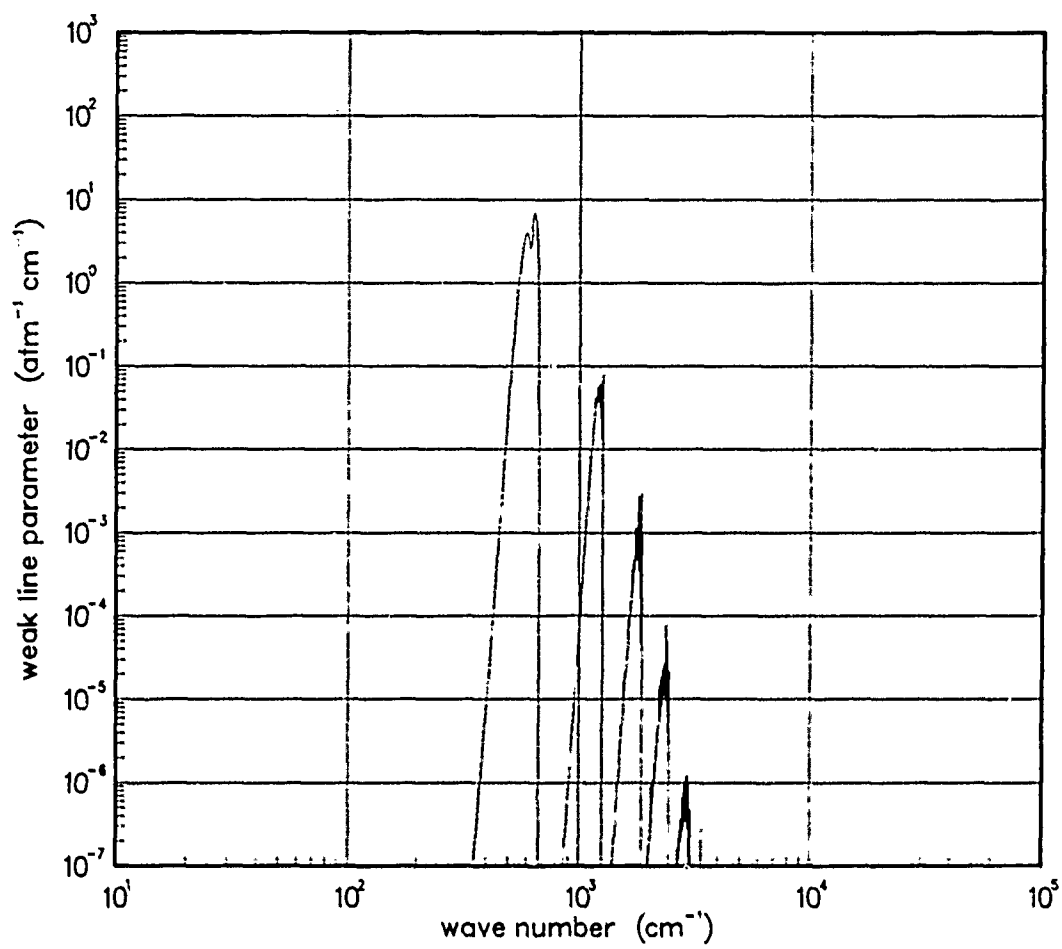


Figure 319. Weak-line parameter for CuO at 750°K.

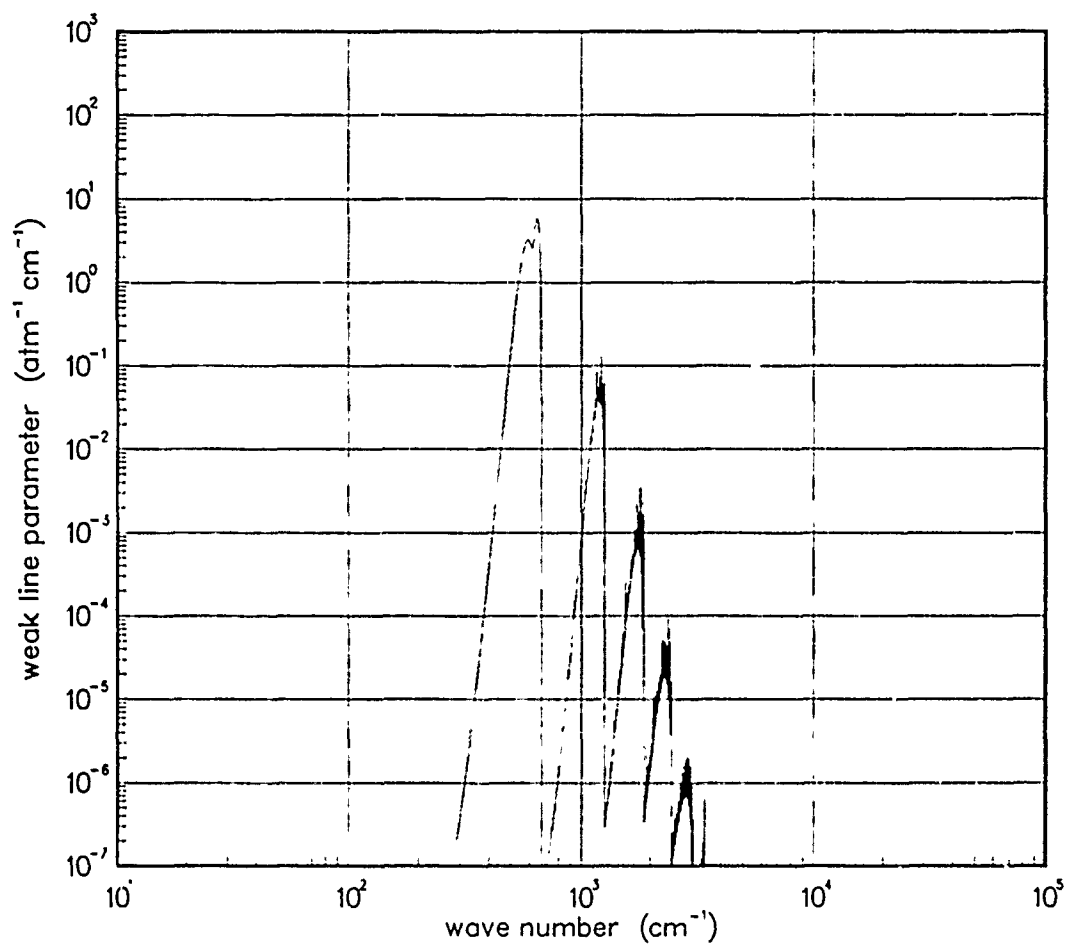


Figure 320. Weak-line parameter for CuO at 1000°K.

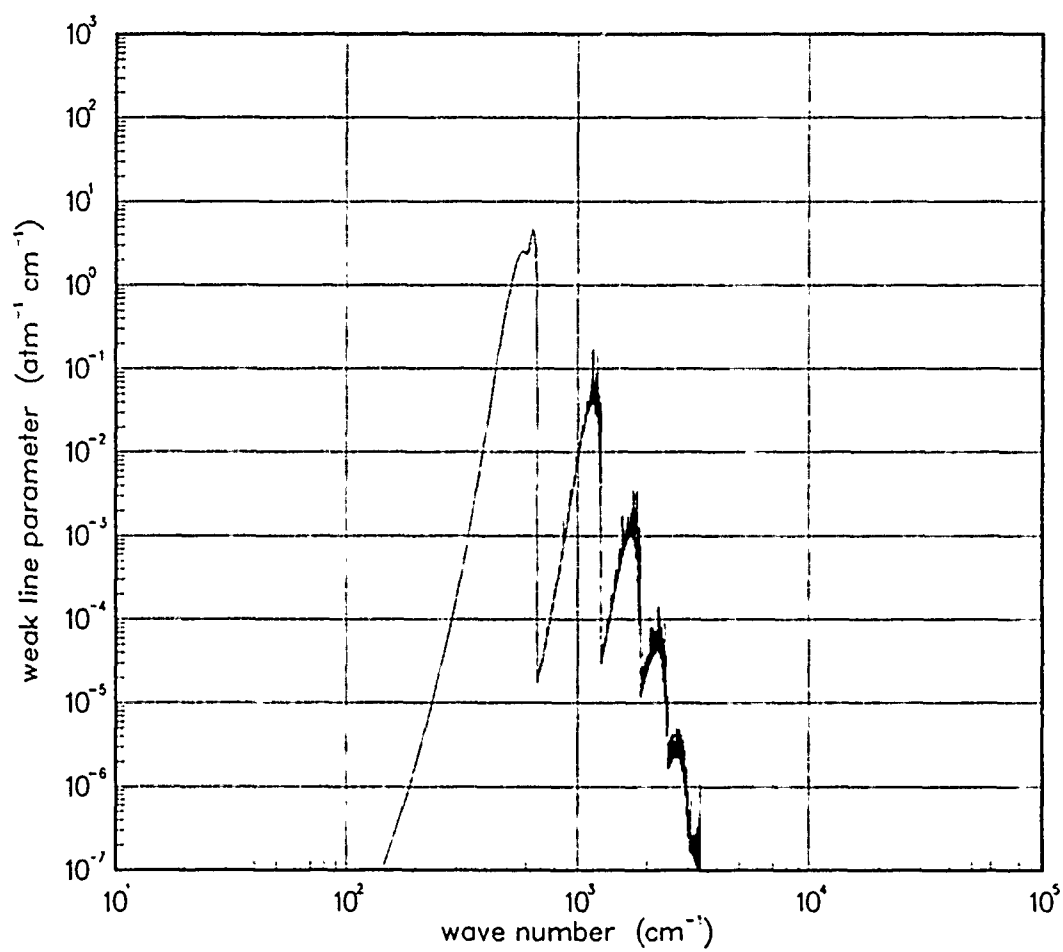


Figure 321. Weak-line parameter for CuO at 1500°K.

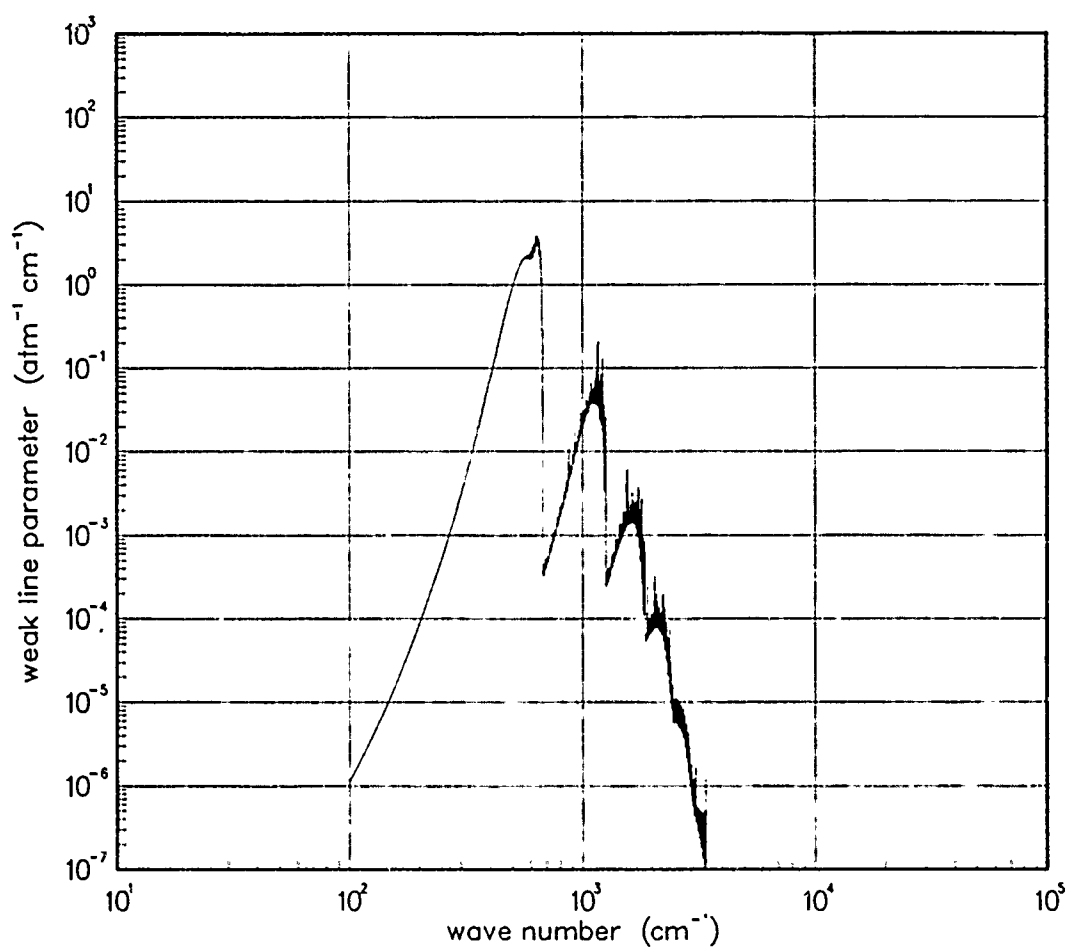


Figure 322. Weak-line parameter for CuO at 2000°K.

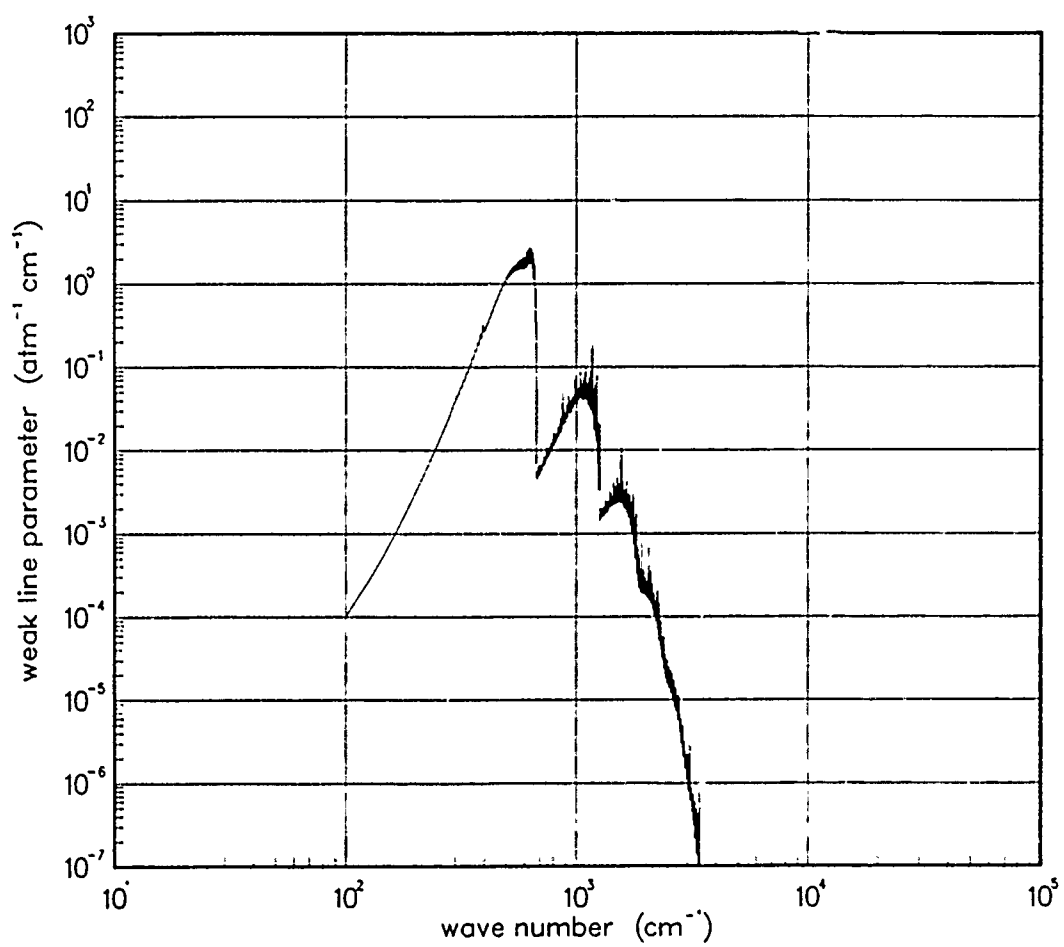


Figure 323. Weak-line parameter for CuO at 3000°K.

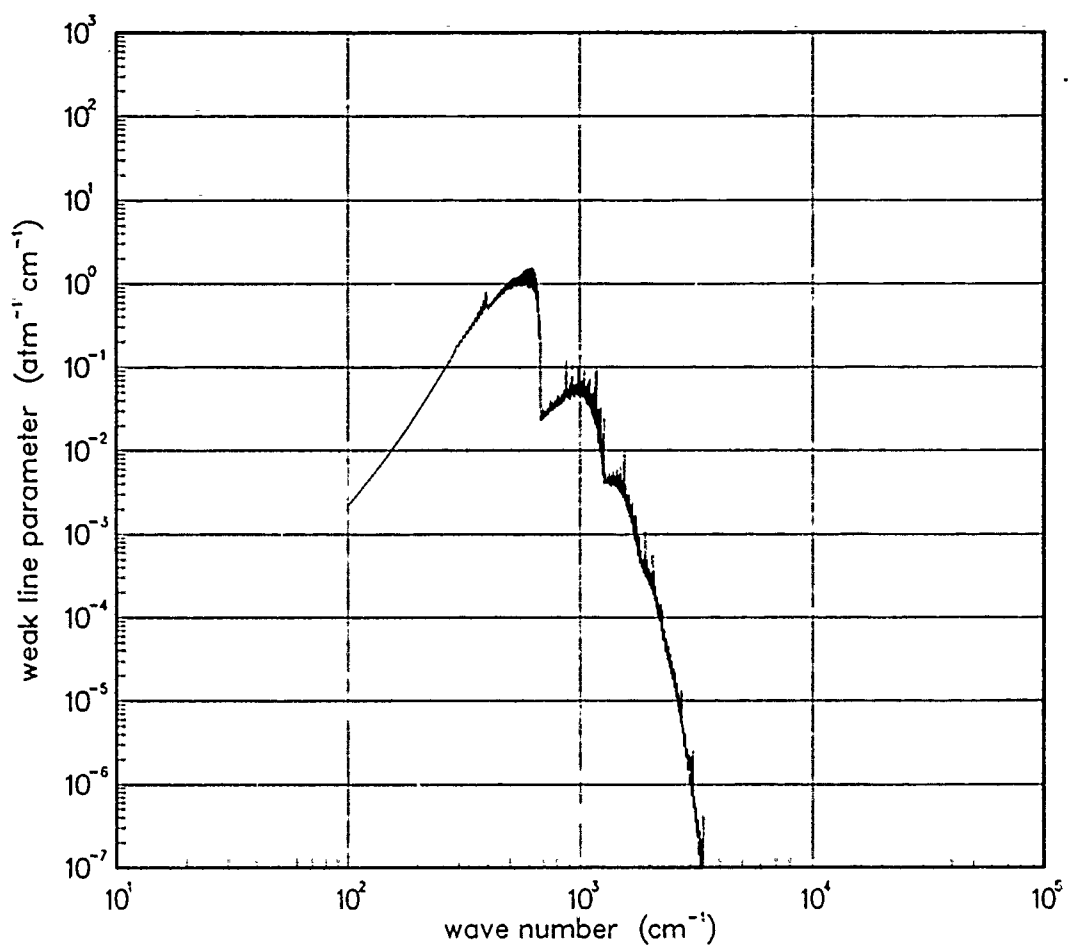


Figure 324. Weak-line parameter for CuO at 5000°K.

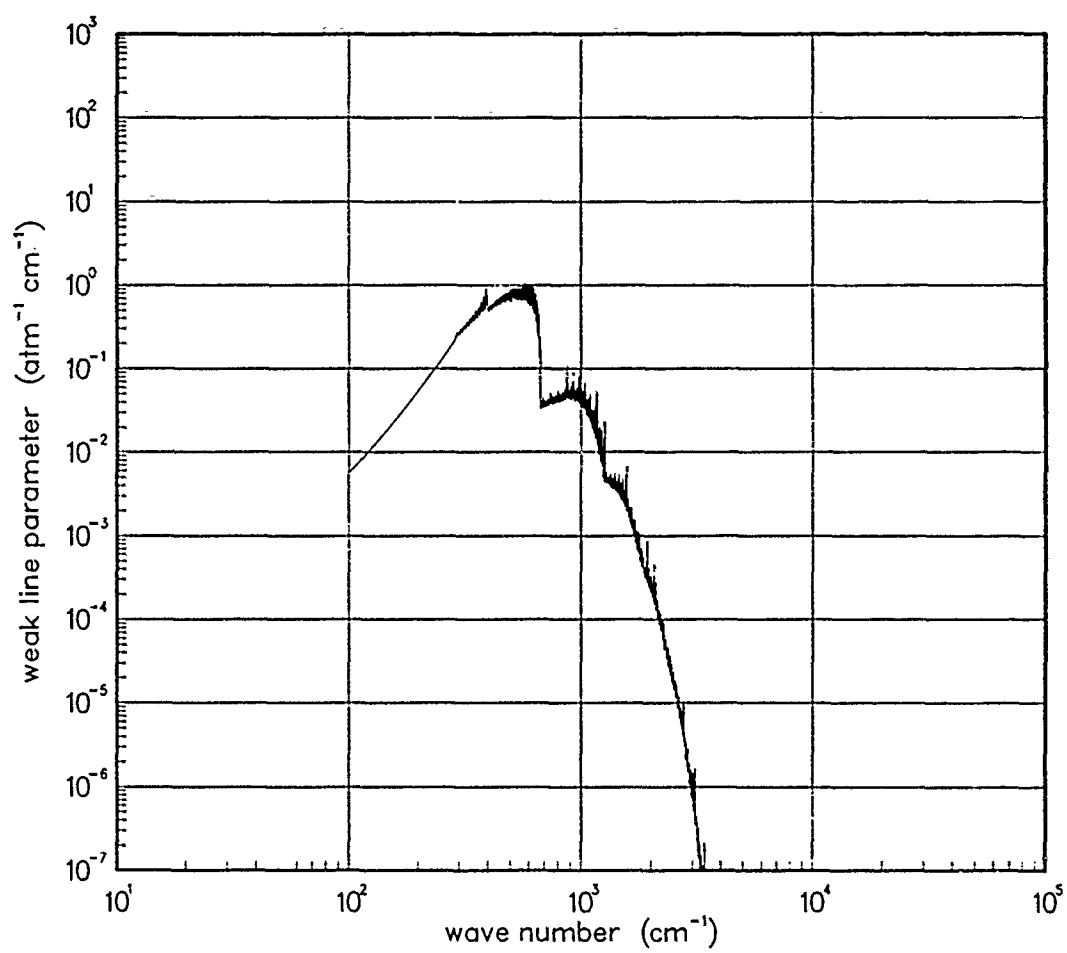


Figure 325. Weak-line parameter for CuO at 7000°K.

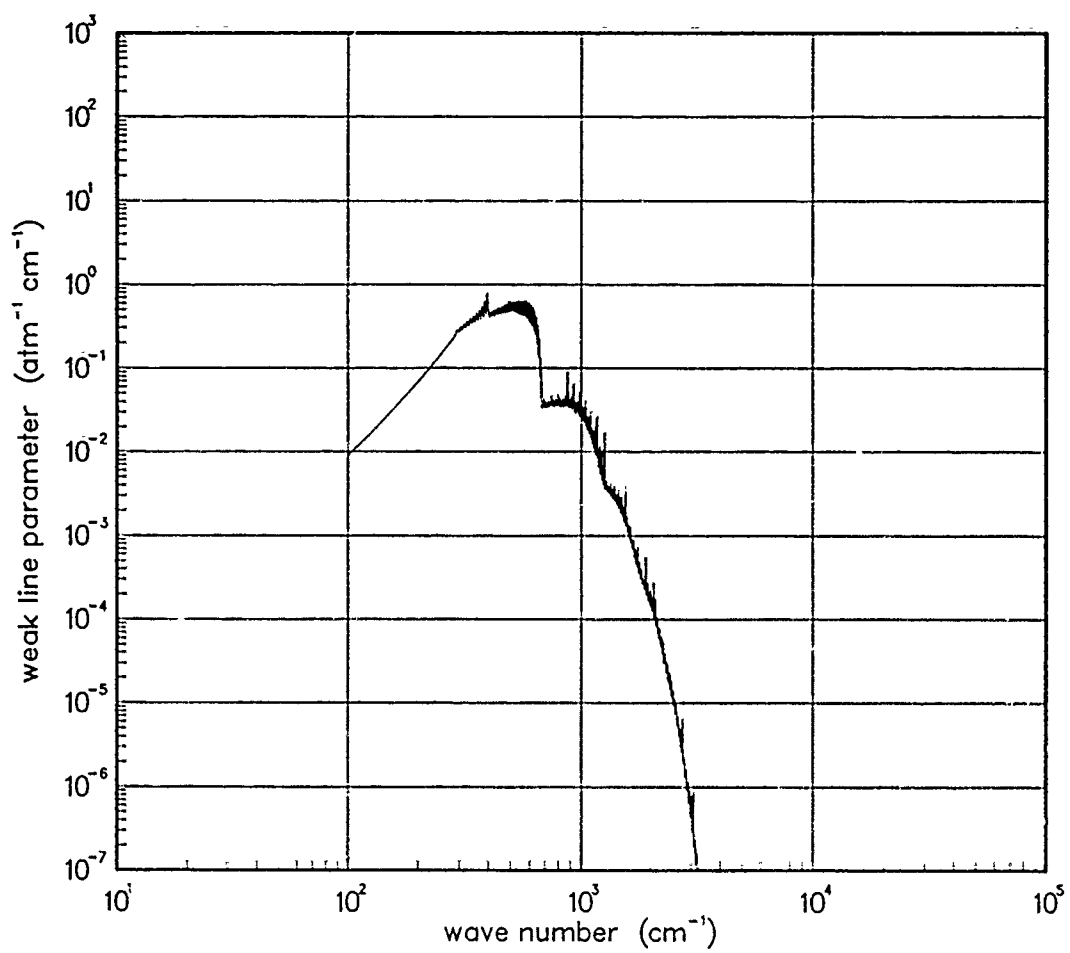


Figure 326. Weak-line parameter for CuO at 10000°K.

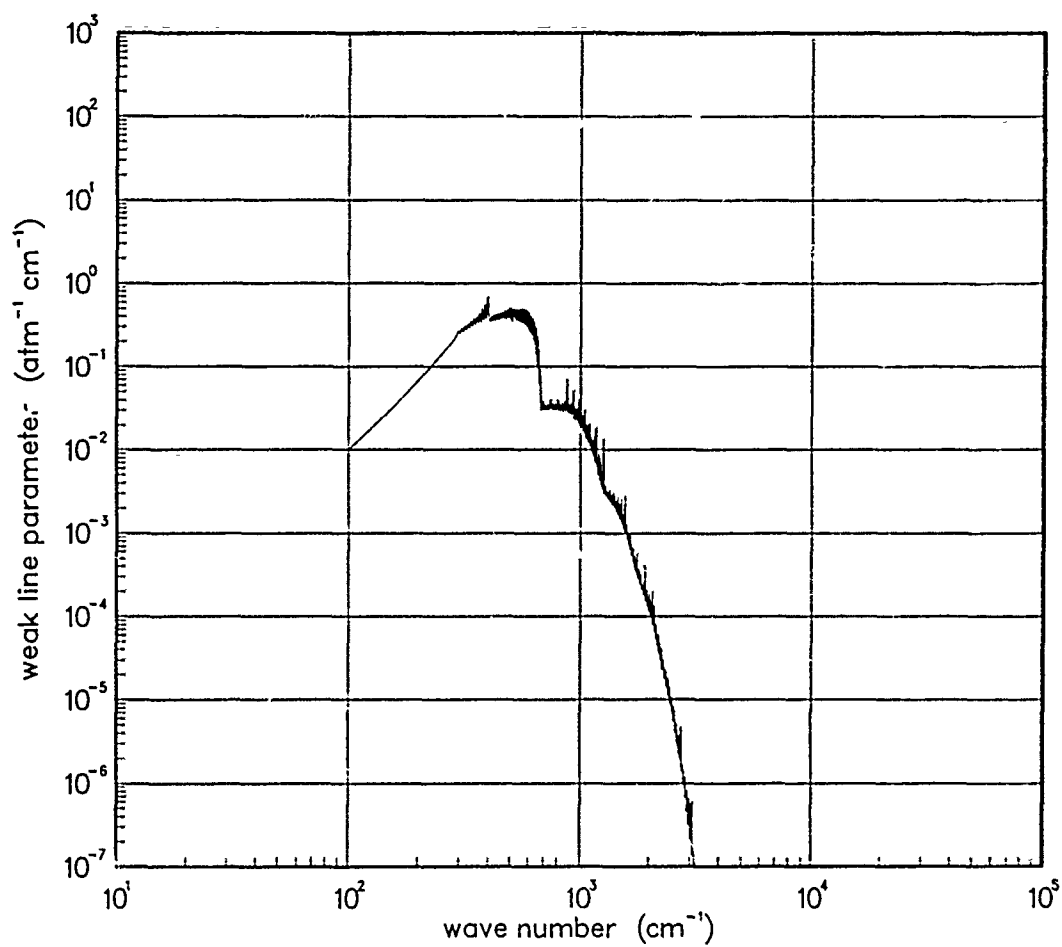


Figure 327. Weak-line parameter for CuO at 12000°K.

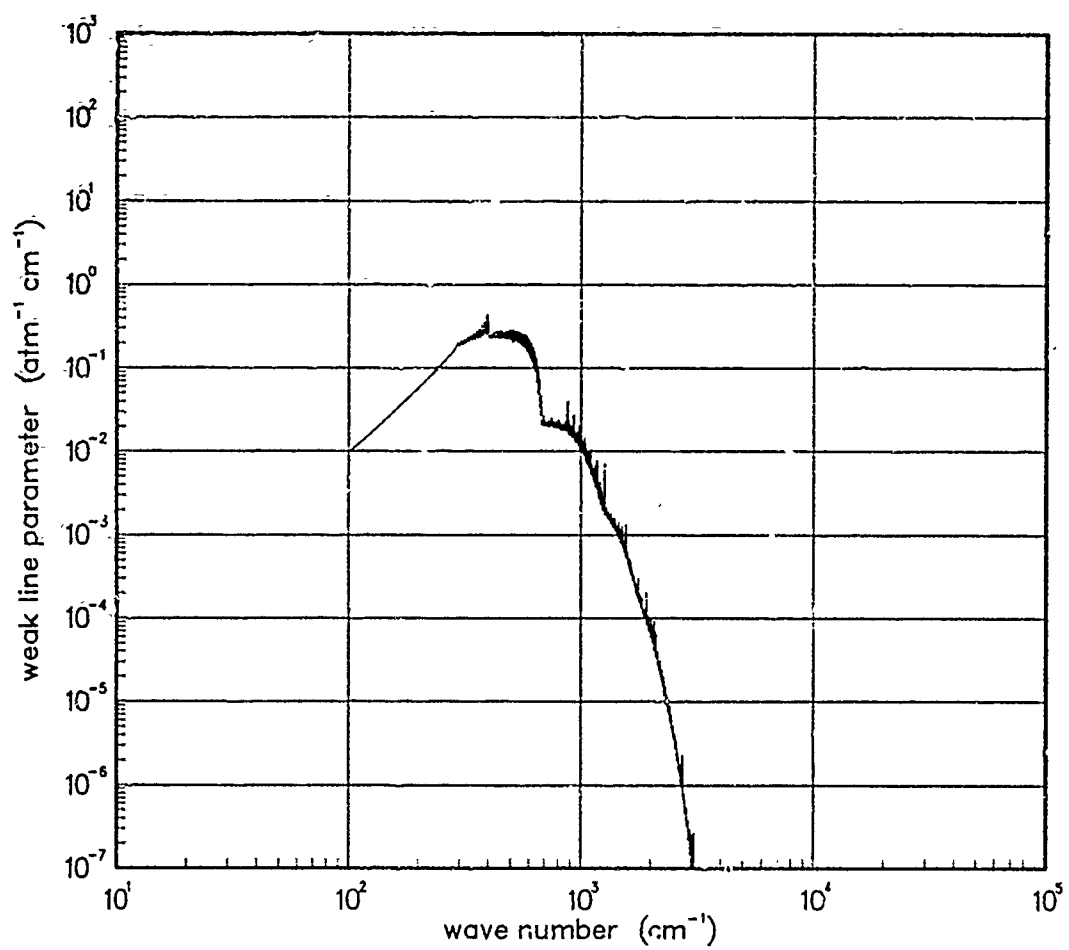


Figure 328. Weak-line parameter for CuO at 18000°K.

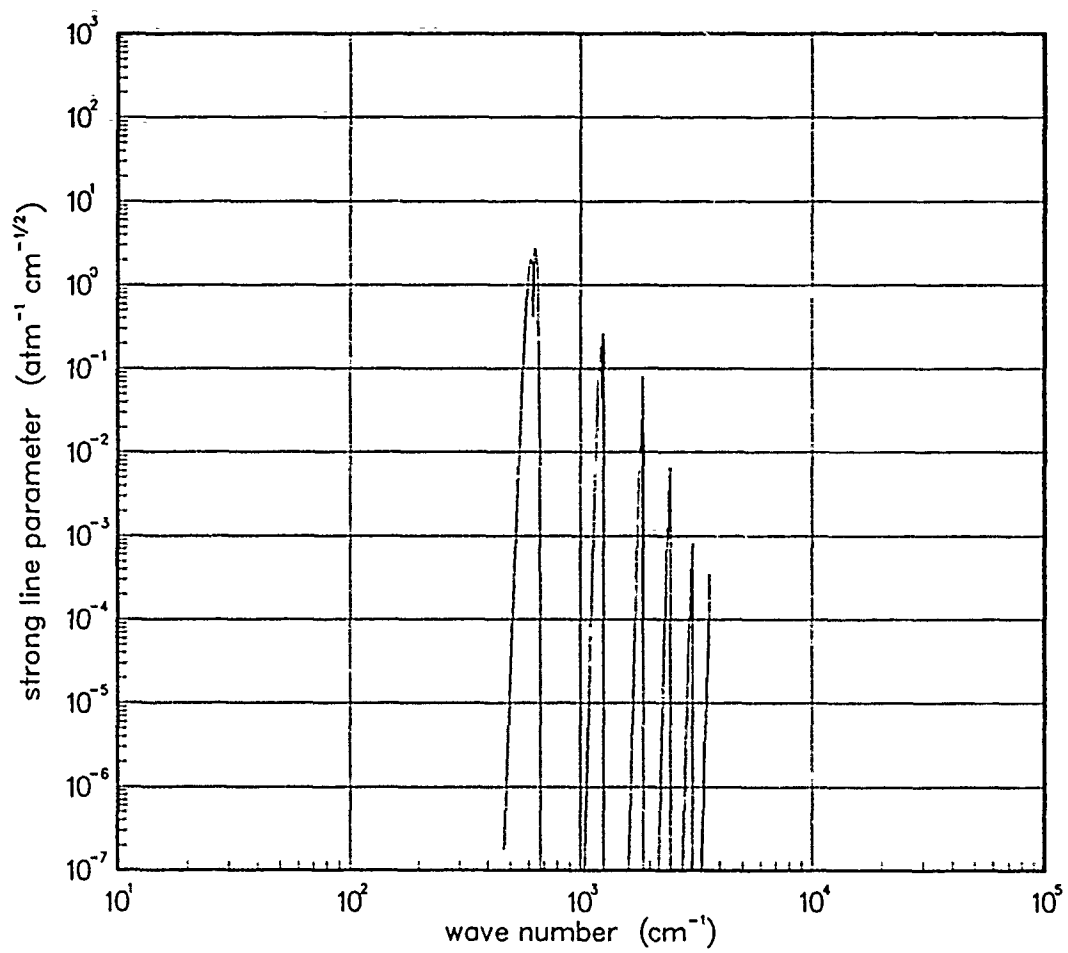


Figure 329. Strong-line parameter for CuO at 200°K.

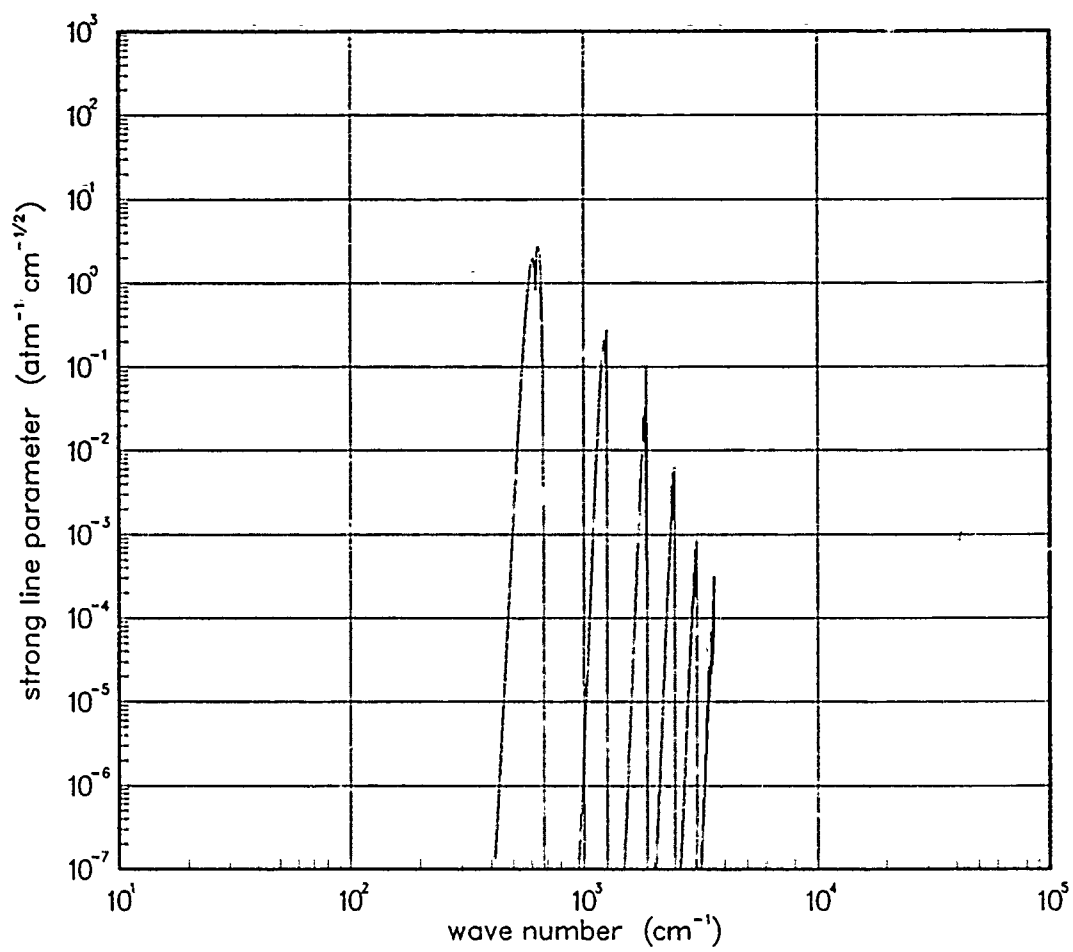


Figure 330. Strong-line parameter for CuO at 300°K.

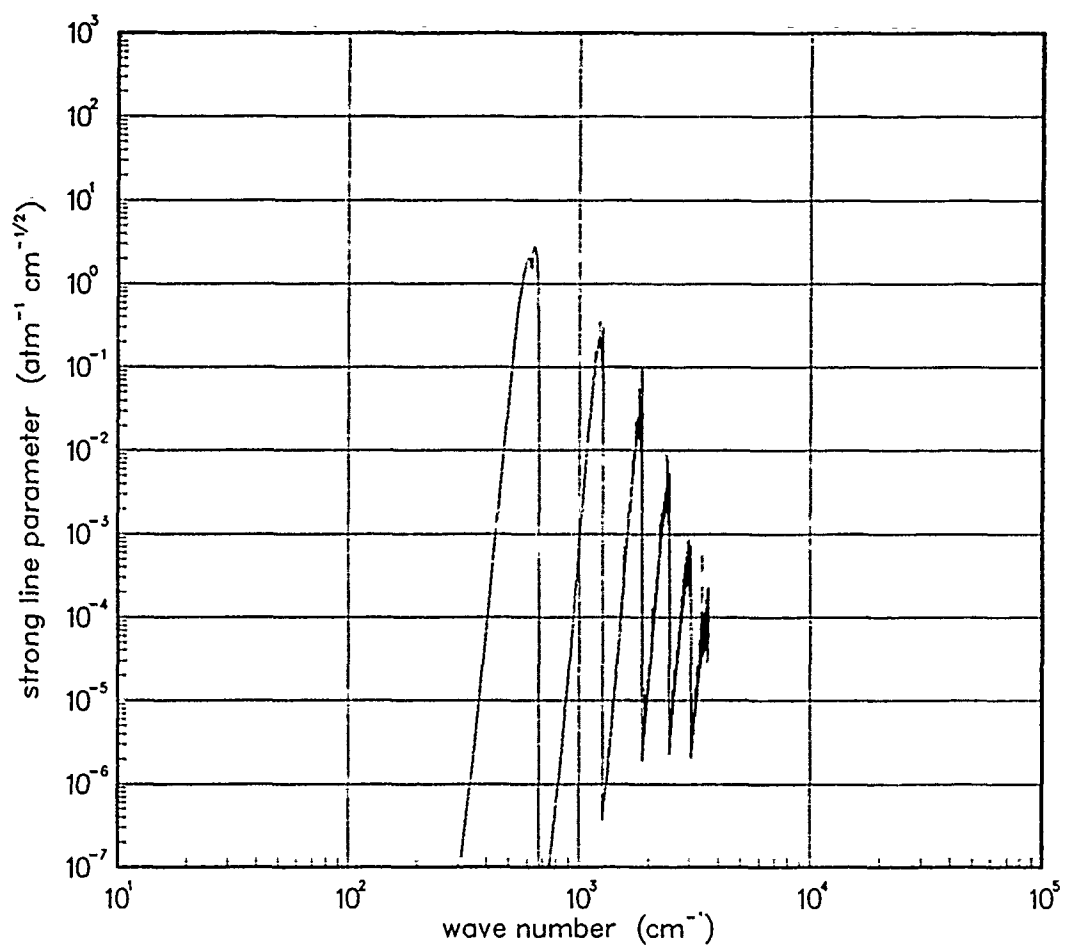


Figure 331. Strong-line parameter for CuO at 500°K.

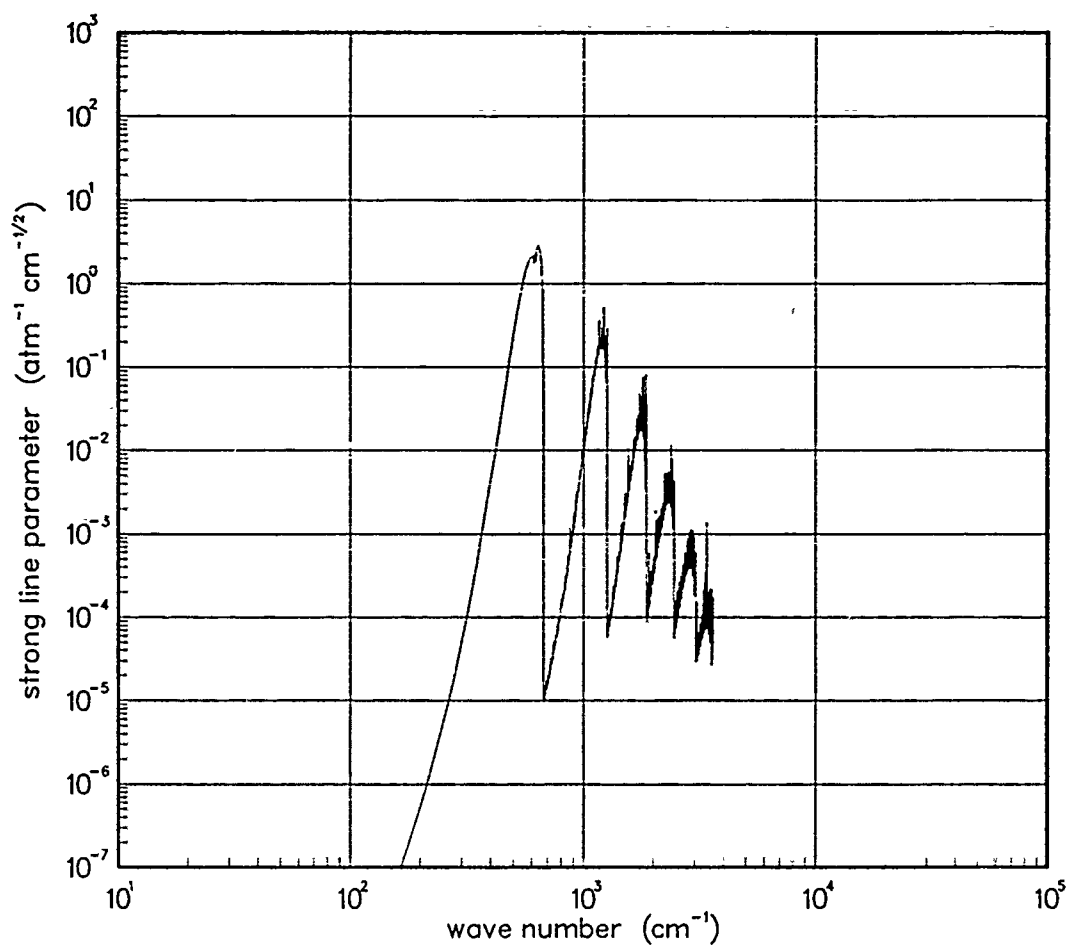


Figure 332. Strong-line parameter for CuO at 750°K.

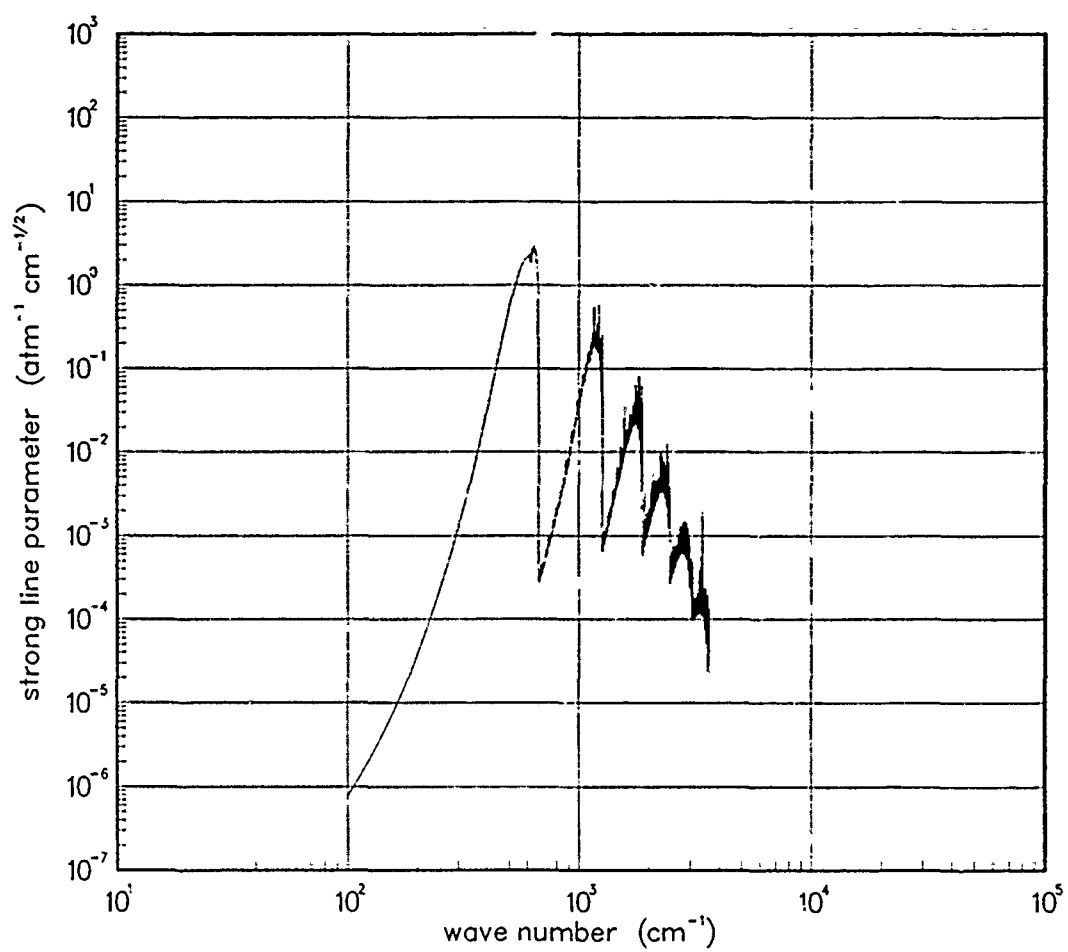


Figure 333. Strong-line parameter for CuO at 1000°K.

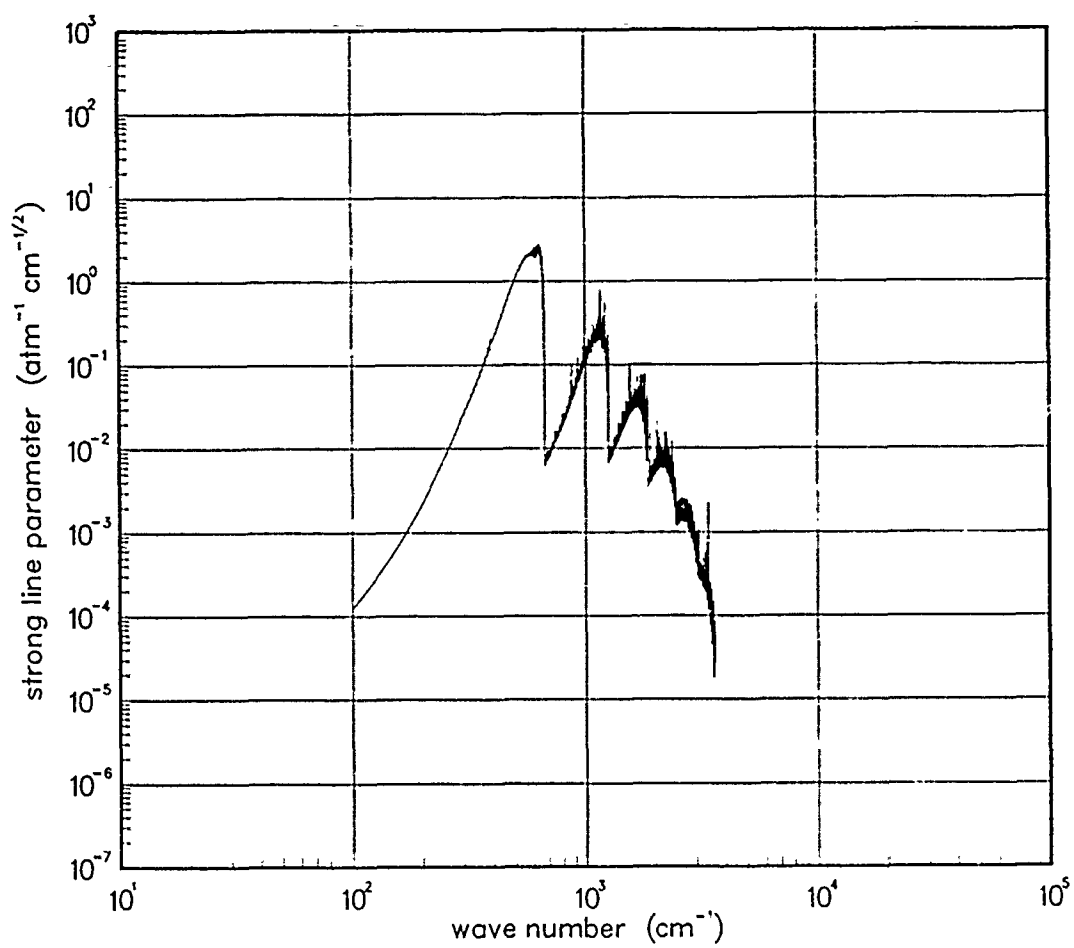


Figure 334. Strong-line parameter for CuO at 1500°K.

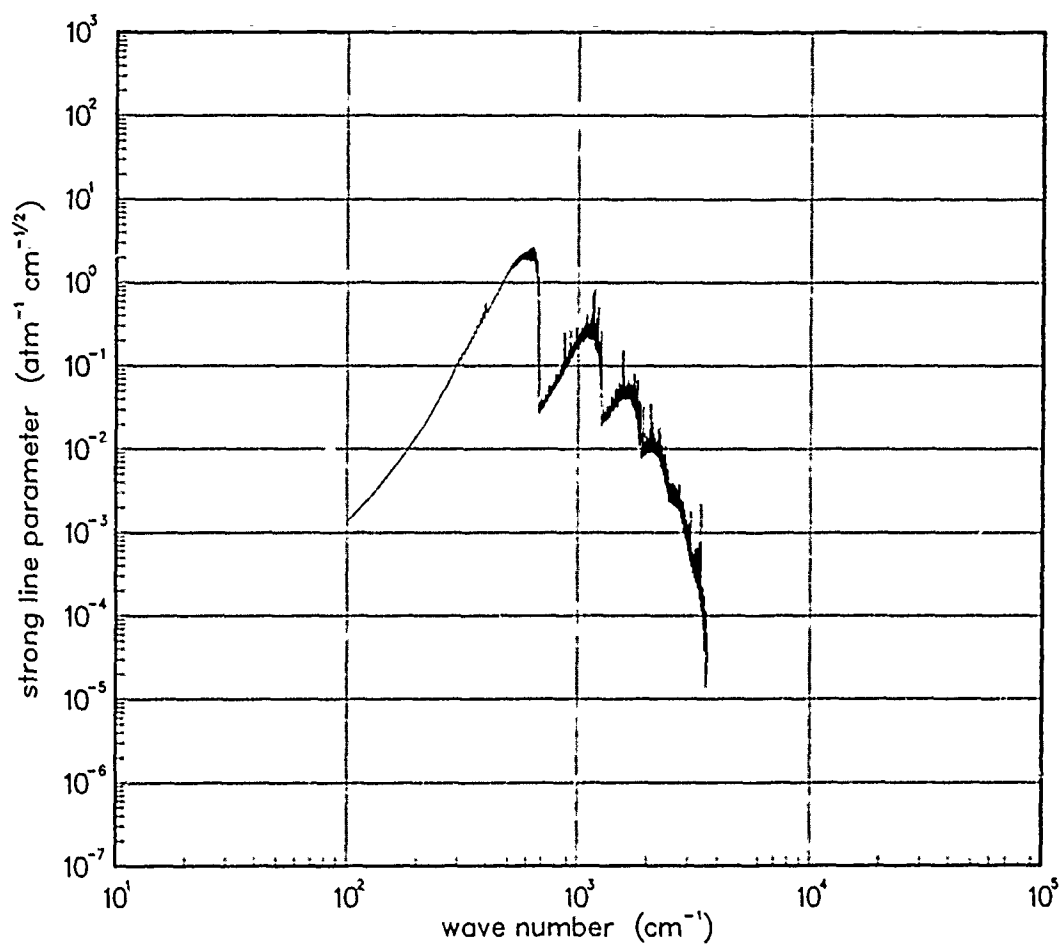


Figure 335. Strong-line parameter for CuO at 2000°K.

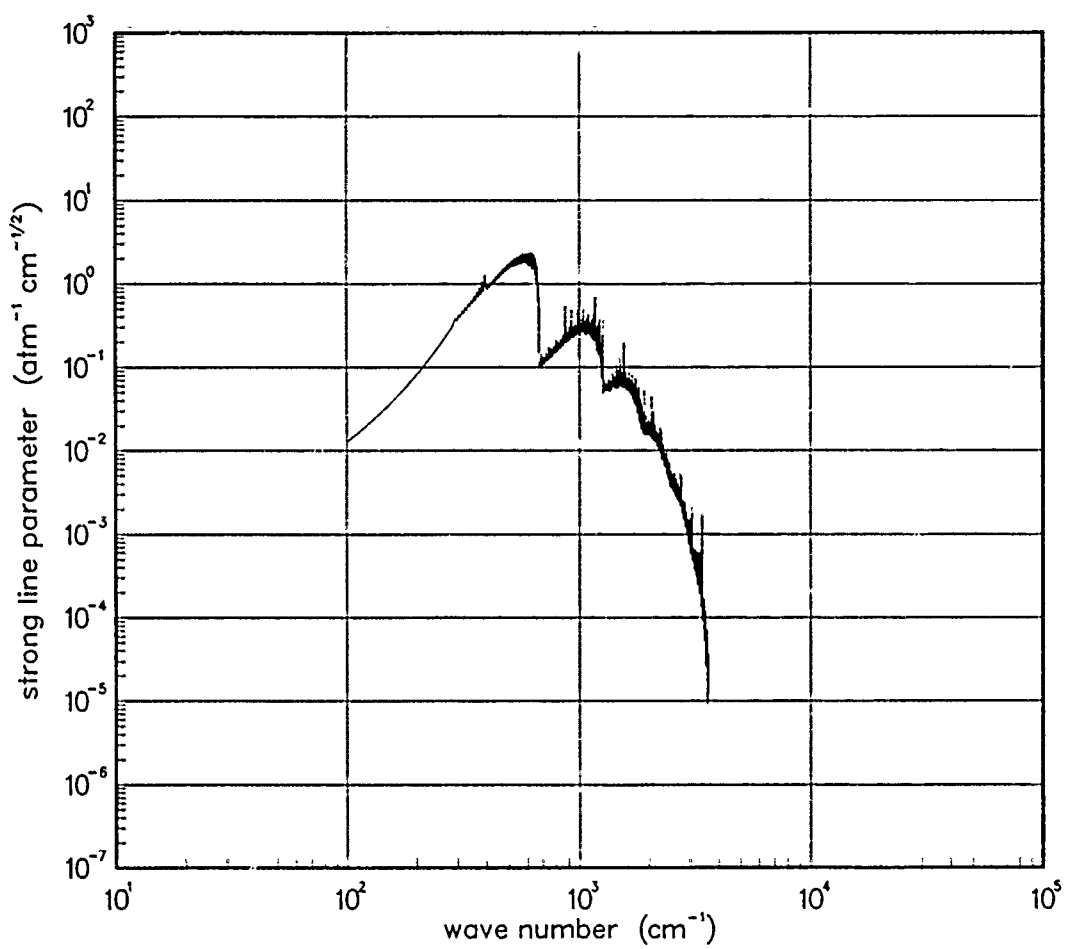


Figure 336. Strong-line parameter for CuO at 3000°K.

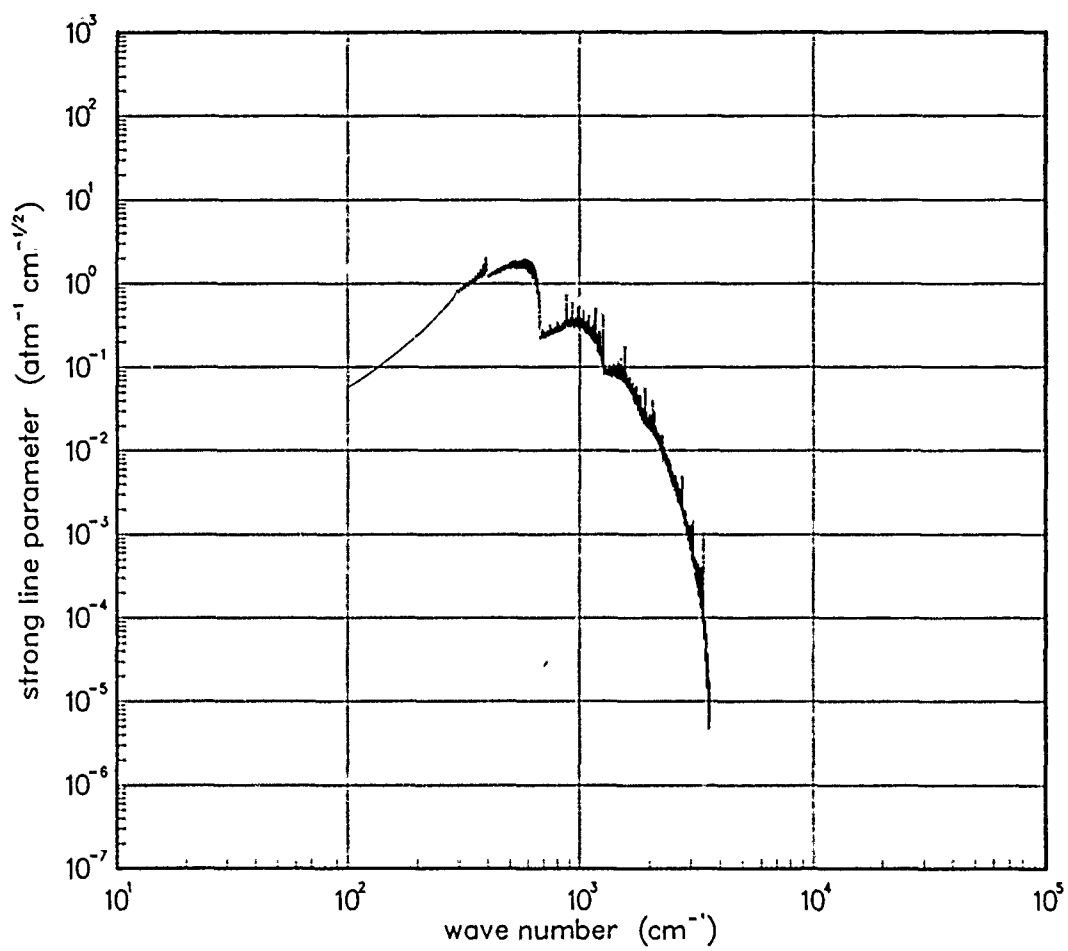


Figure 337. Strong-line parameter for CuO at 5000°K.

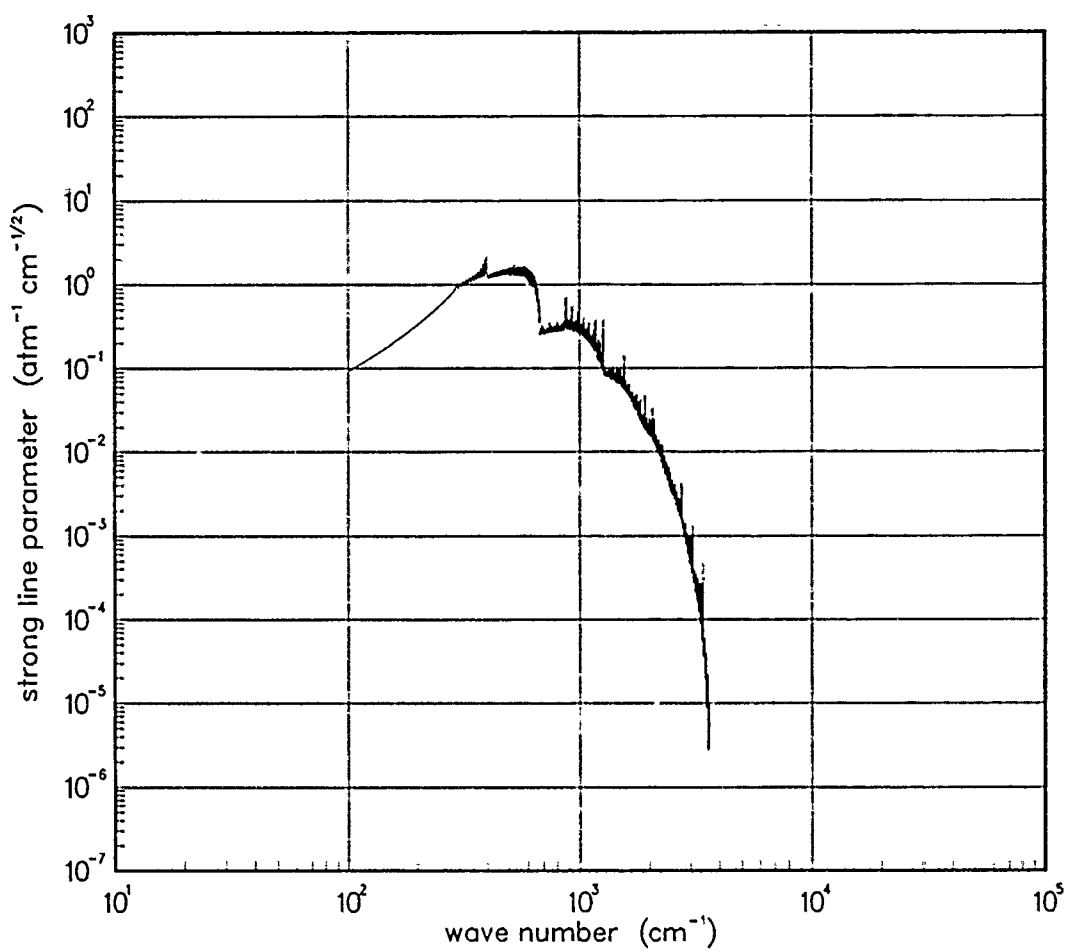


Figure 338. Strong-line parameter for CuO at 7000°K.

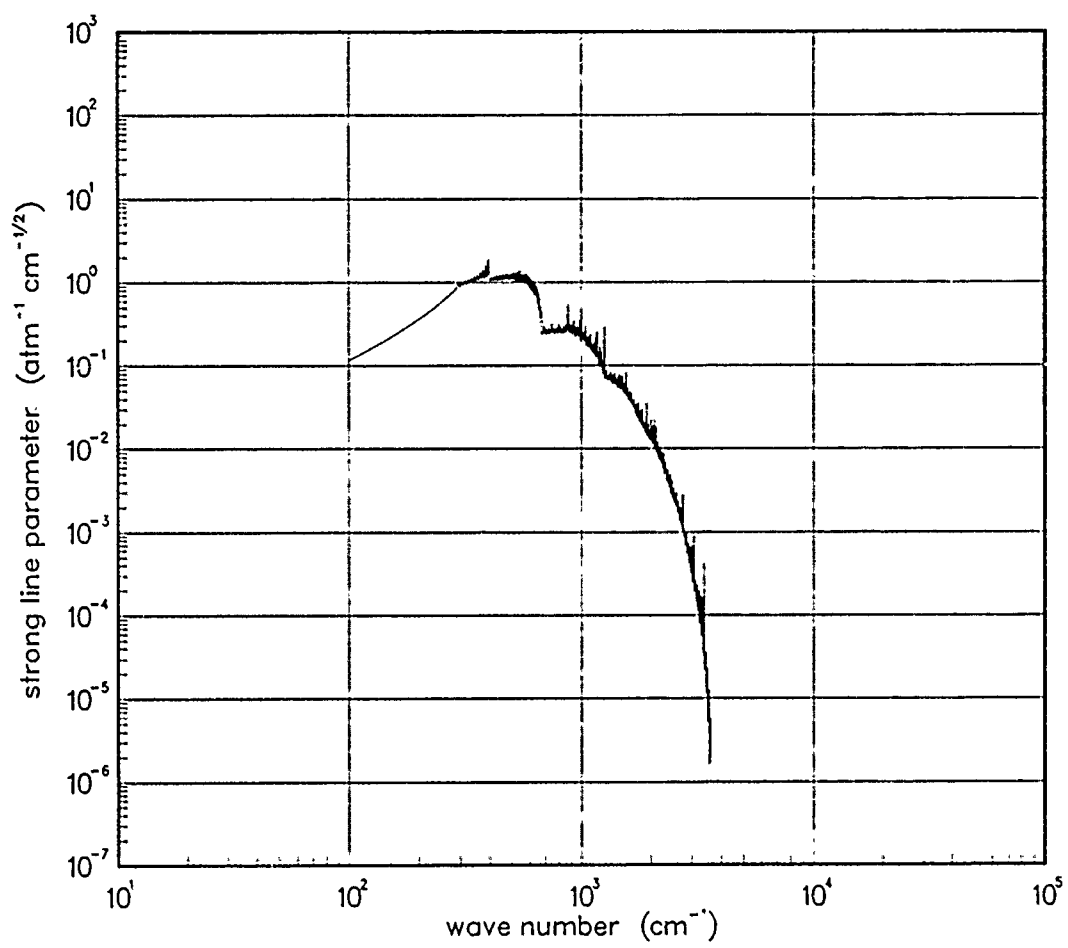


Figure 339. Strong-line parameter for CuO at 10000°K.

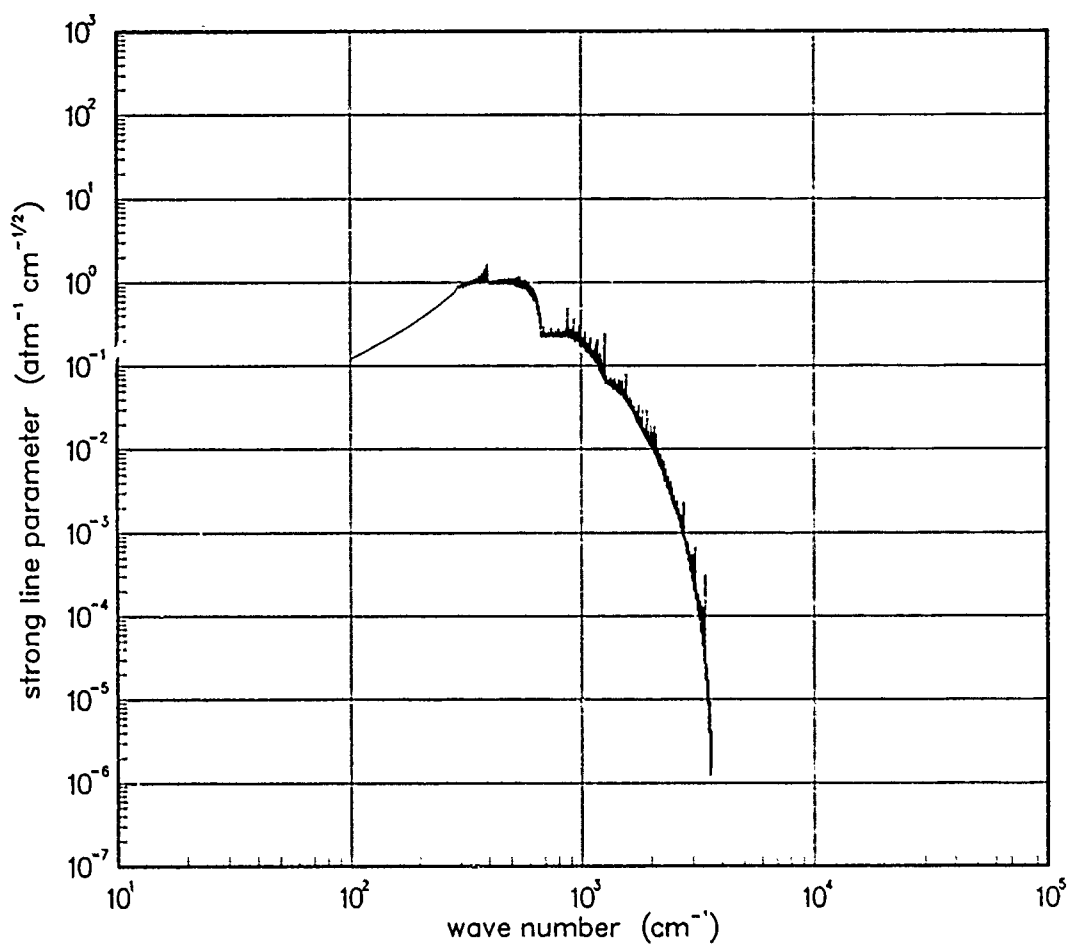


Figure 340. Strong-line parameter for CuO at 12000°K.

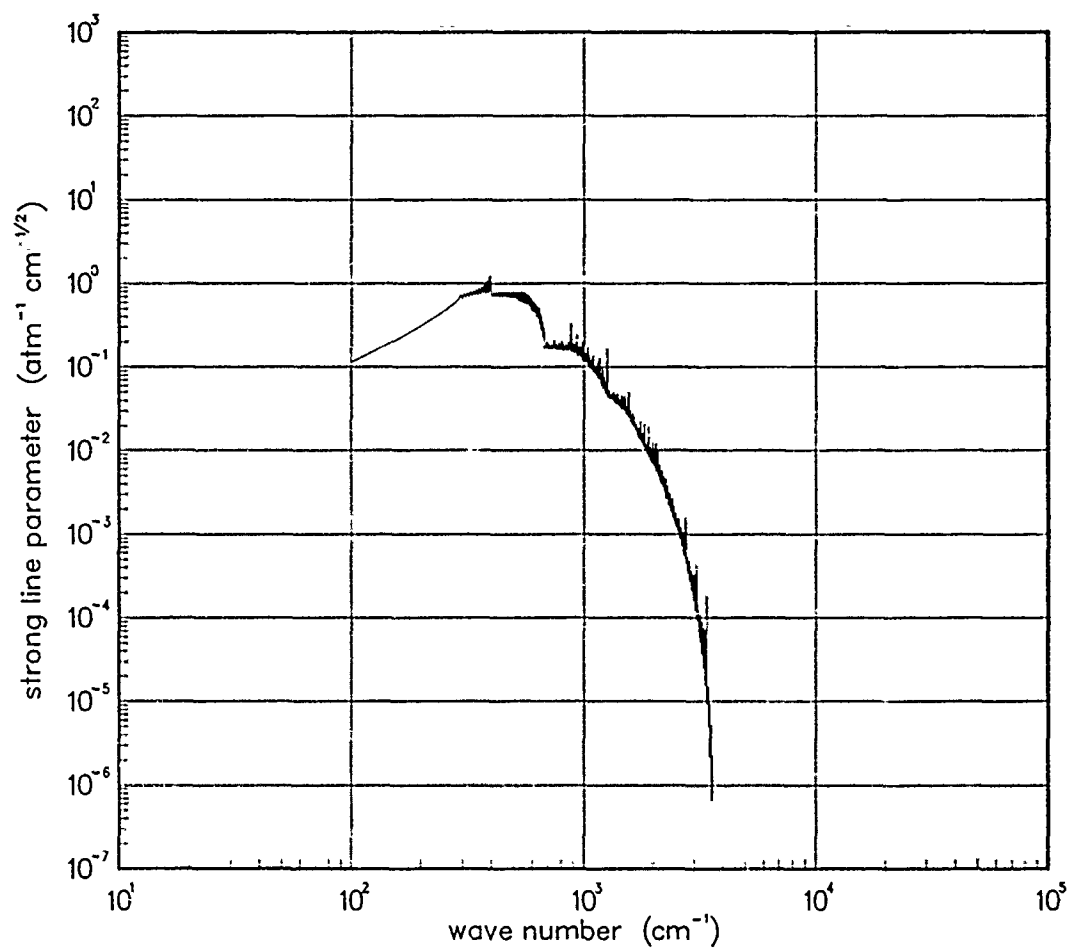


Figure 341. Strong-line parameter for CuO at 18000°K.

6.3 IRON OXIDE (FeO).

Table 9. Spectroscopic data for FeO.

$X \ ^2\Sigma$	
$\omega_e = 880.53^*$	$\omega_e x_e = 4.63^*$
$\alpha_e = 0.00376^*$	$B_e = 0.51271^*$
$S_{10} = 450^\dagger$	
$\gamma_t(300 \text{ }^\circ\text{K}) = 0.04^\ddagger$	

Data Source:

*R.F. Barrow, and M. Senior, Nature 223 1359 (1969).

†K. Wray, AVCO, Mass., Contribution to DASA/ARPA Working Group, p. 26
Palo Alto, Ca. (October 1970).

‡Estimate.

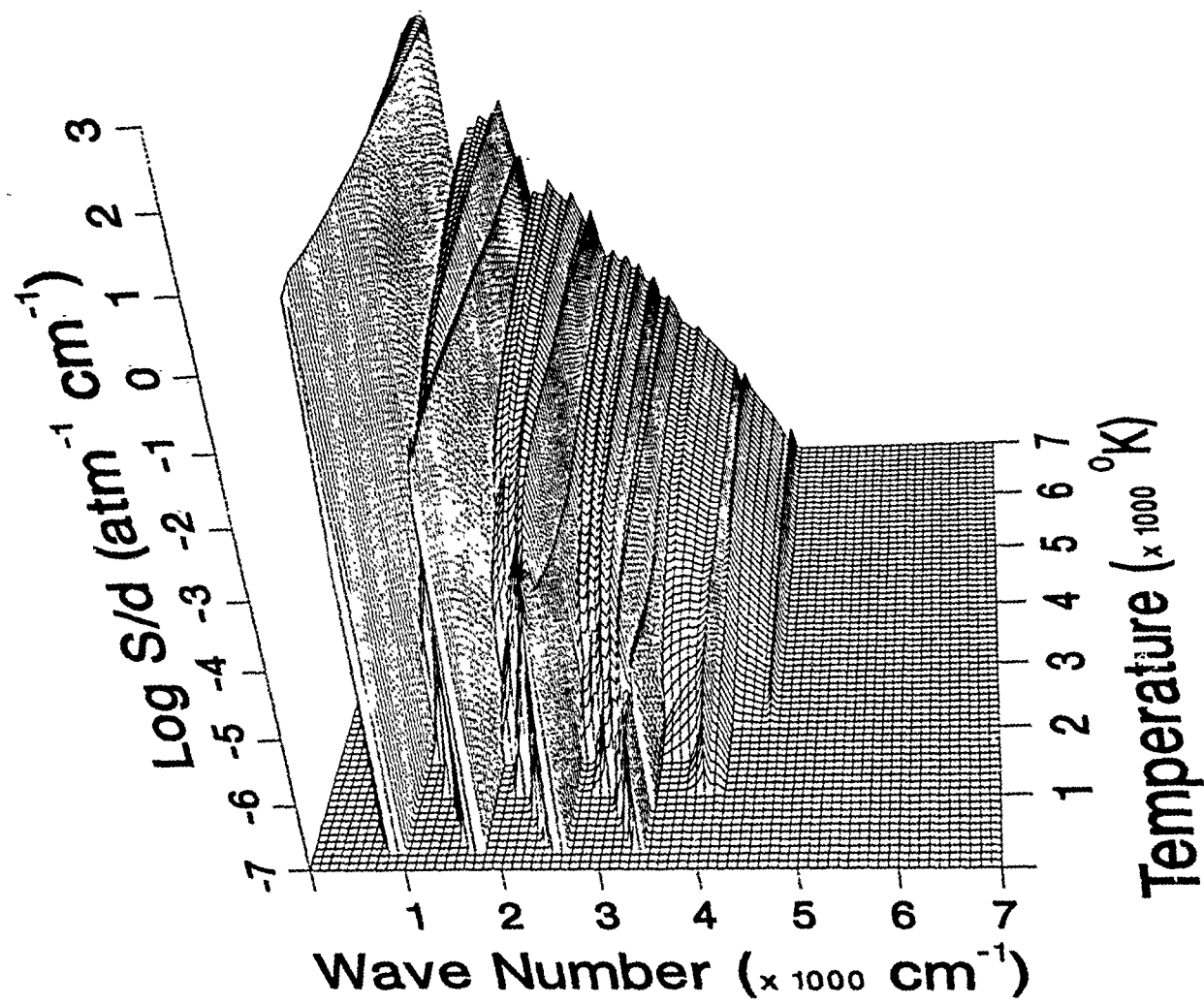


Figure 342. Weak-line parameter for FeO.

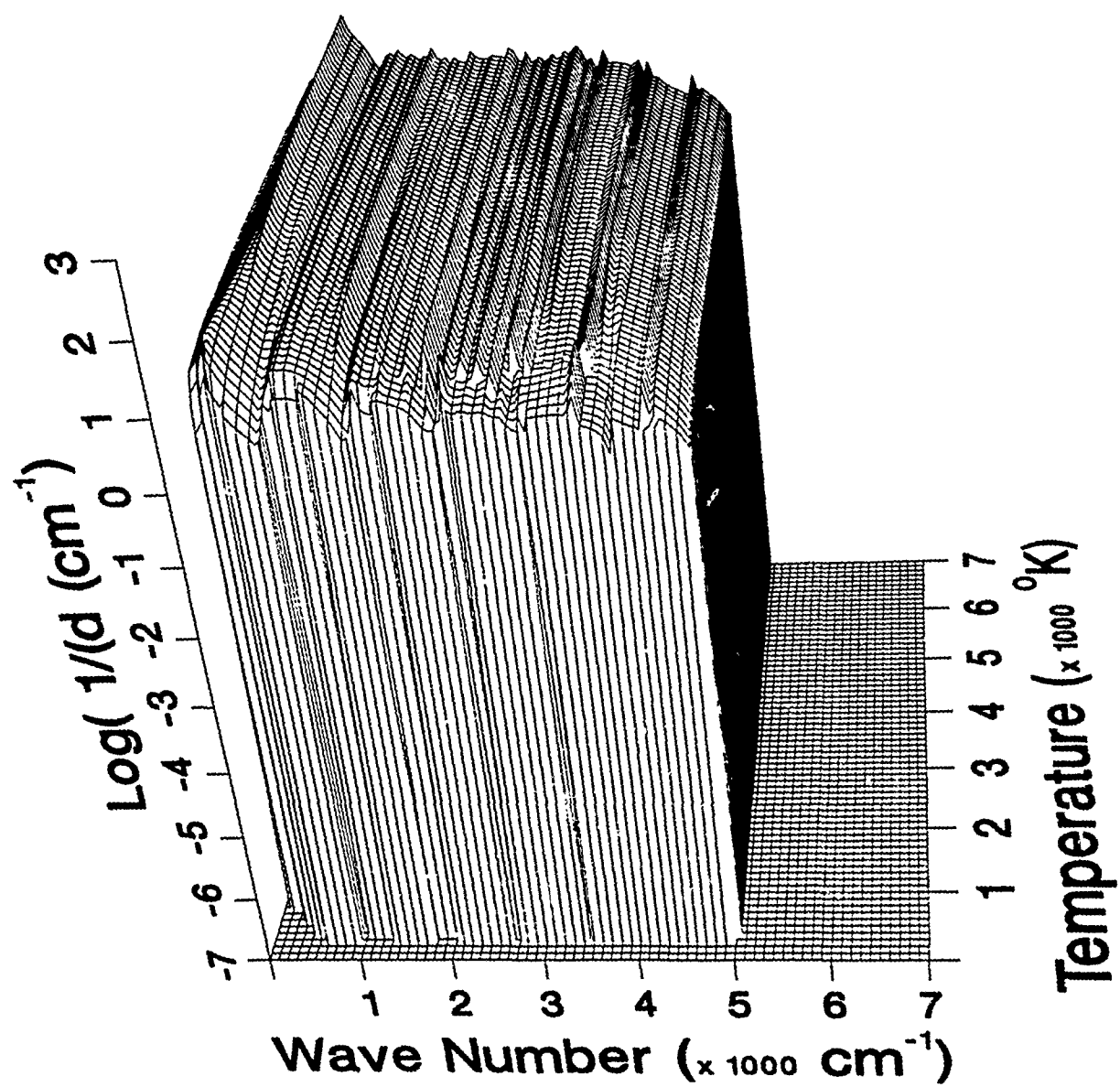


Figure 343. Inverse line spacing for FeO.

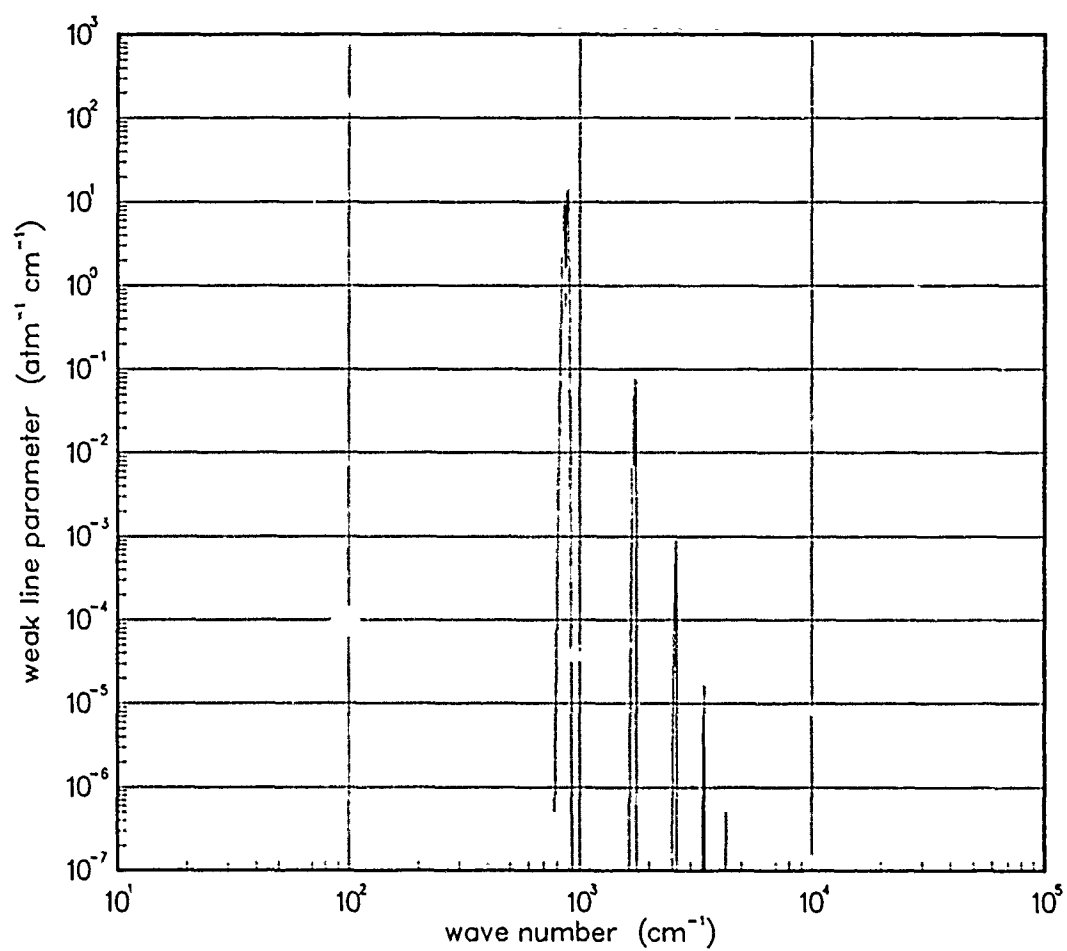


Figure 344. Weak-line parameter for FeO at 200°K.

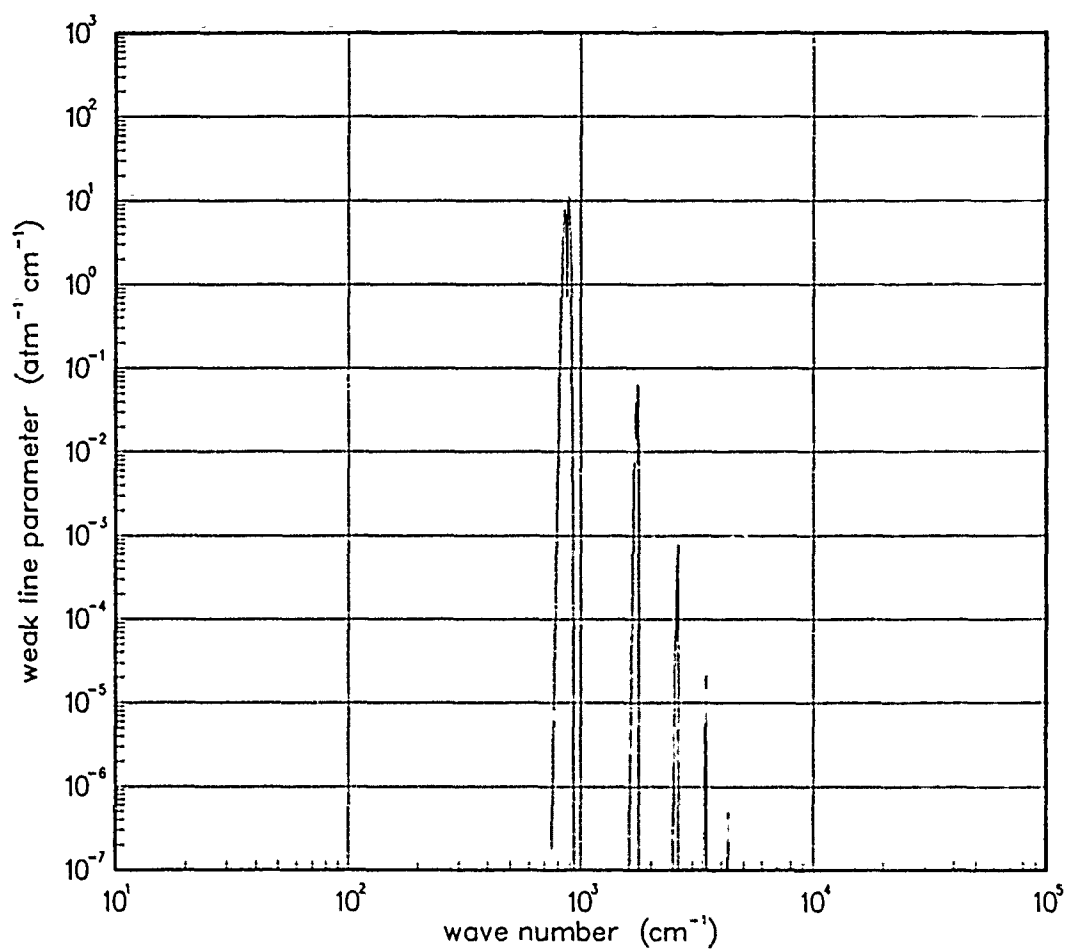


Figure 345. Weak-line parameter for FeO at 300°K.

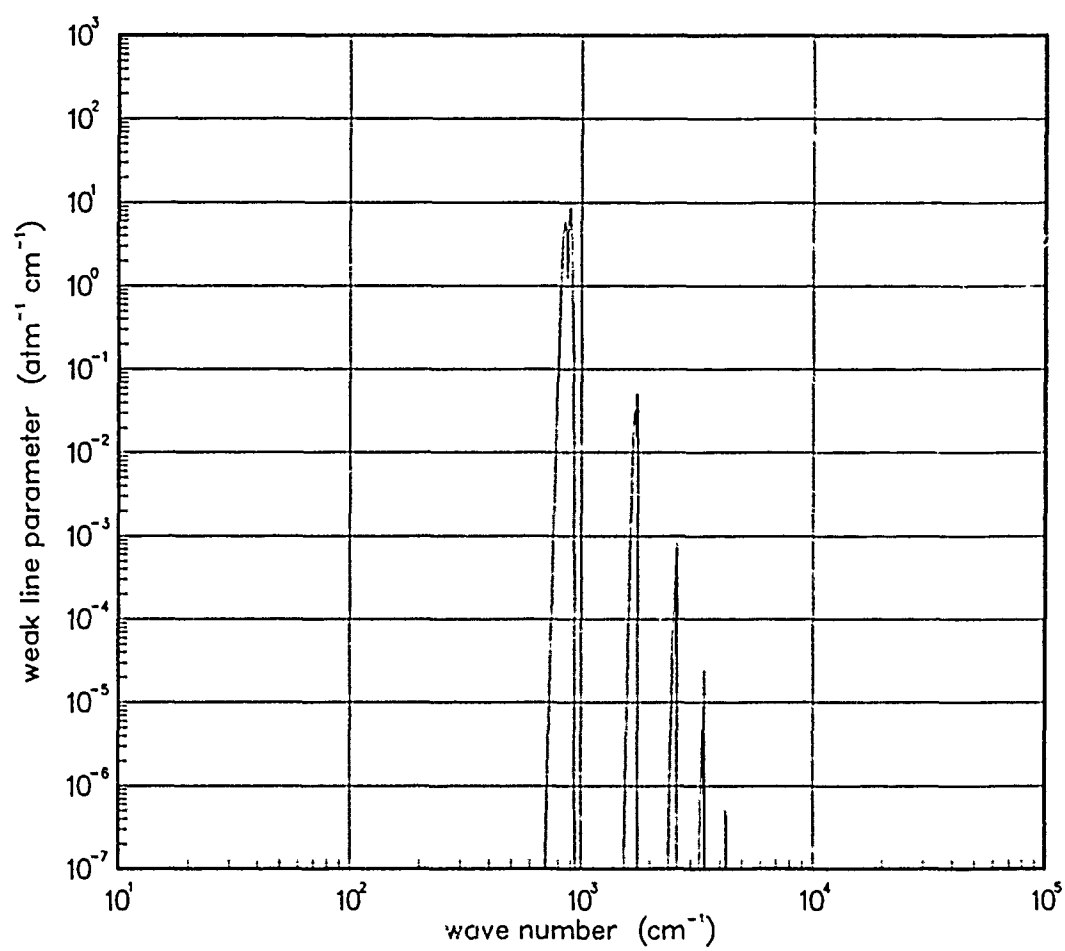


Figure 346. Weak-line parameter for FeO at 500°K.

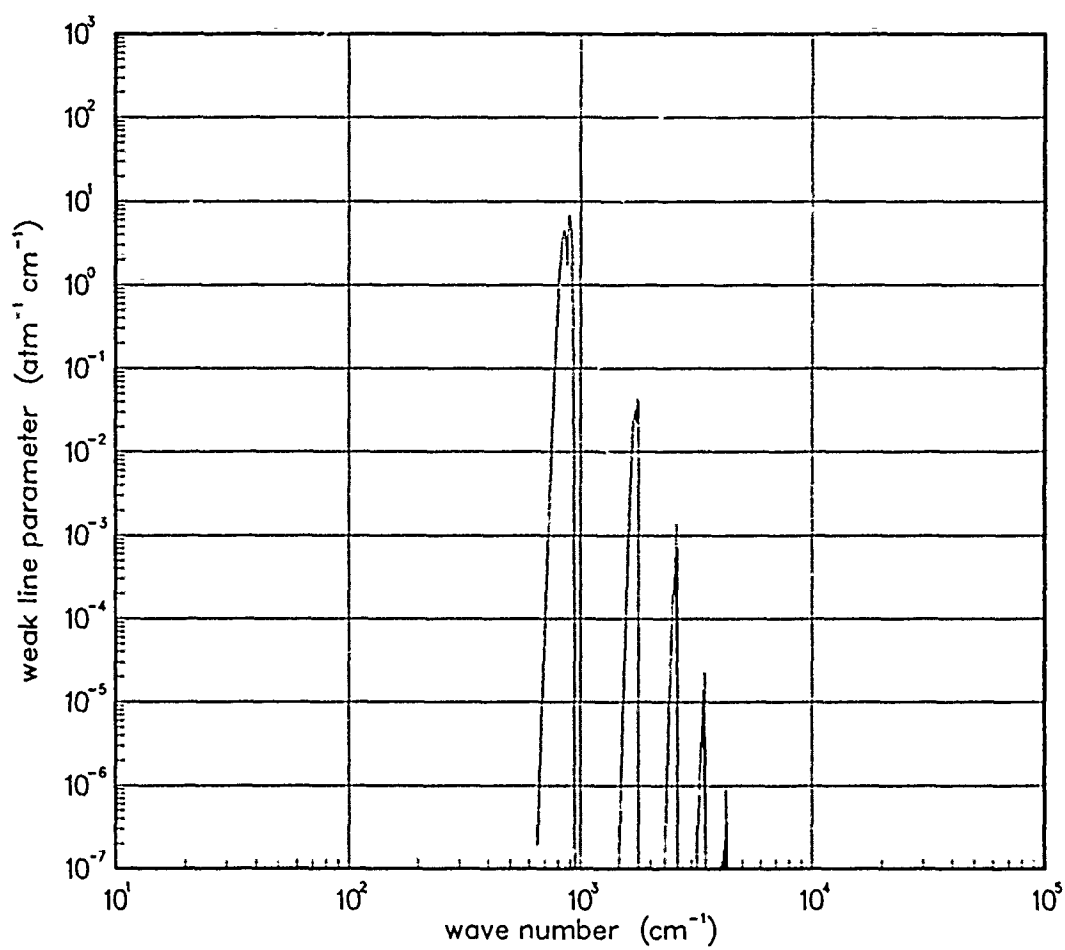


Figure 347. Weak-line parameter for FeO at 750°K.

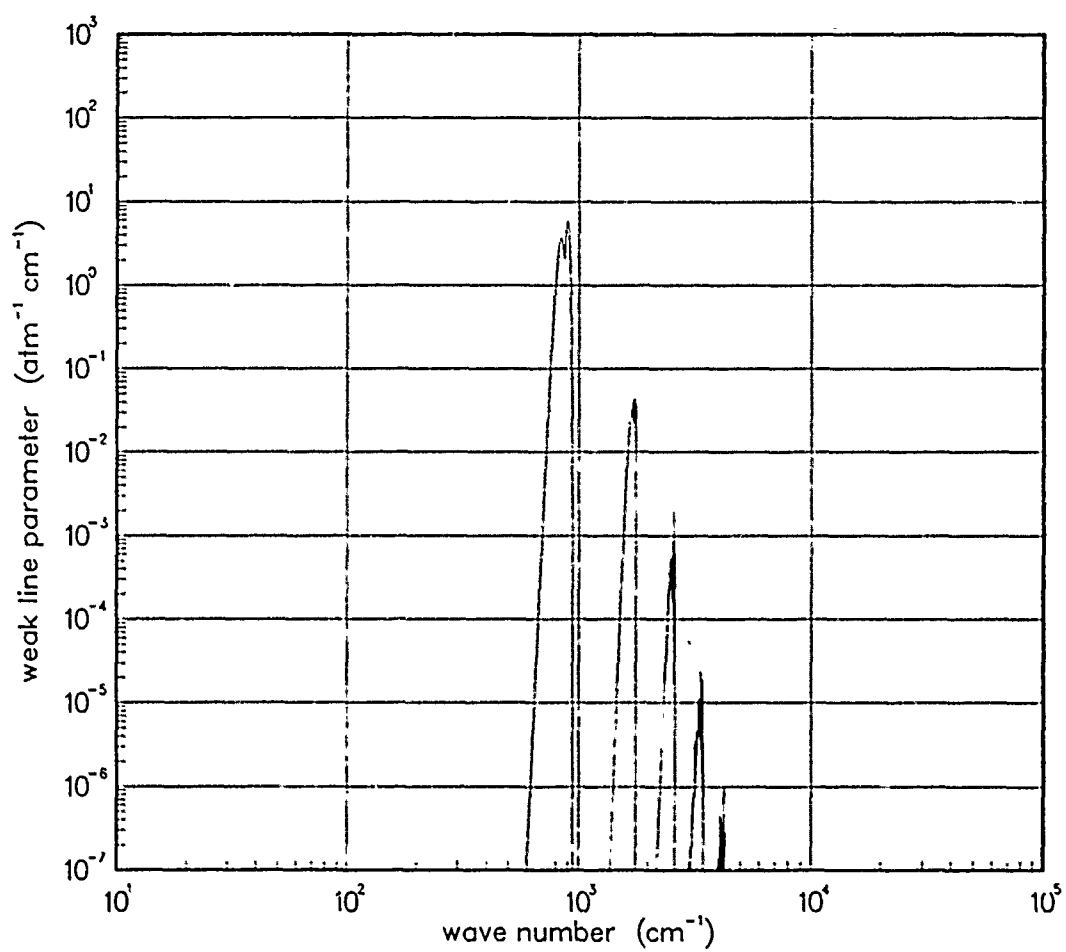


Figure 348. Weak-line parameter for FeO at 1000°K.

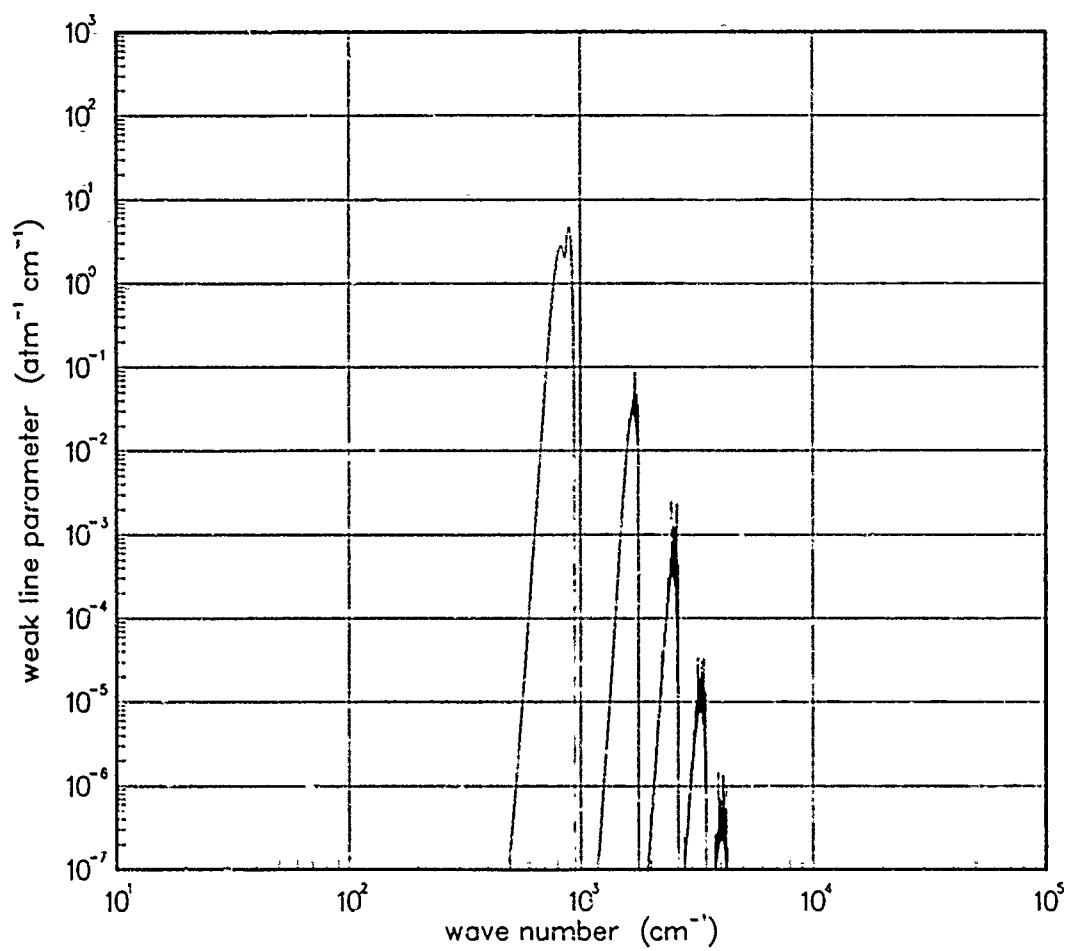


Figure 349. Weak-line parameter for FeO at 1500°K.

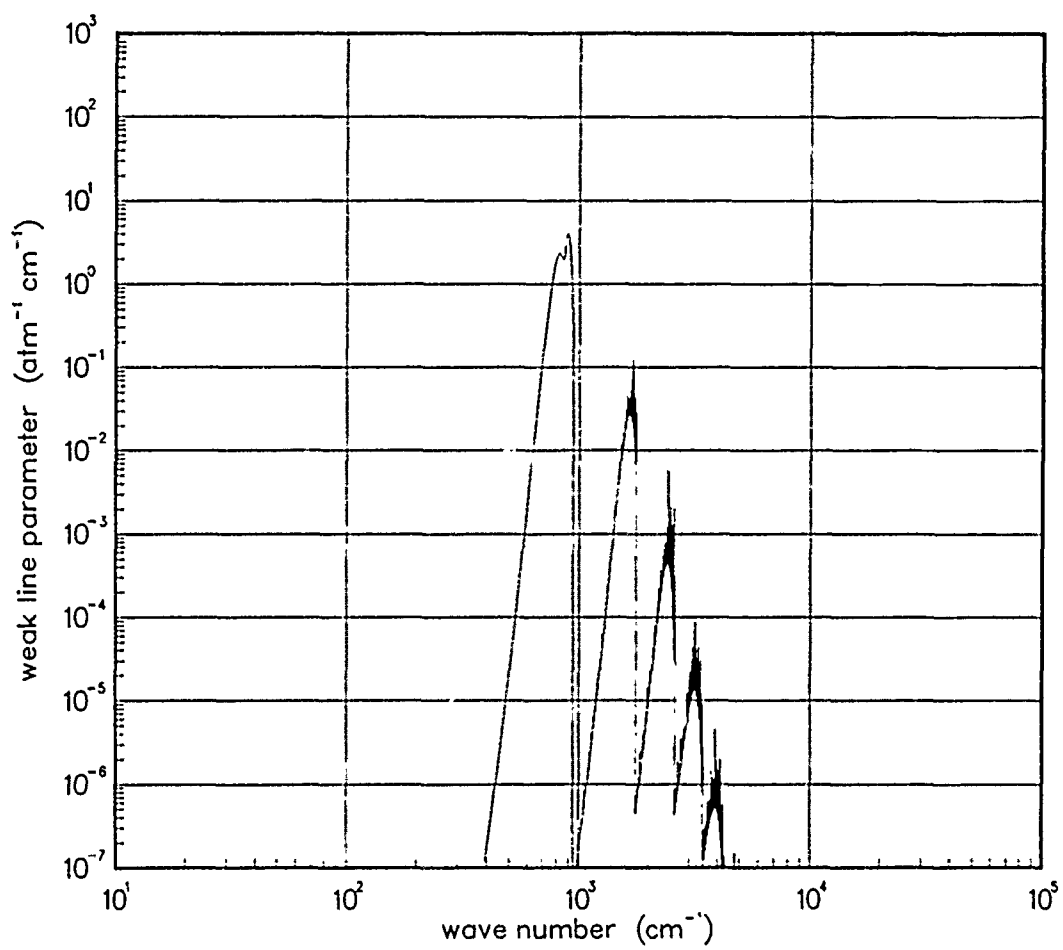


Figure 350. Weak-line parameter for FeO at 2000°K.

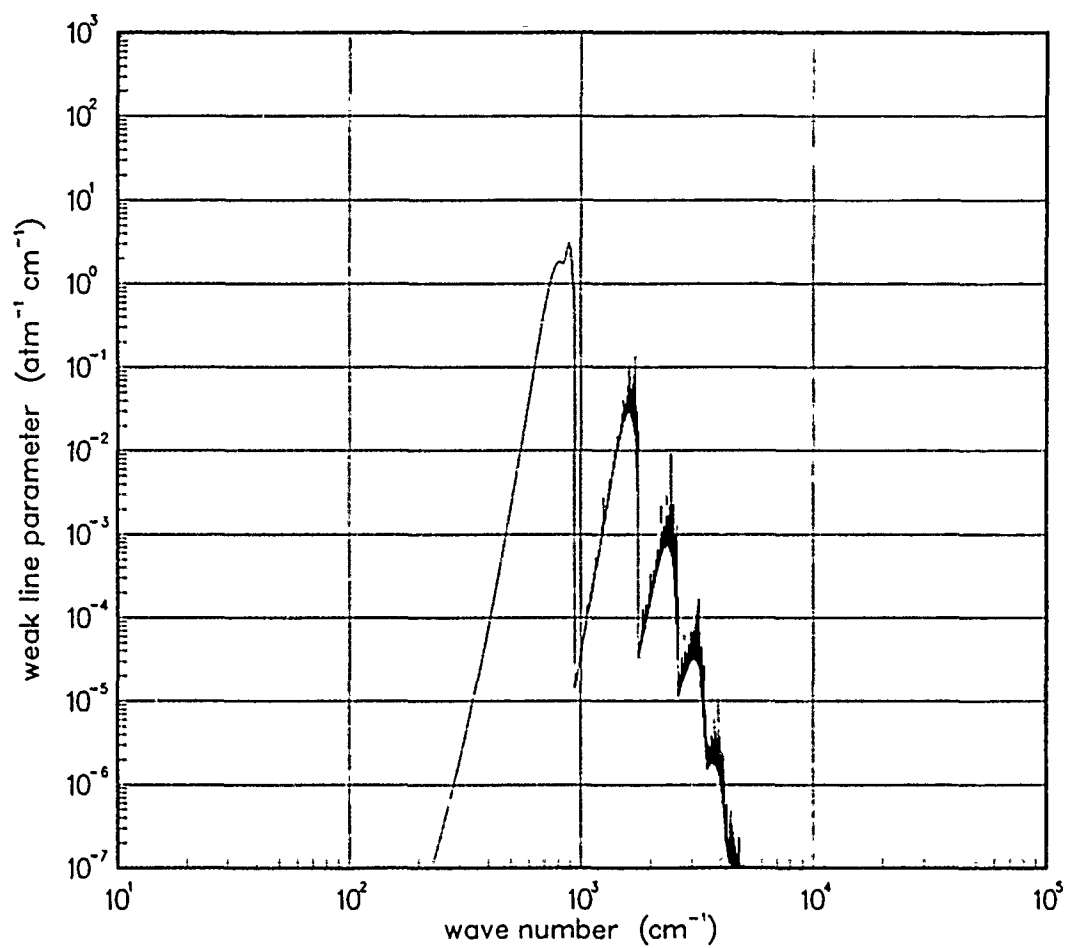


Figure 351. Weak-line parameter for FeO at 3000°K.

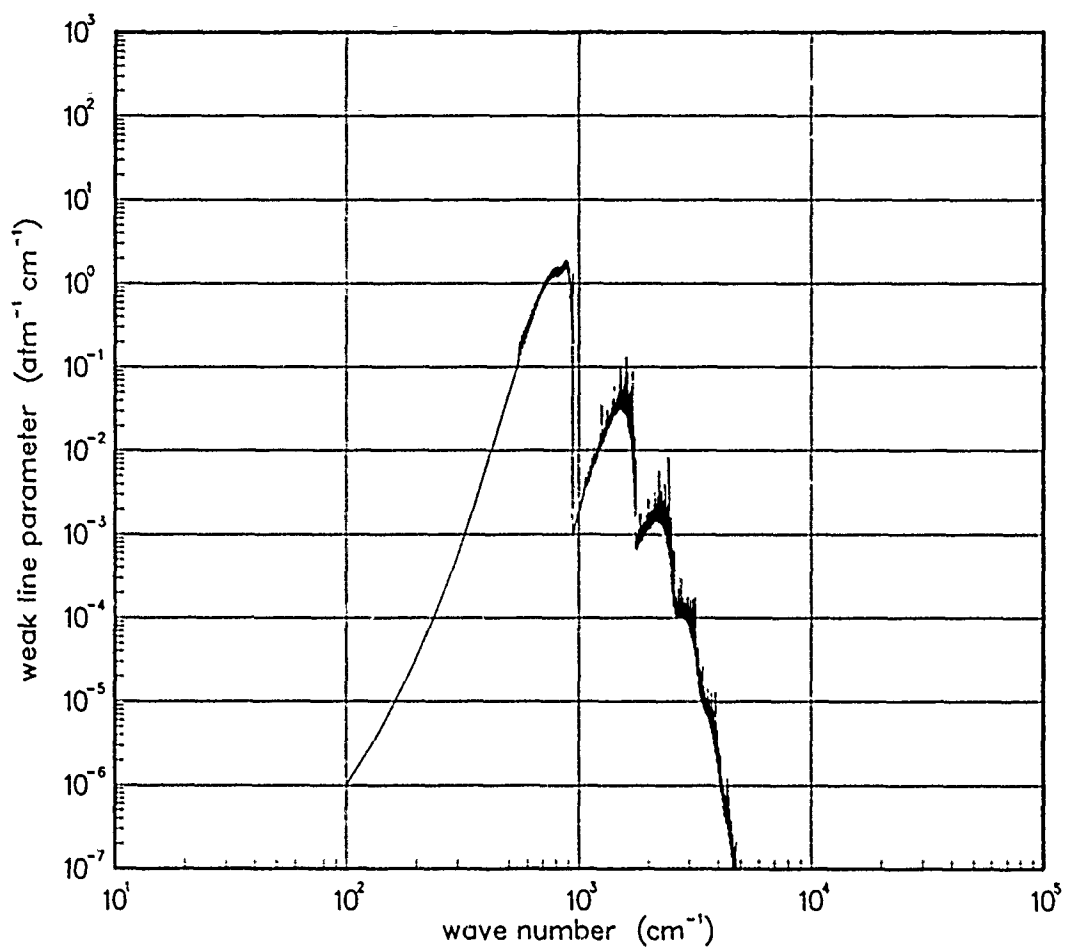


Figure 352. Weak-line parameter for FeO at 5000°K.

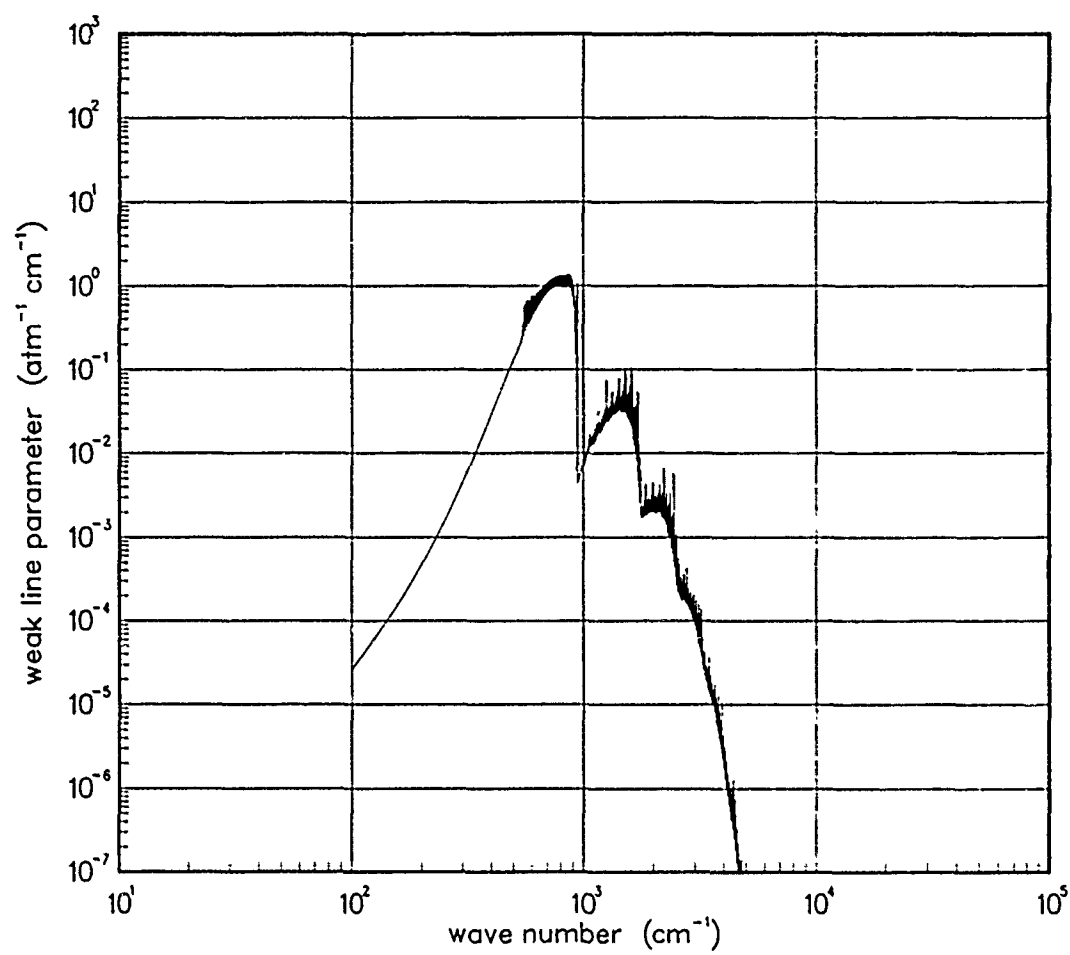


Figure 353. Weak-line parameter for FeO at 7000°K.

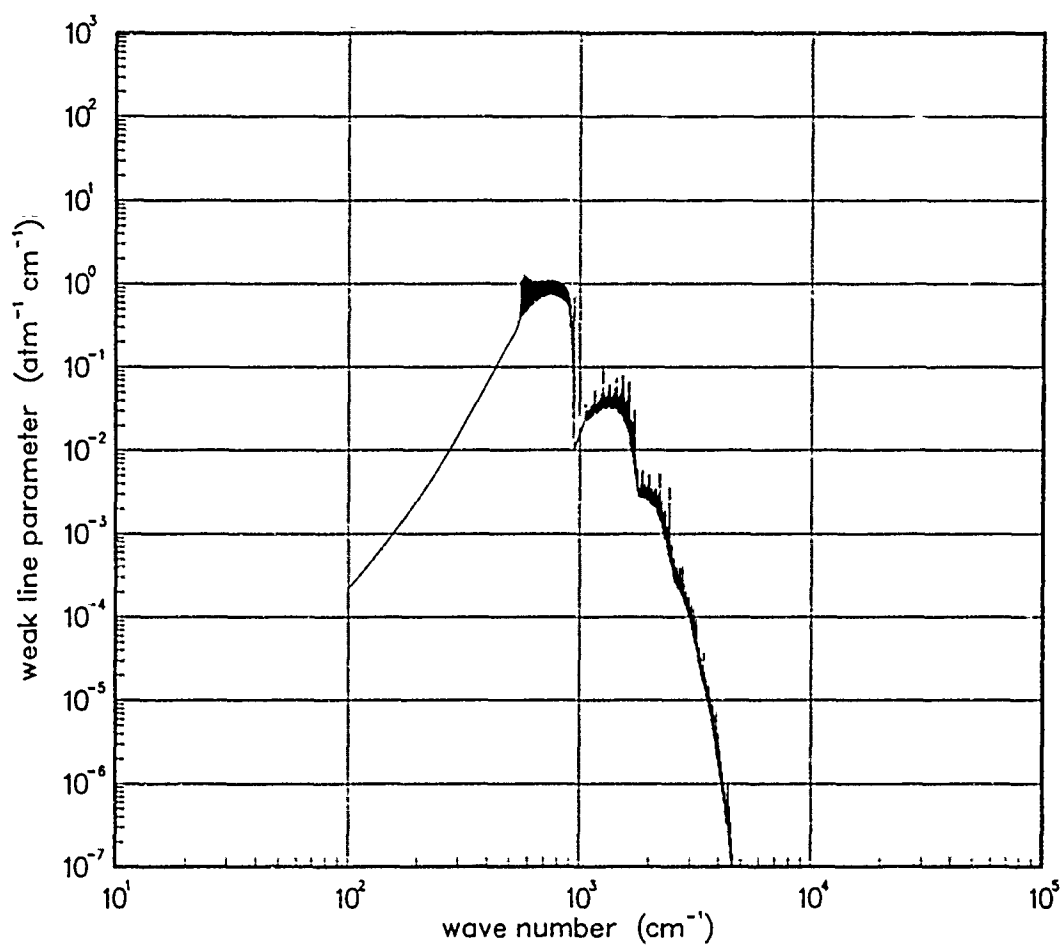


Figure 354. Weak-line parameter for FeO at 10000°K.

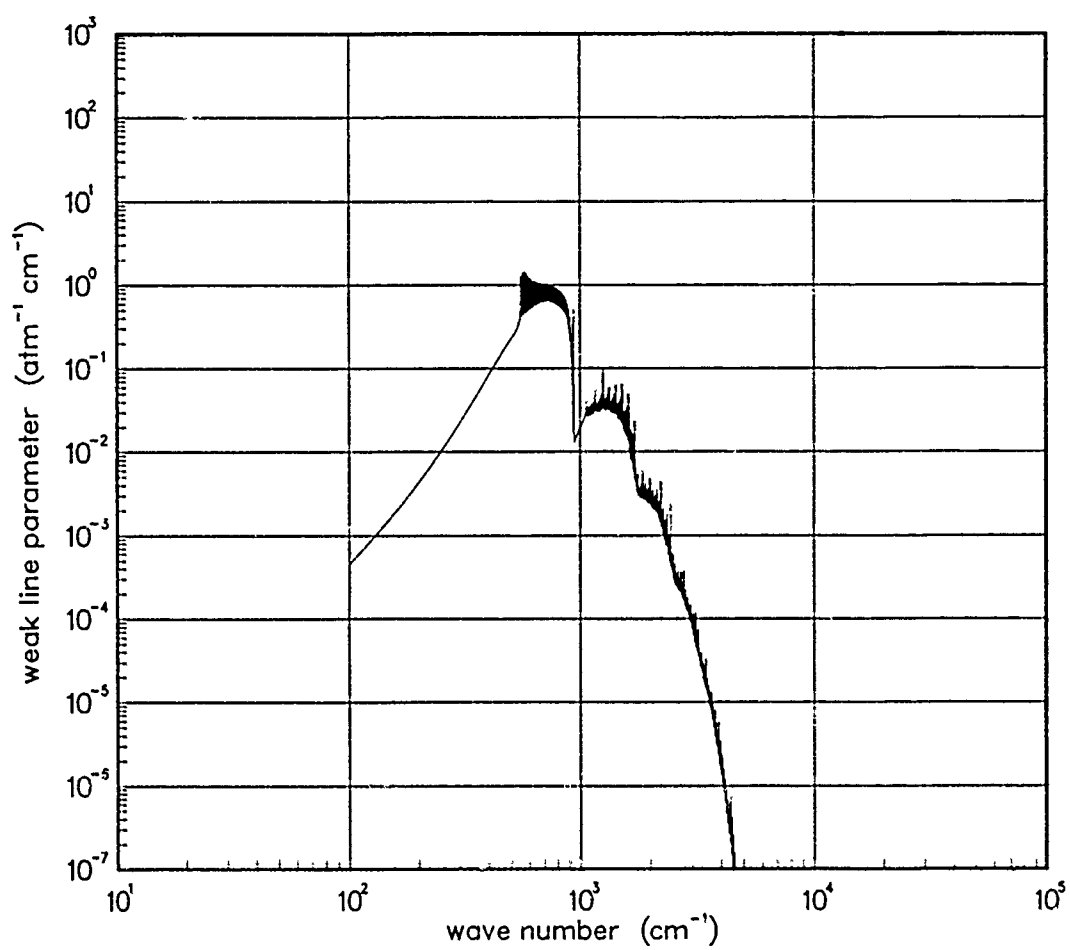


Figure 355. Weak-line parameter for FeO at 12000°K.

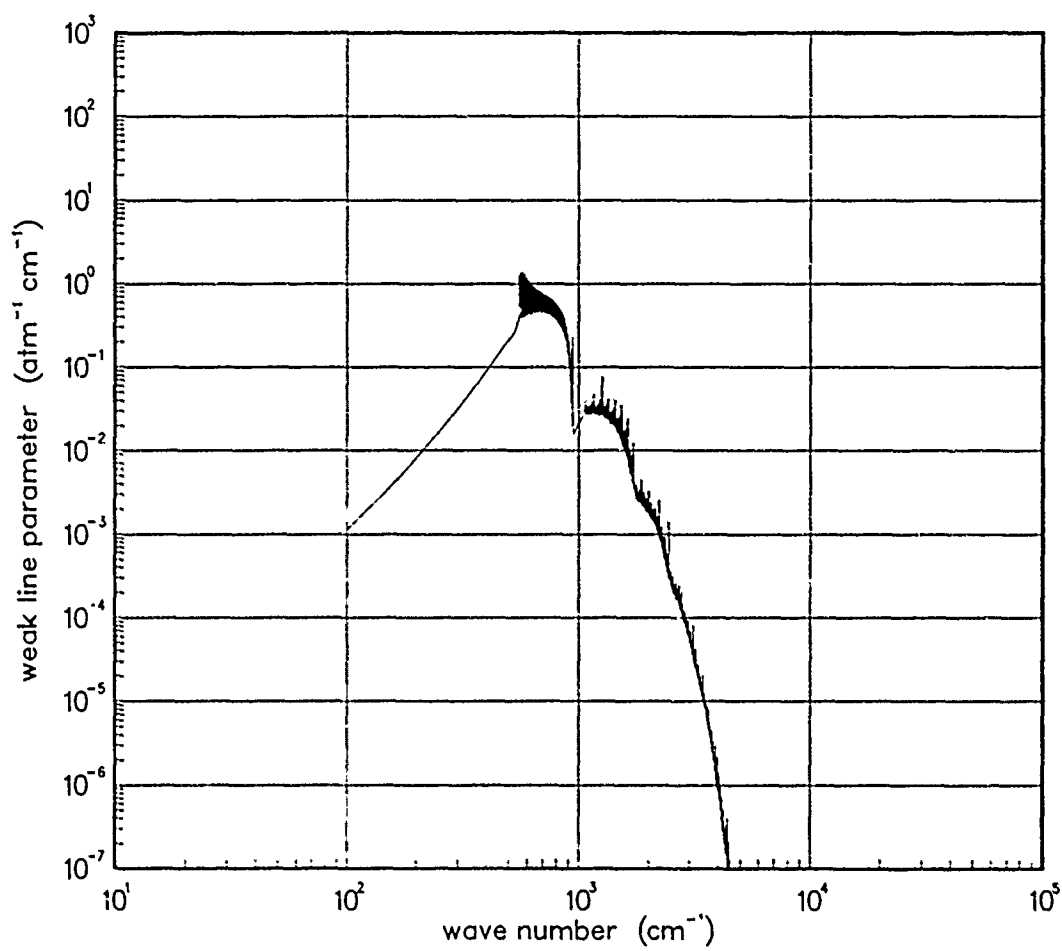


Figure 356. Weak-line parameter for FeO at 18000°K.

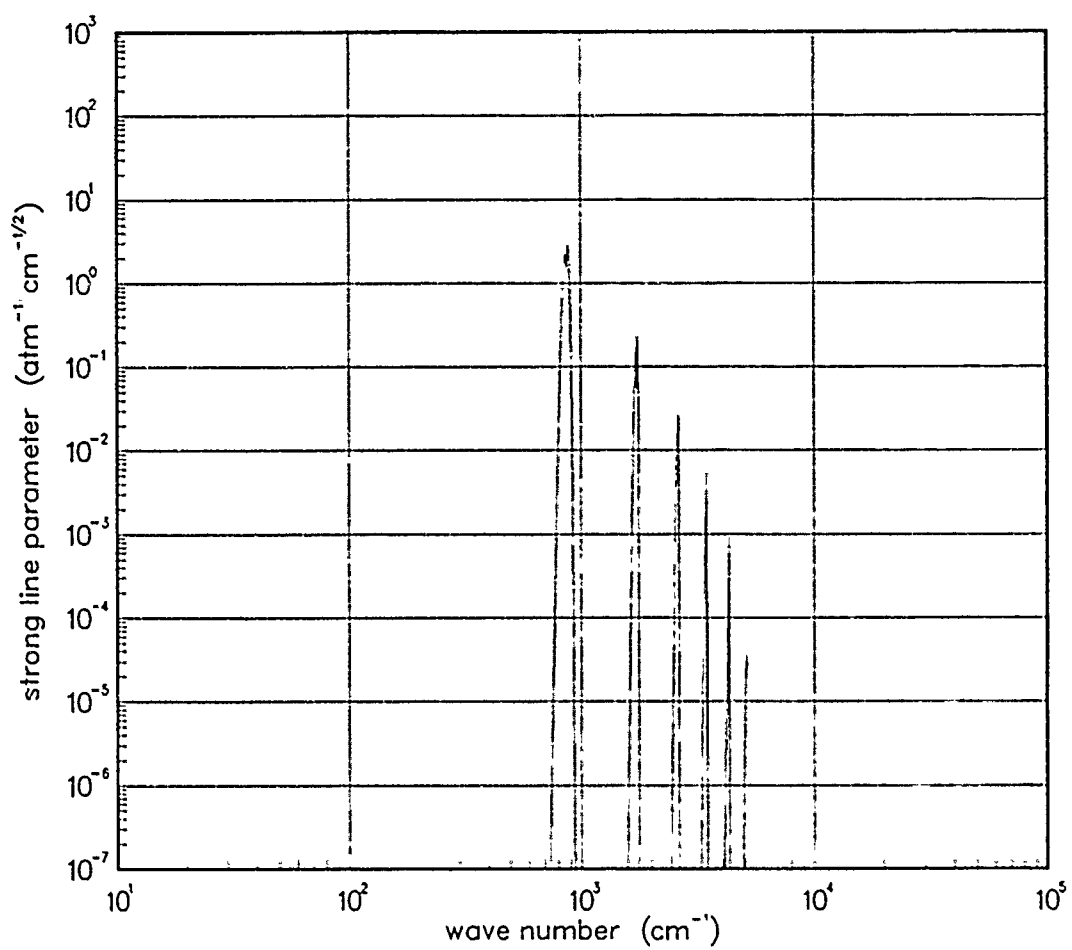


Figure 357. Strong-line parameter for FeO at 200°K.

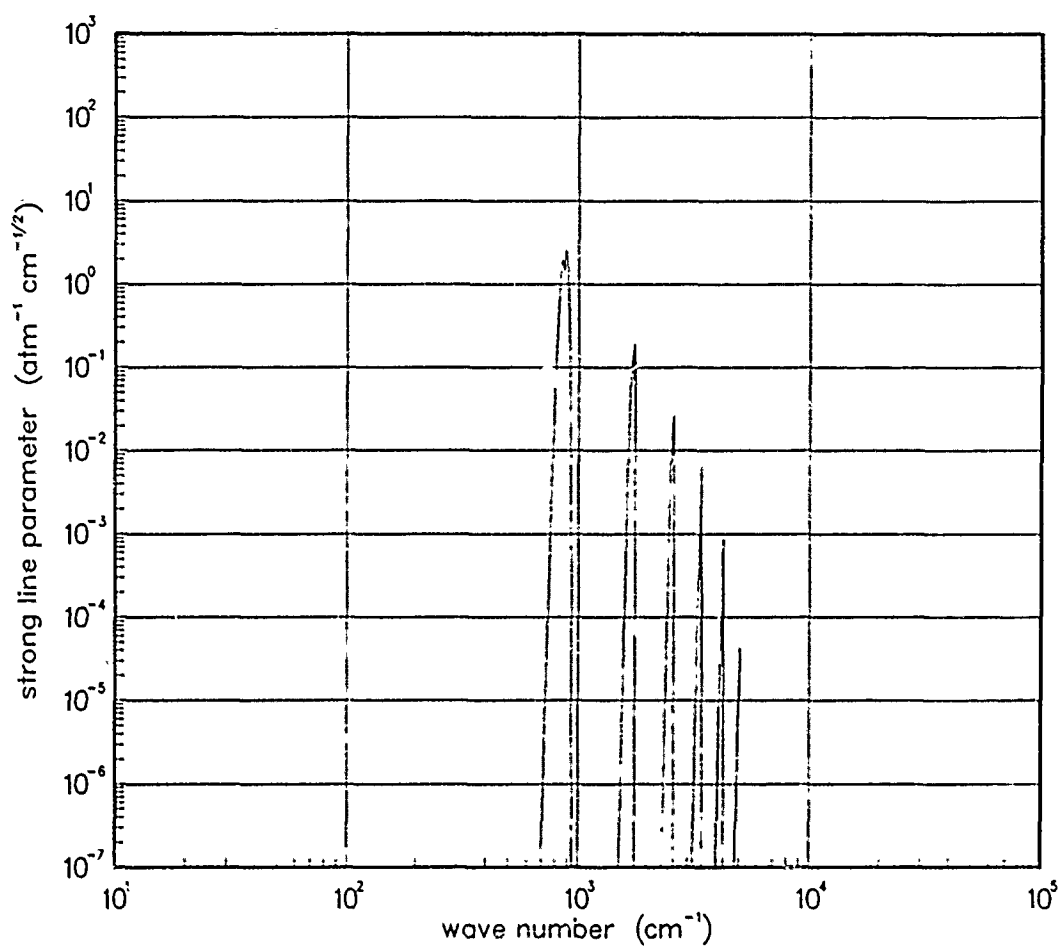


Figure 358. Strong-line parameter for FeO at 300°K.

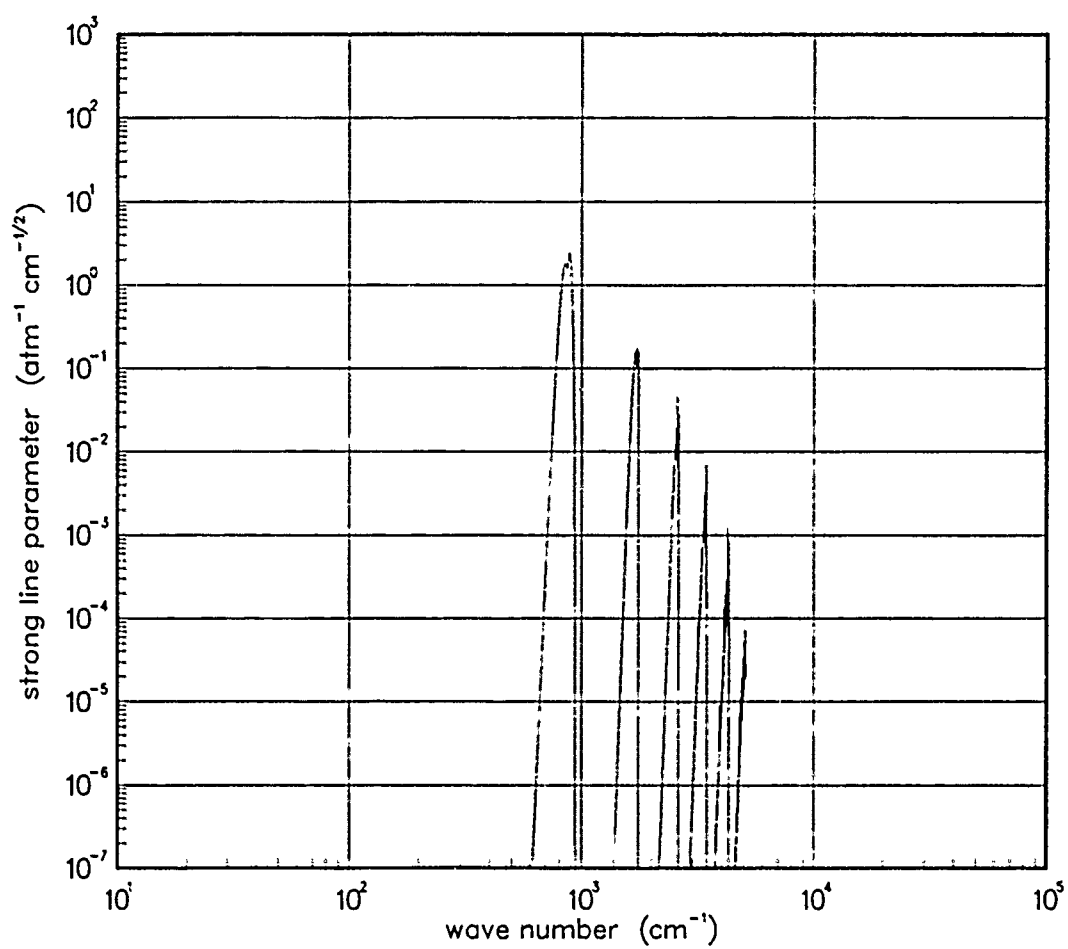


Figure 359. Strong-line parameter for FeO at 500°K.

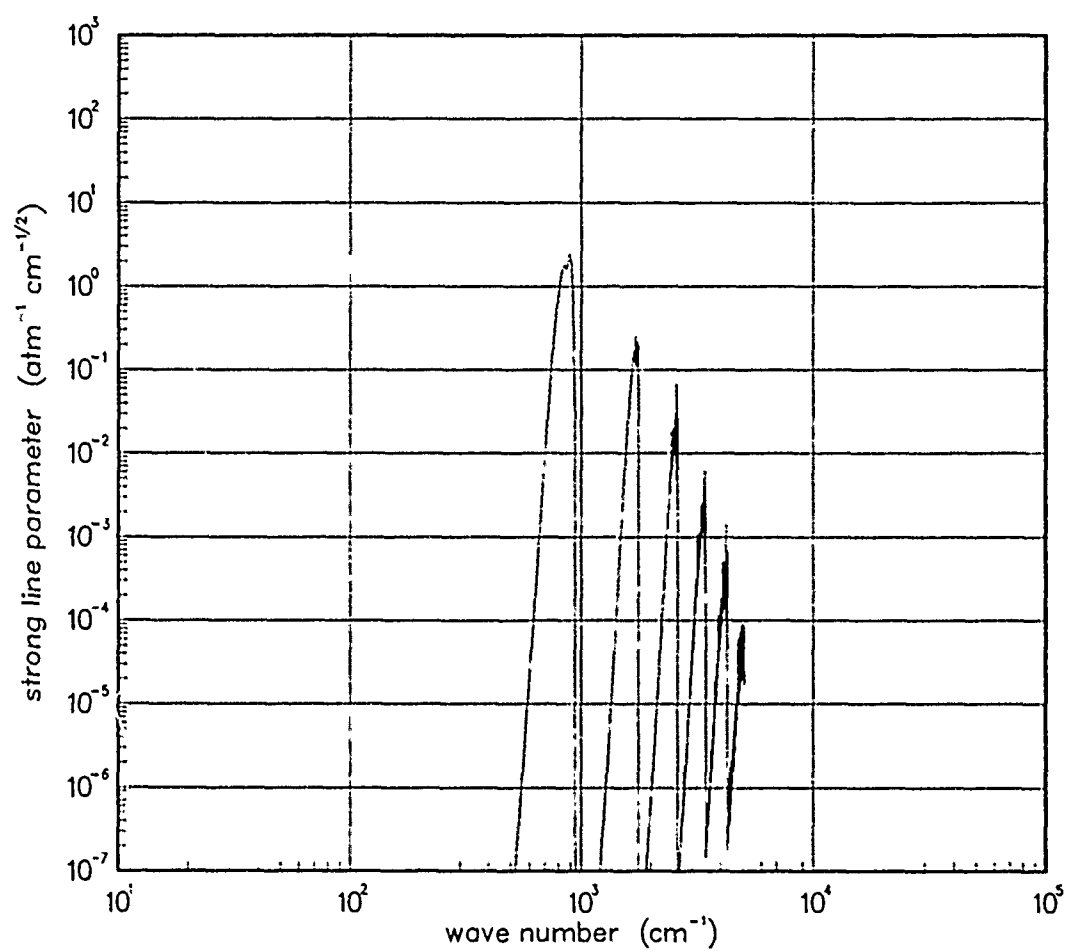


Figure 360. Strong-line parameter for FeO at 750°K.

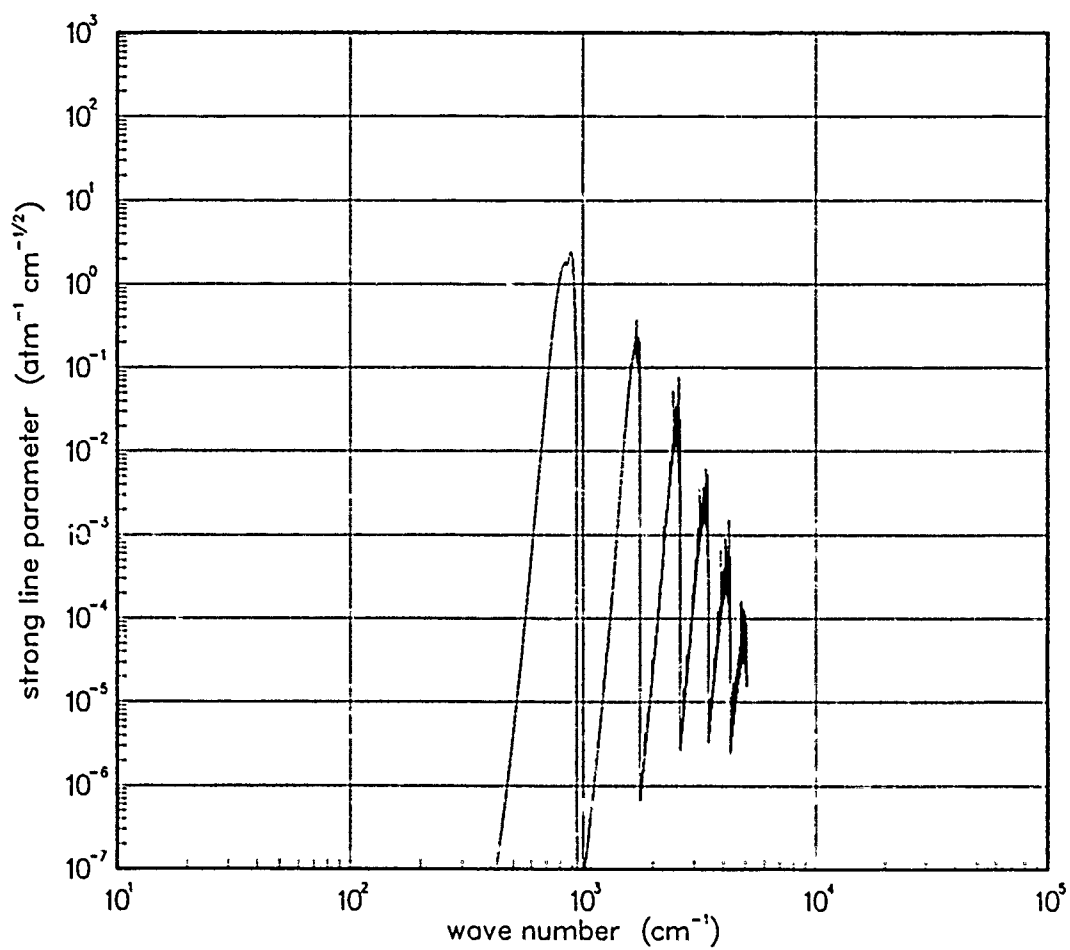


Figure 361. Strong-line parameter for FeO at 1000°K.

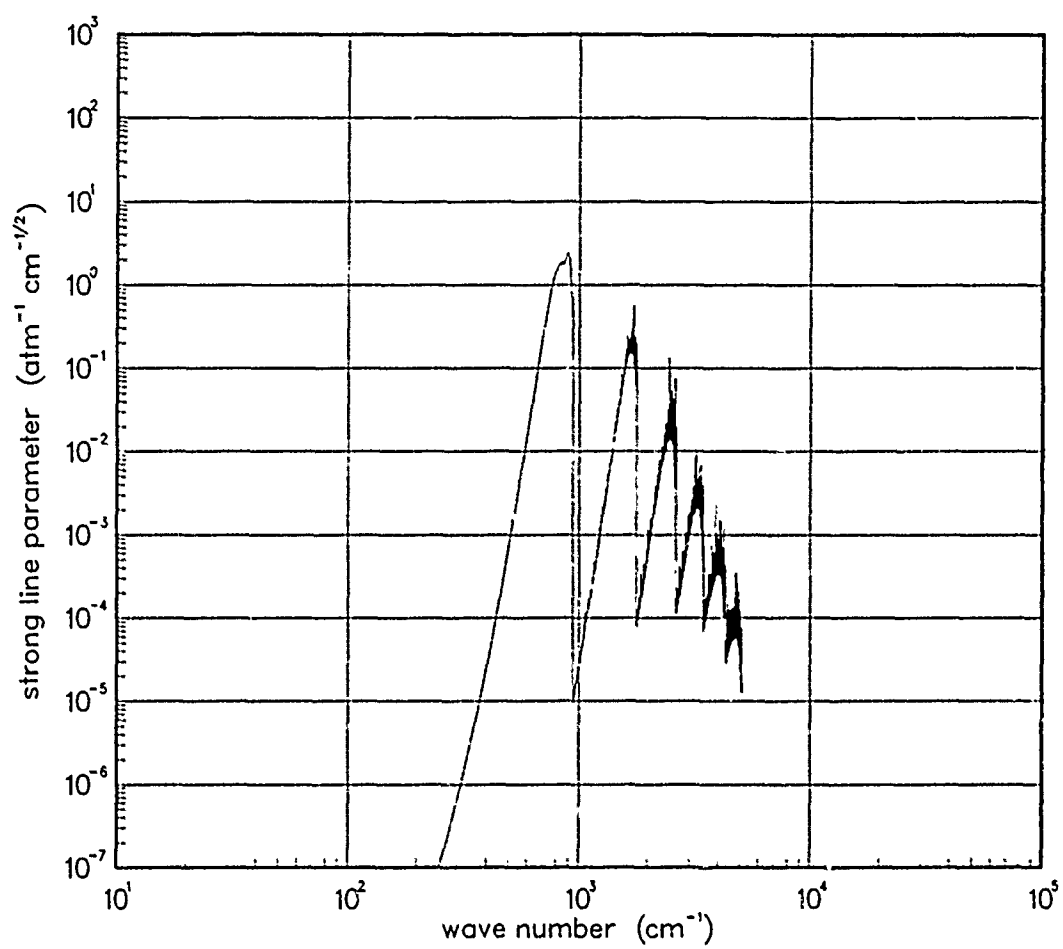


Figure 362. Strong-line parameter for FeO at 1500°K.

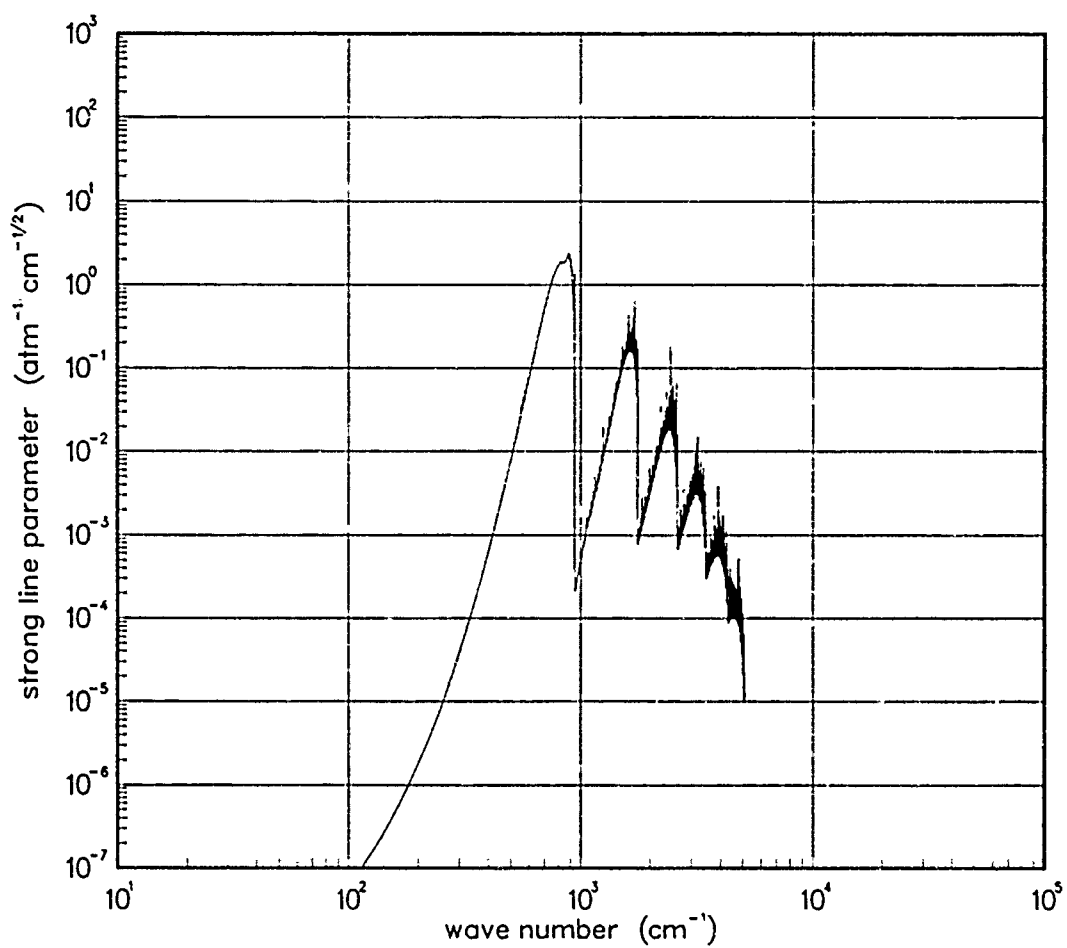


Figure 363. Strong-line parameter for FeO at 2000°K.

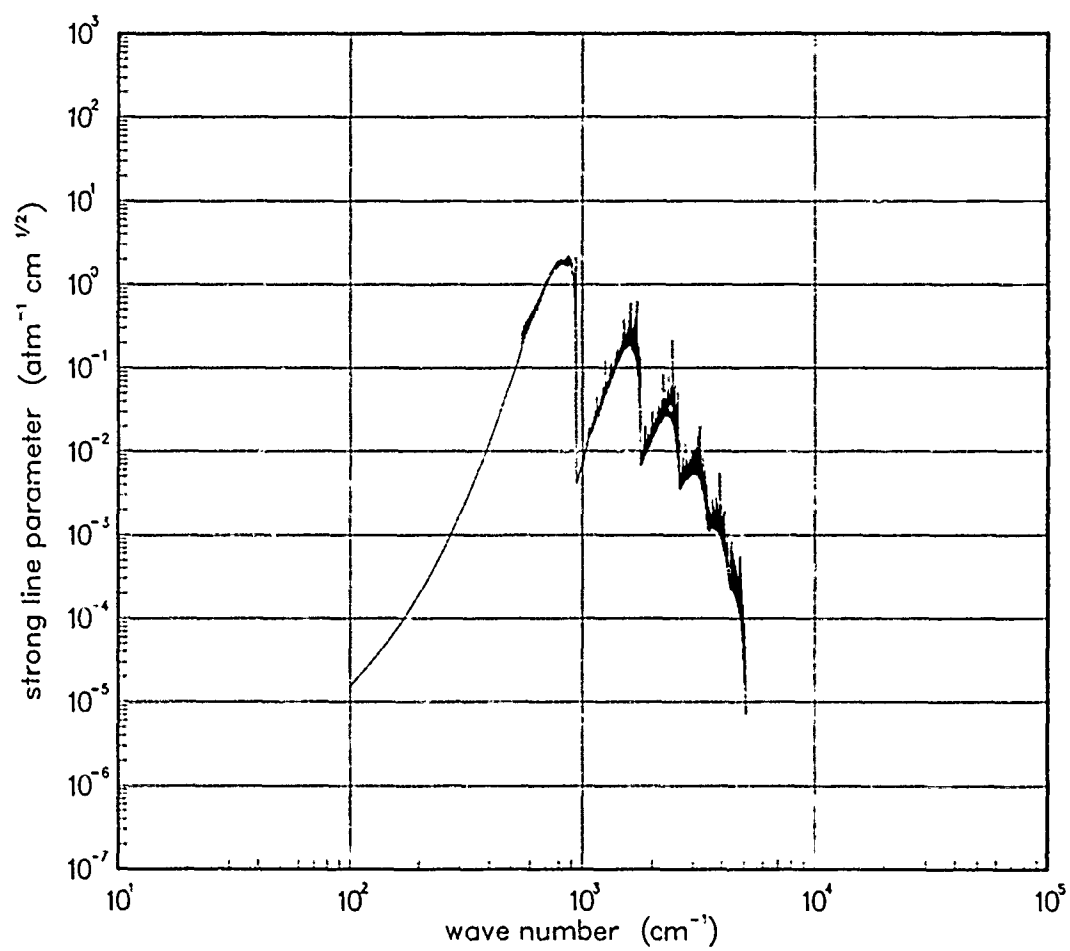


Figure 364. Strong-line parameter for FeO at 3000°K.

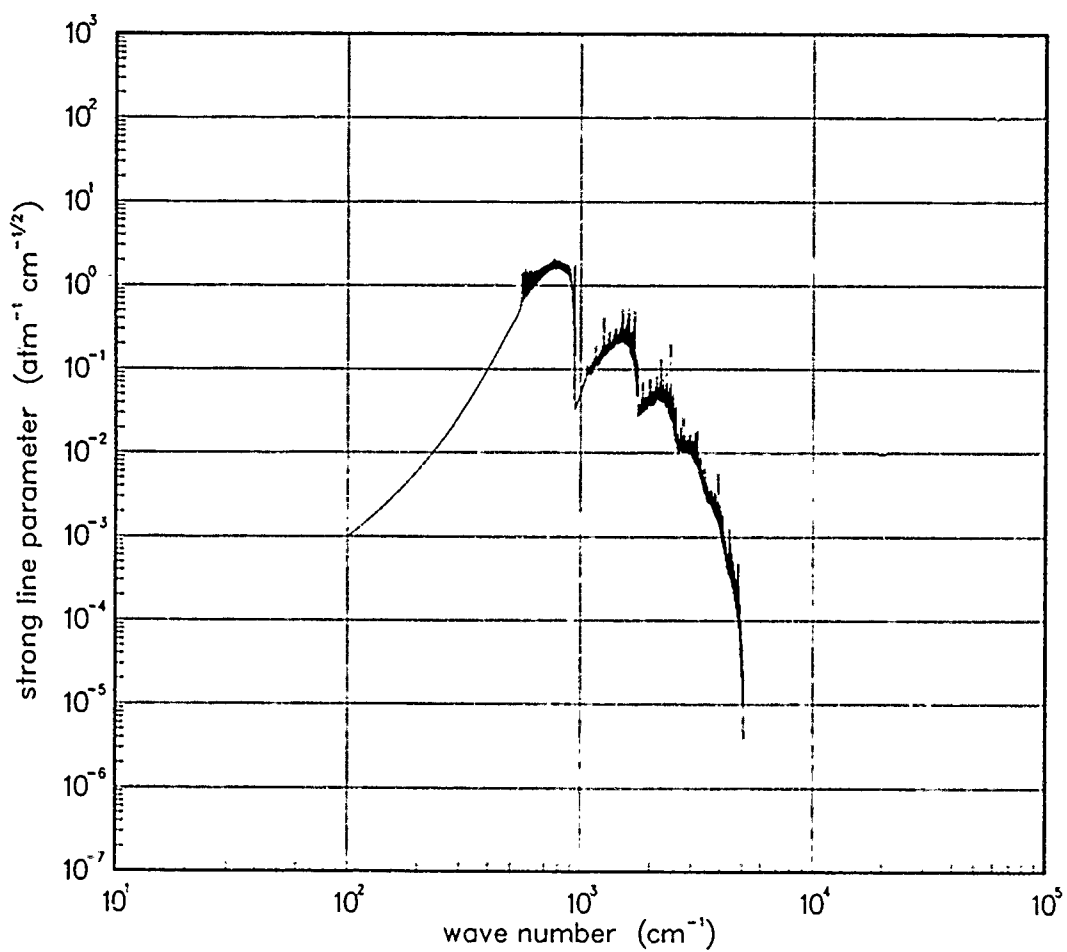


Figure 365. Strong-line parameter for FeO at 5000°K.

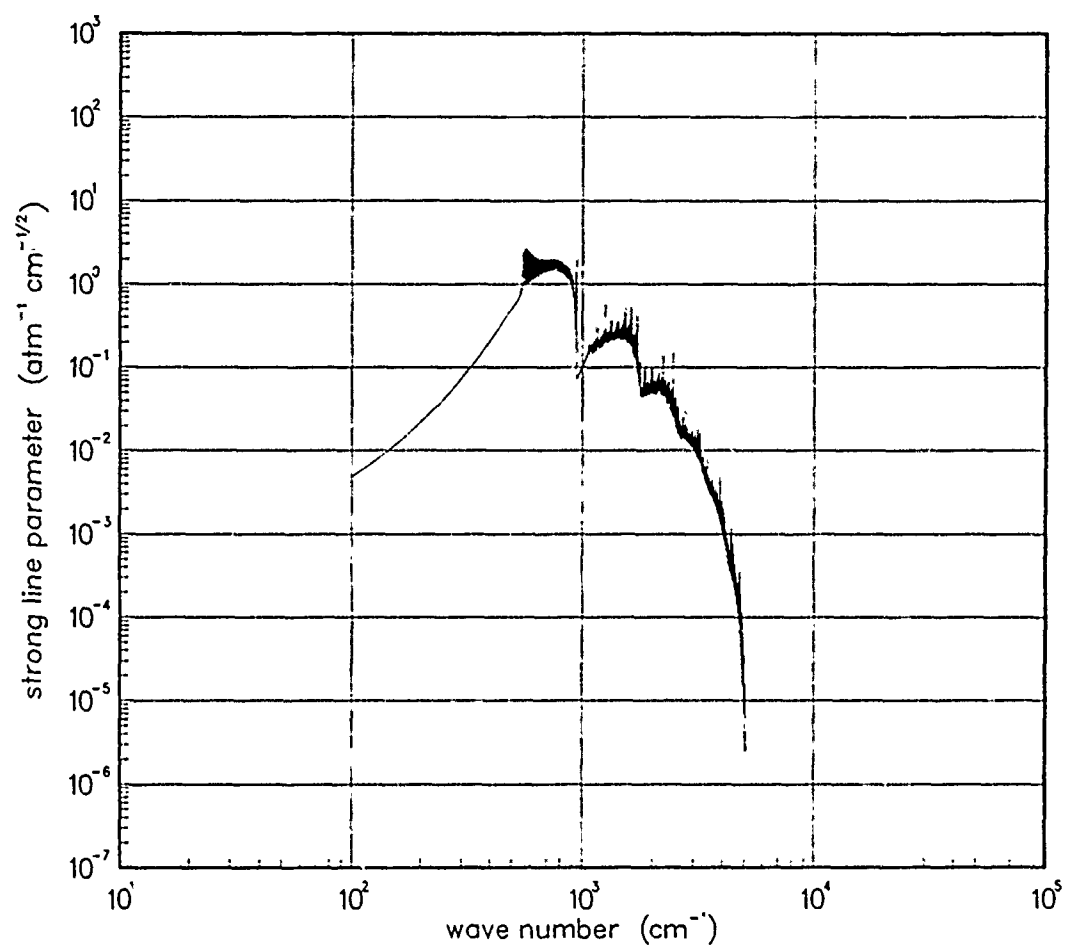


Figure 366. Strong-line parameter for FeO at 7000°K.

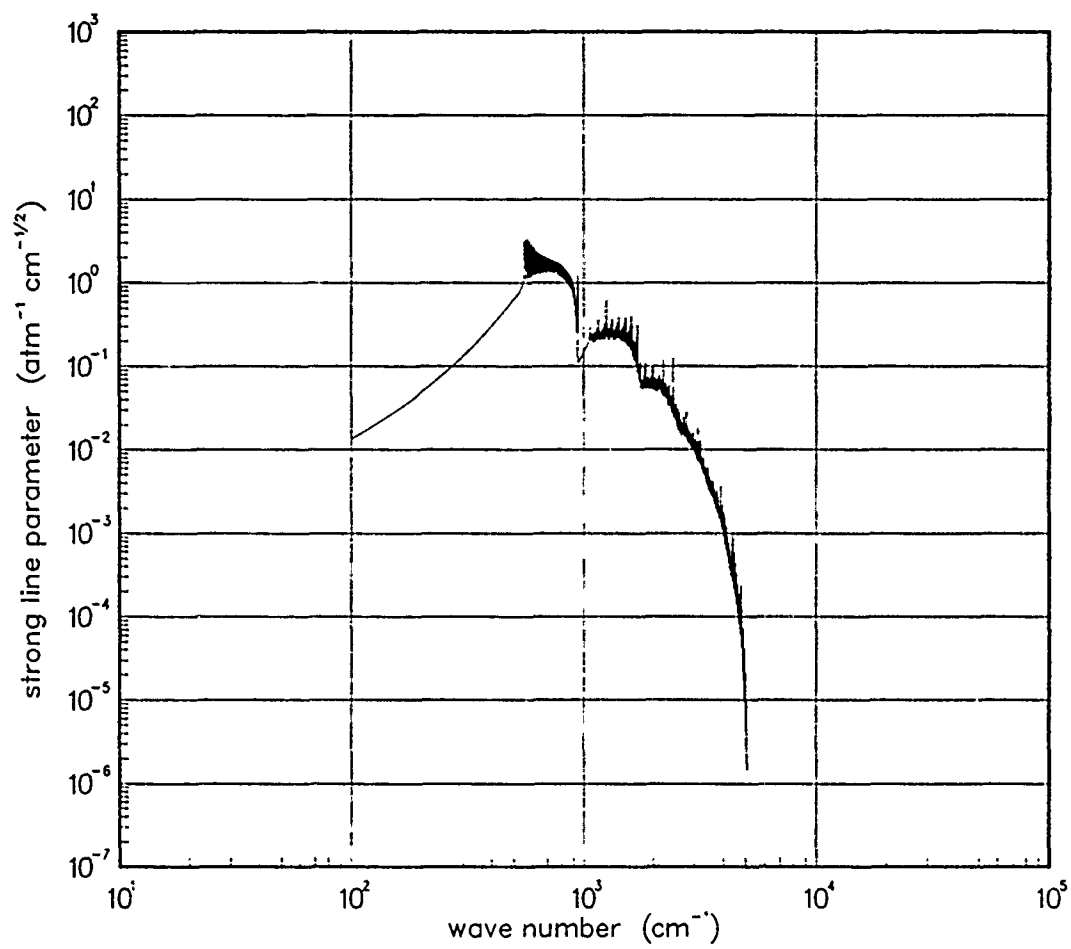


Figure 367. Strong-line parameter for FeO at 10000°K.

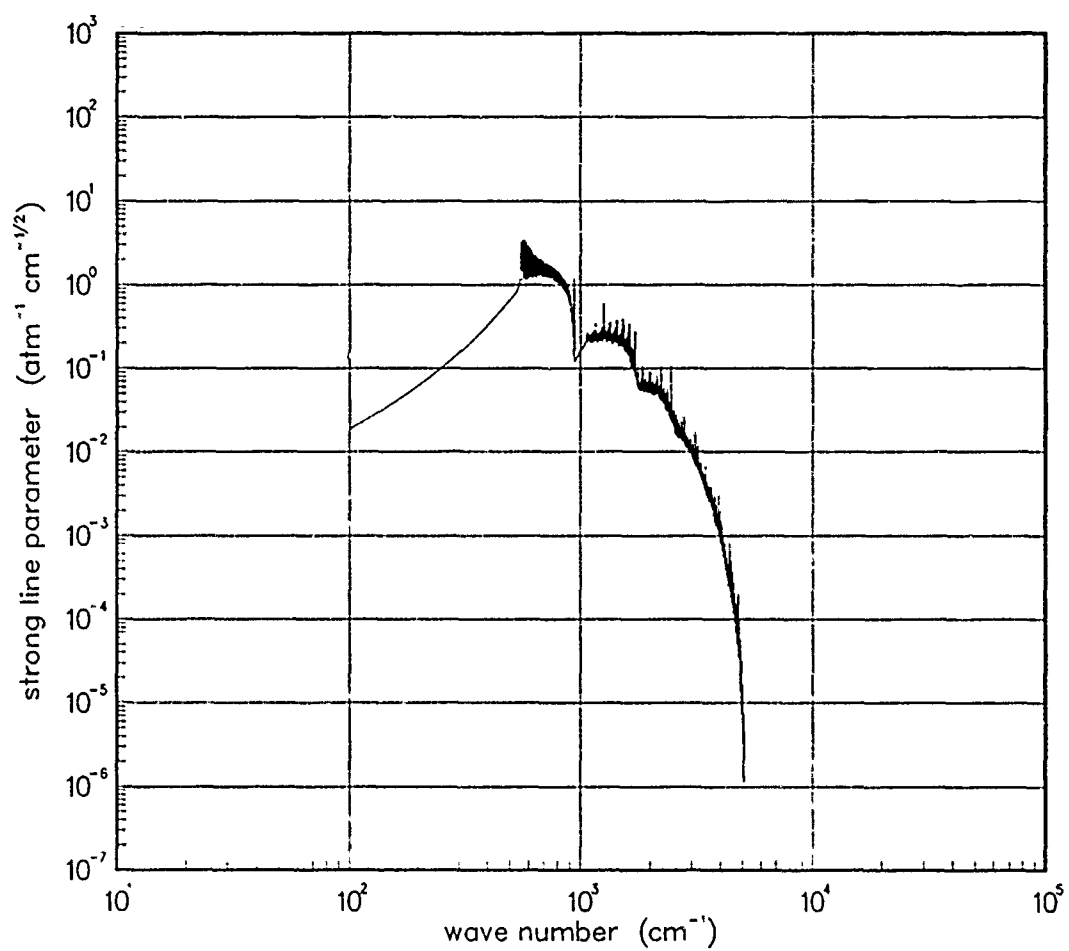


Figure 368. Strong-line parameter for FeO at 12000°K.

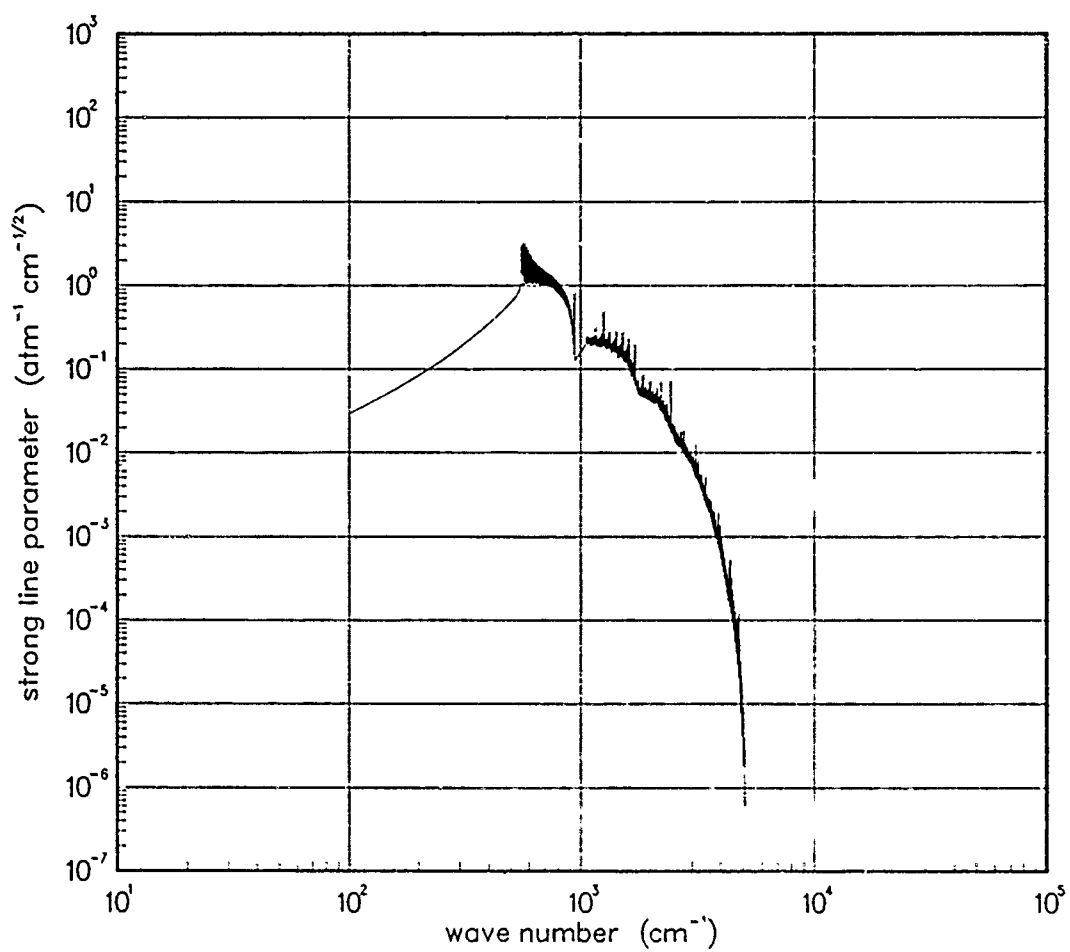


Figure 369. Strong-line parameter for FeO at 18000°K.

6.4 LITHIUM OXIDE (LiO).

Table 10. Spectroscopic data for LiO.

X $^2\Pi$

$$\begin{array}{lll} \omega_e = 848.6^* & \omega_e x_e = 5.4^\dagger & E_e = 0.0 \\ \alpha_e = 0.012^\dagger & A_e = -112.0^* & B_e = 1.222^* \end{array}$$

$$S_{10} = 450.^\dagger$$

$$\gamma_t(300^\circ\text{K}) = 0.04^\dagger$$

A $^2\Sigma^+$

$$\begin{array}{lll} \omega_e = 871.0^* & \omega_e x_e = 5.6^\dagger & E_e = 2800.^* \\ \alpha_e = 0.013^\dagger & & B_e = 1.35^* \end{array}$$

$$S_{10} = 450.^\dagger$$

$$\gamma_t(300^\circ\text{K}) = 0.04^\dagger$$

Data Source:

*S.M. Freund, E. Herbst, R.P. Mariella, Jr., and W. Klemperer, Radio Frequency Spectrum of the X $^2\Pi$ State of $^7\text{Li}^{16}\text{O}$, (preprint), Harvard University (1971).

† Estimate.

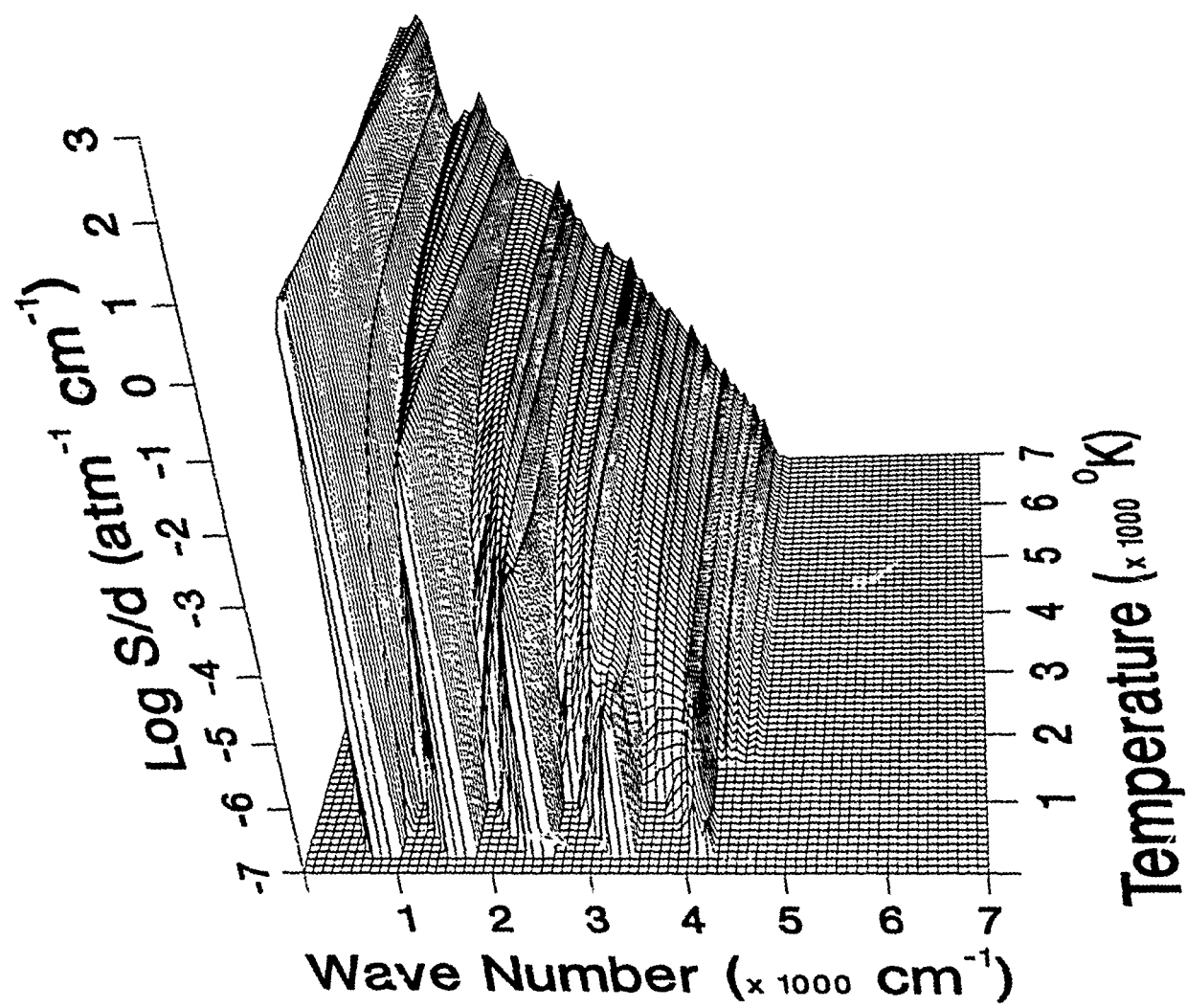


Figure 370. Weak-line parameter for LiO.

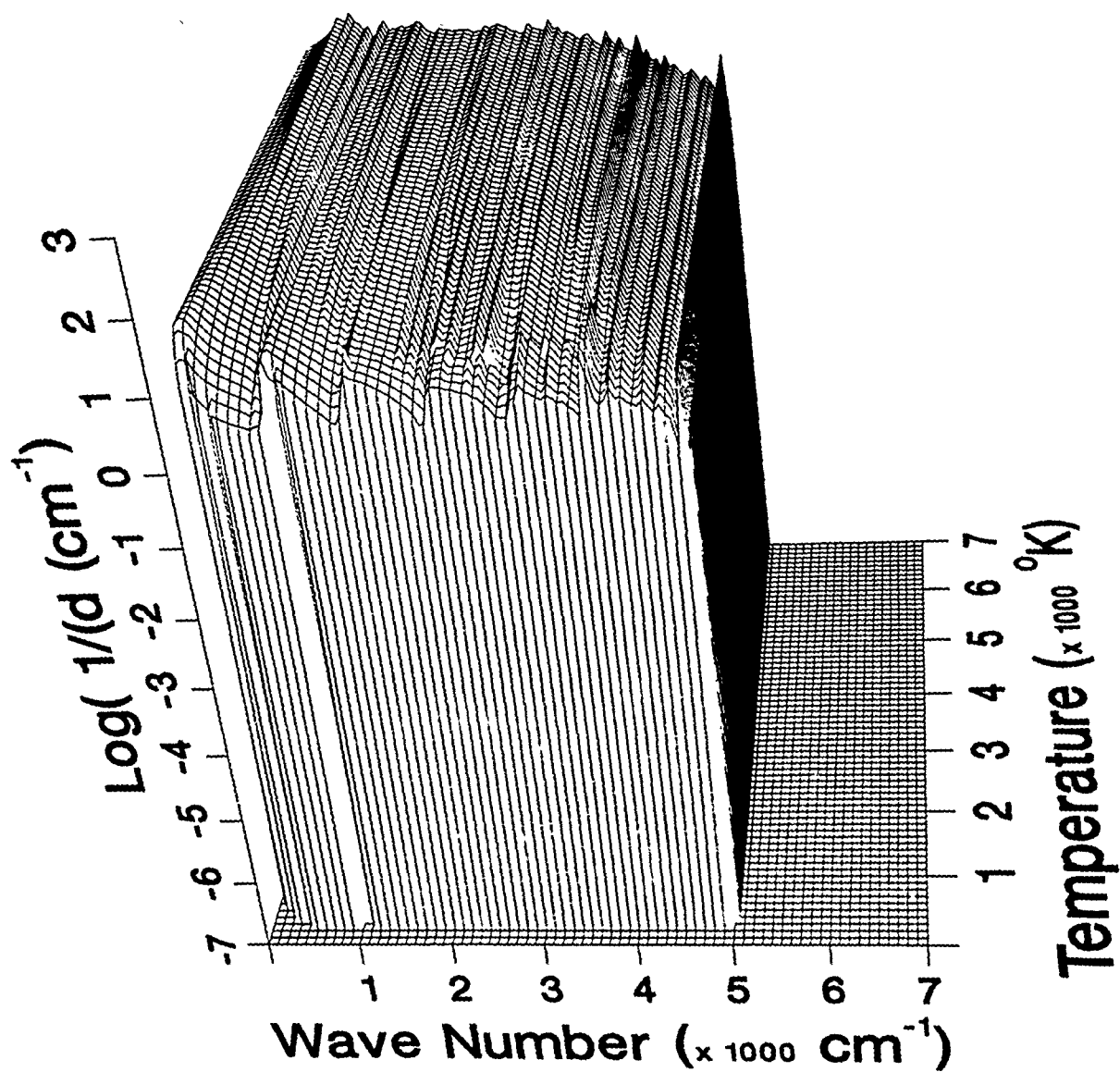


Figure 371. Inverse line spacing for LiO.

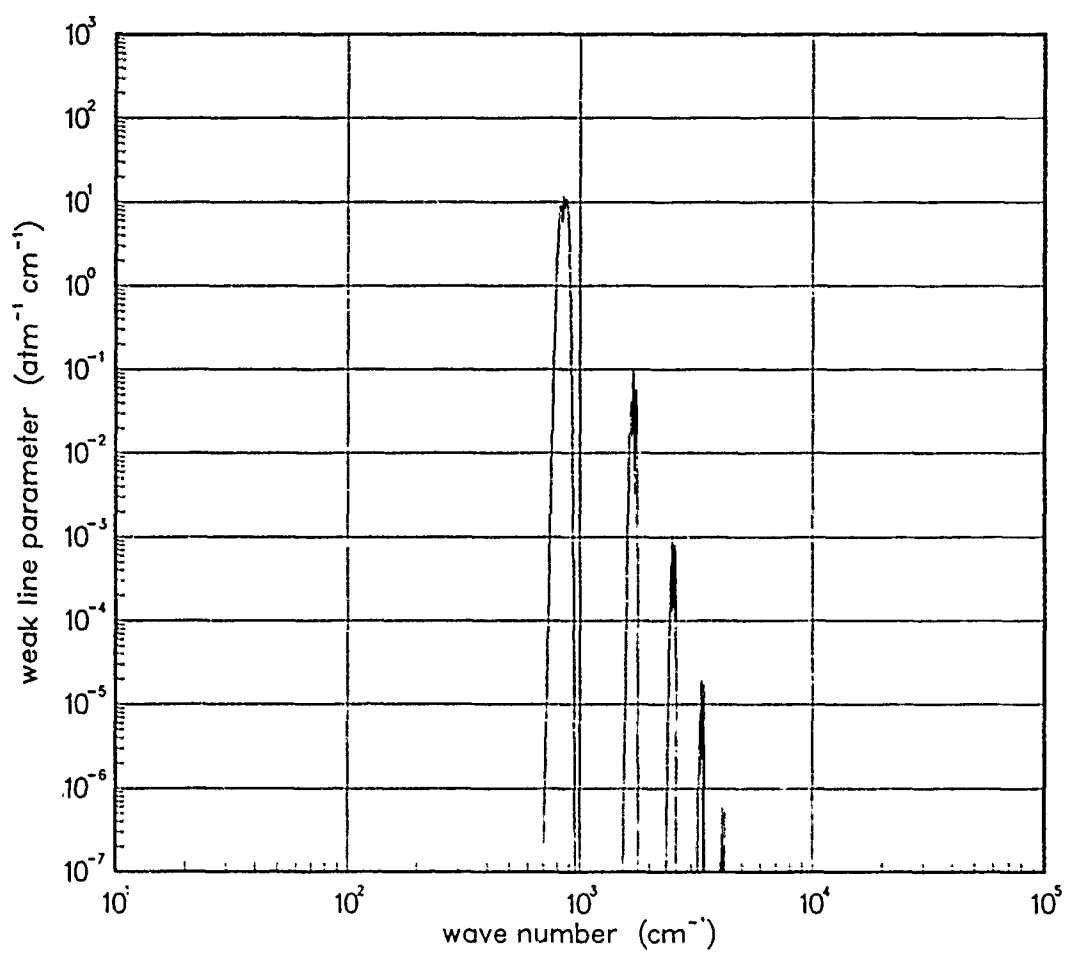


Figure 372. Weak-line parameter for LiO at 200°K.

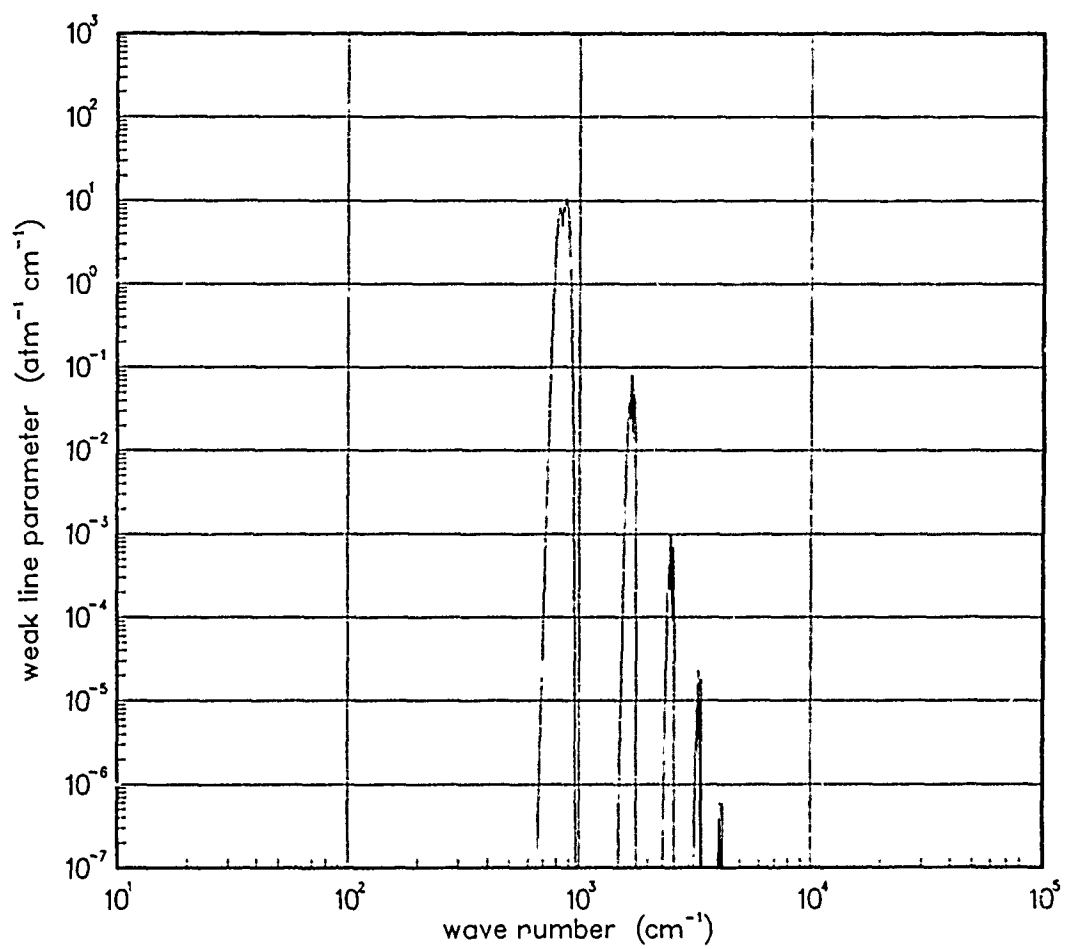


Figure 373. Weak-line parameter for LiO at 300°K.

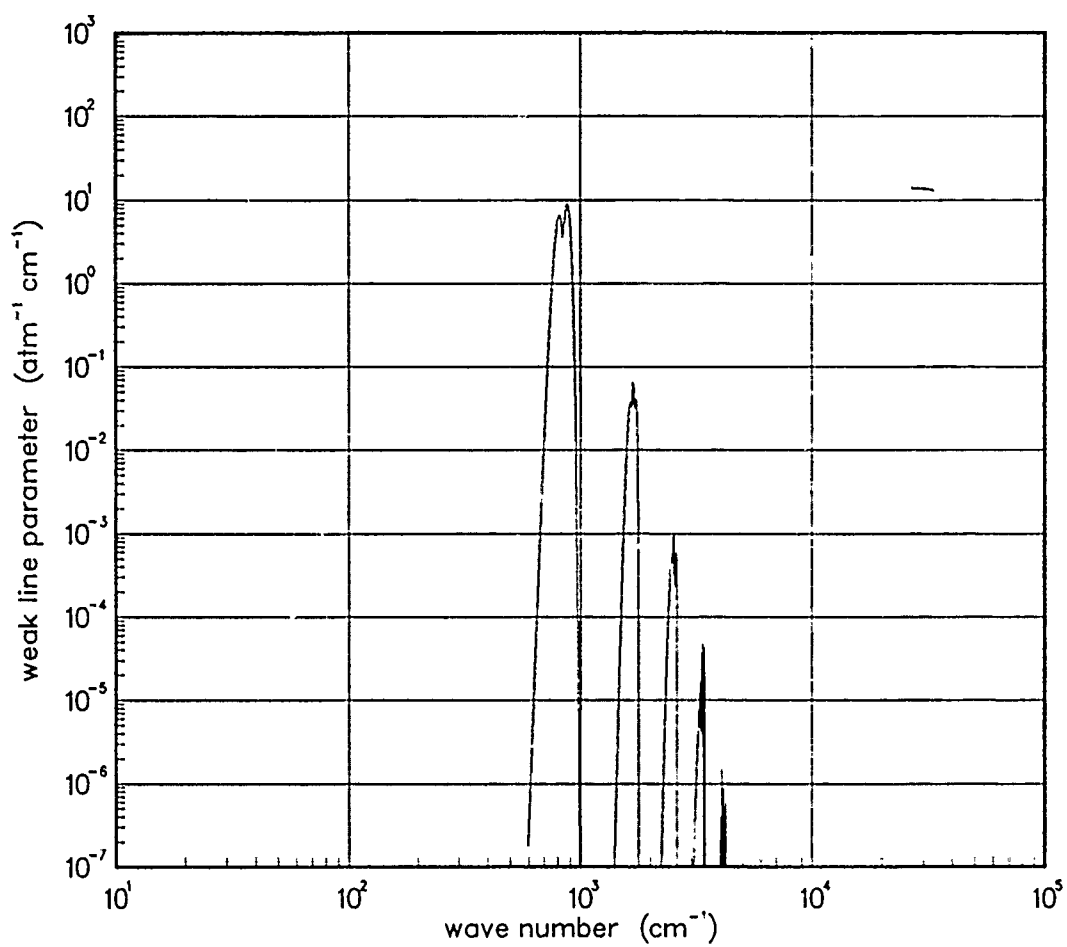


Figure 374. Weak-line parameter for LiO at 500°K.

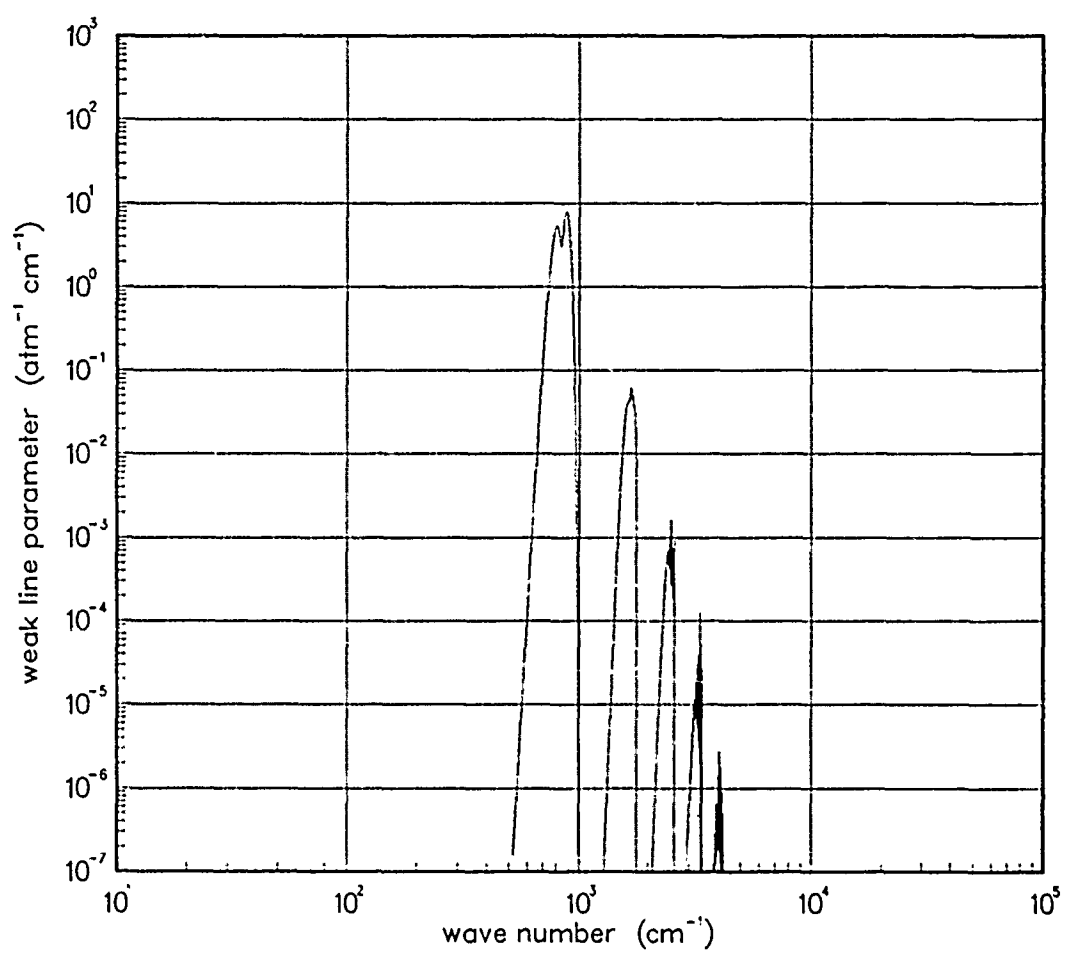


Figure 375. Weak-line parameter for LiO at 750°K.

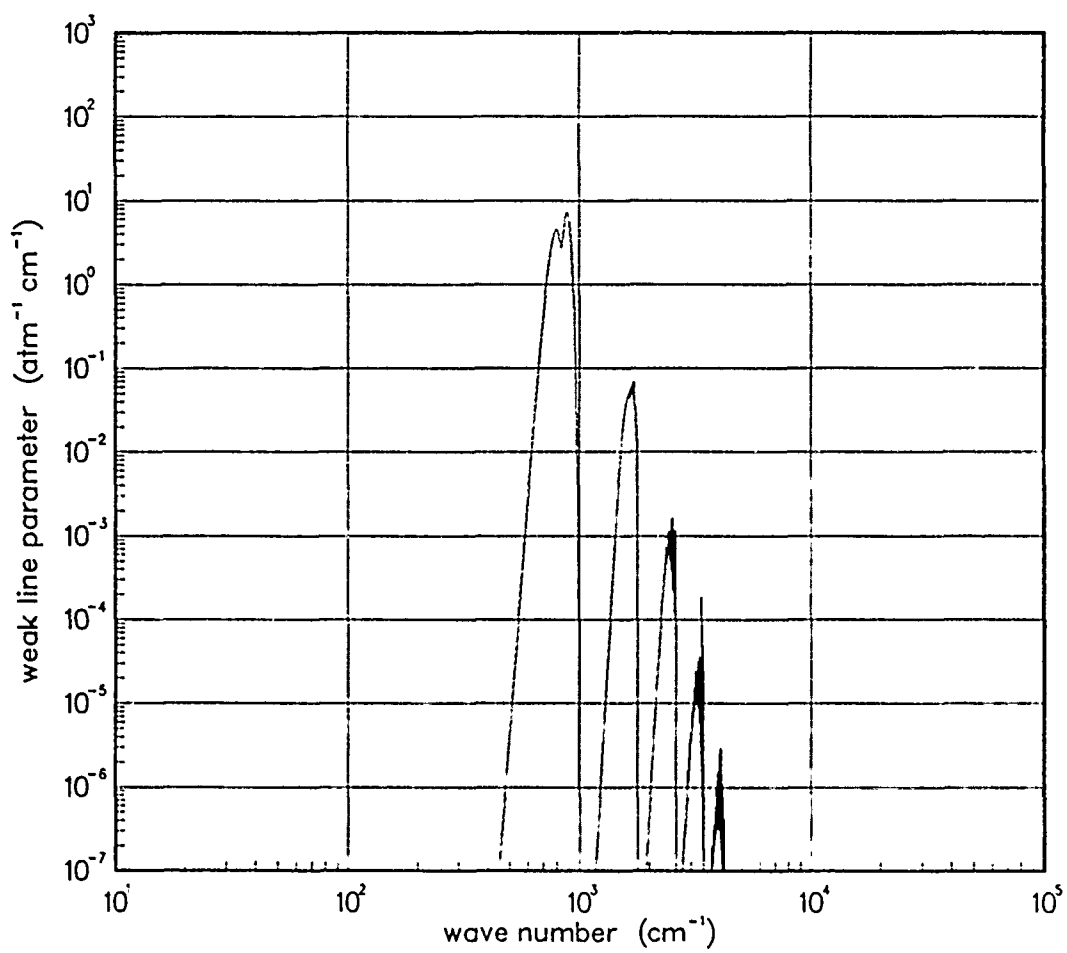


Figure 376. Weak-line parameter for LiO at 1000°K.

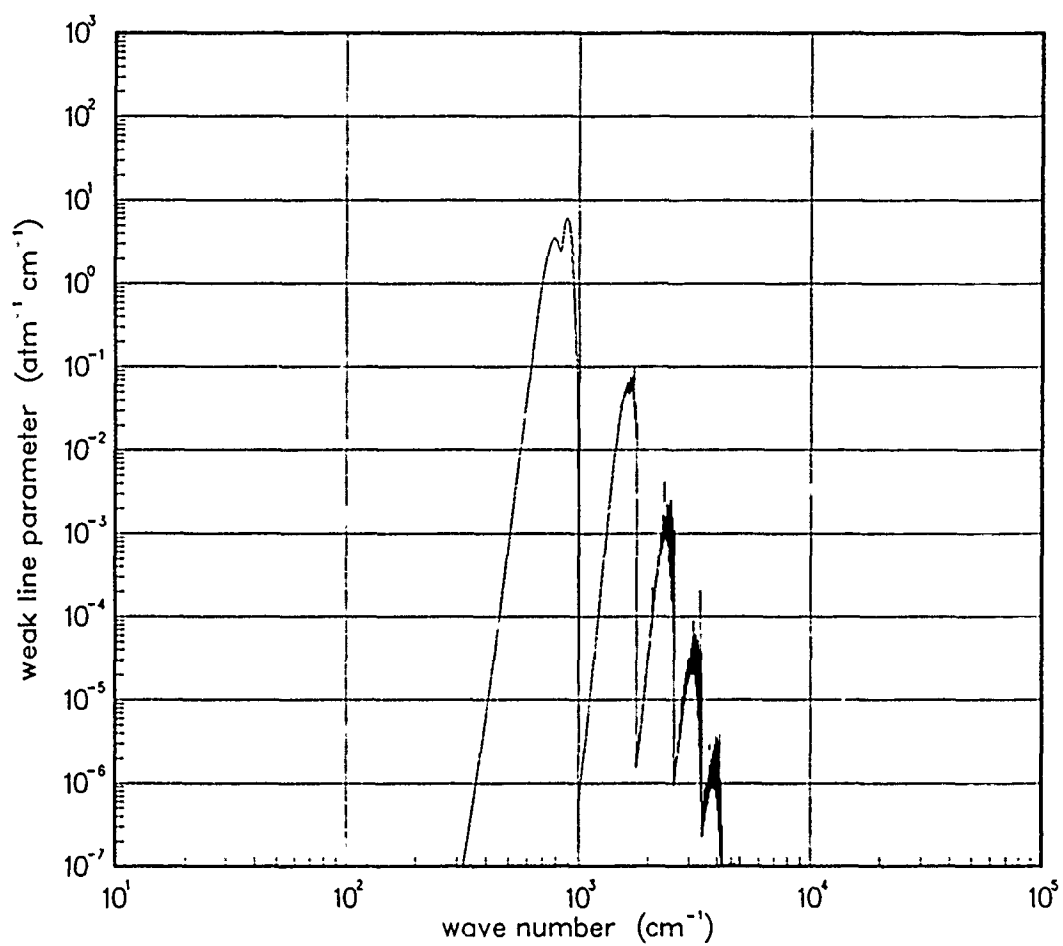


Figure 377. Weak-line parameter for LiO at 1500°K.

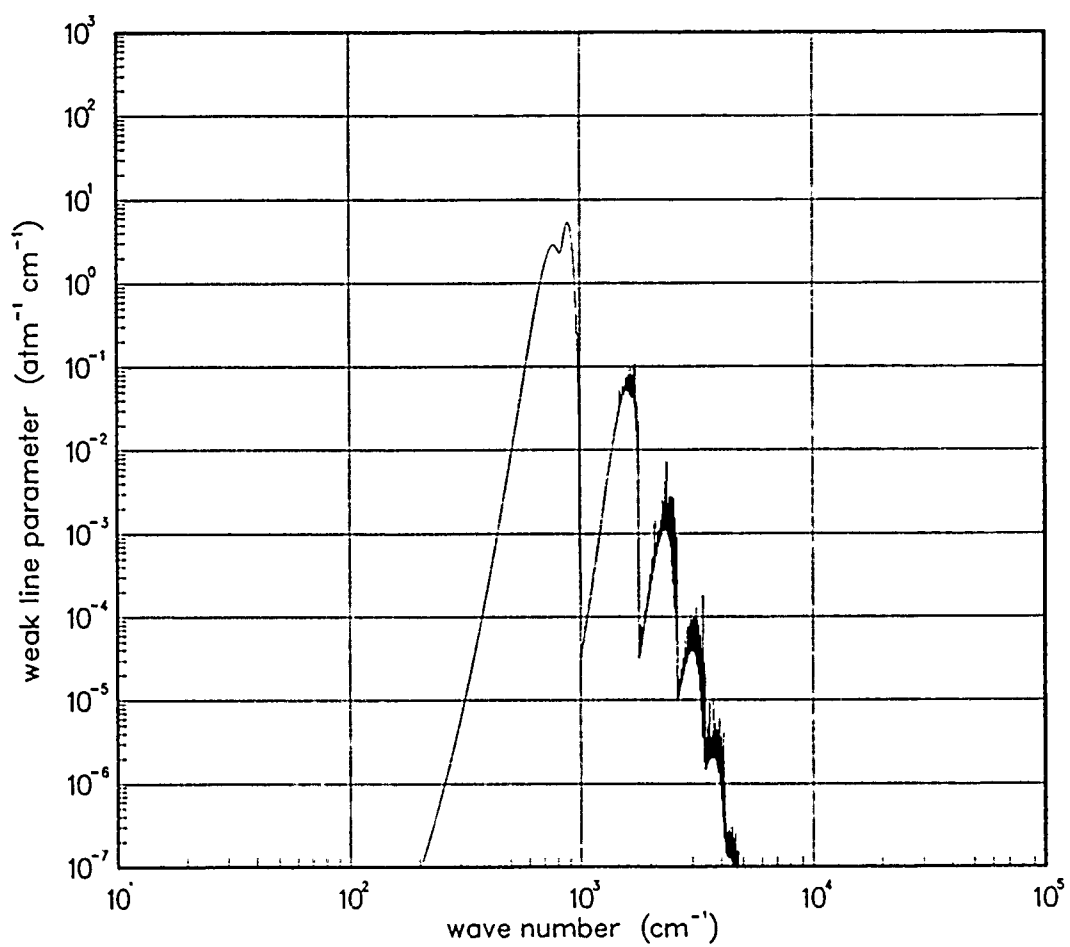


Figure 378. Weak-line parameter for LiO at 2000°K.

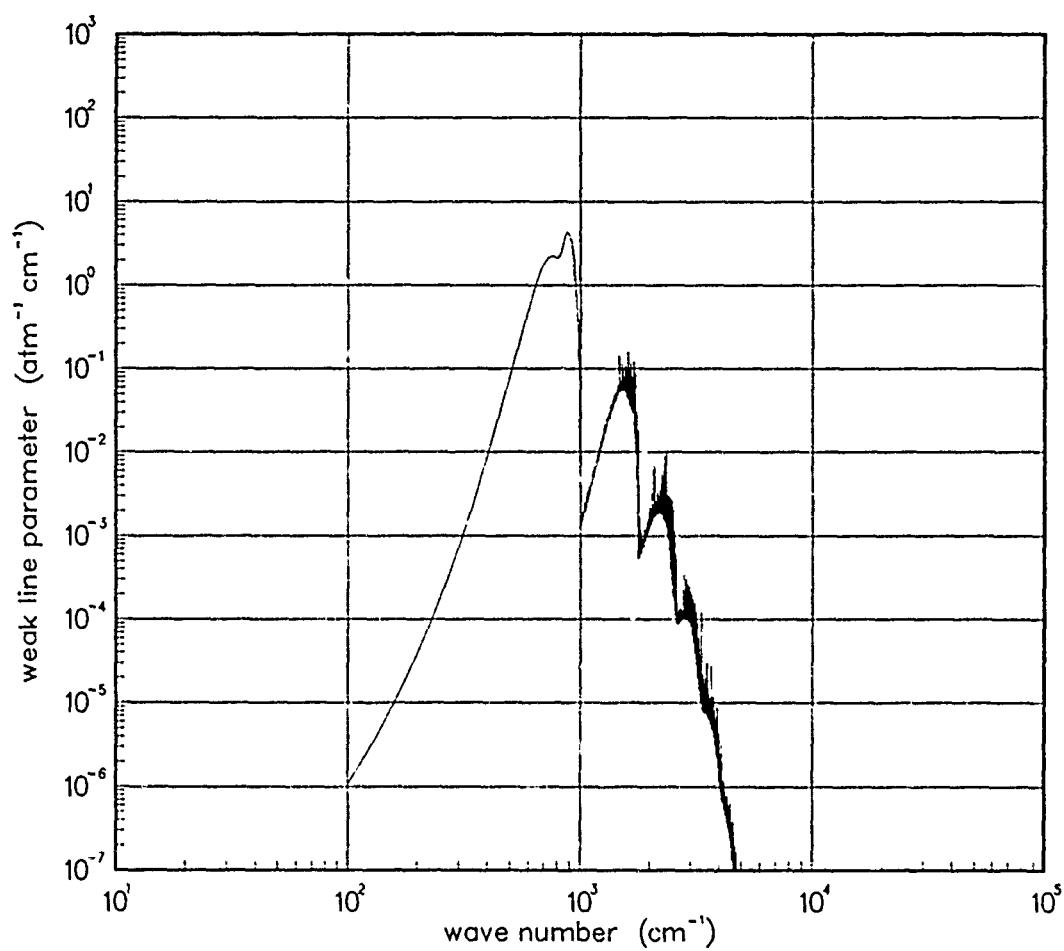


Figure 379. Weak-line parameter for LiO at 3000°K.

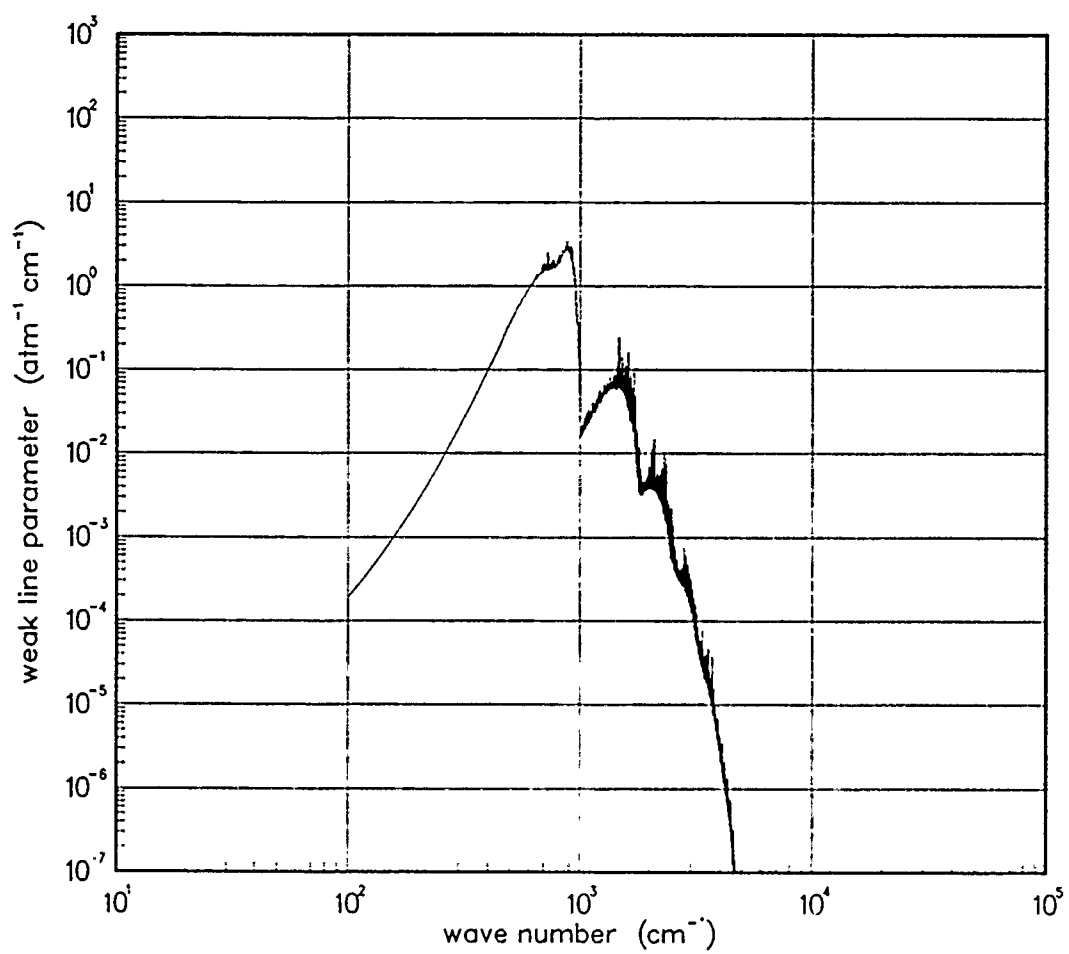


Figure 380. Weak-line parameter for LiO at 5000°K.

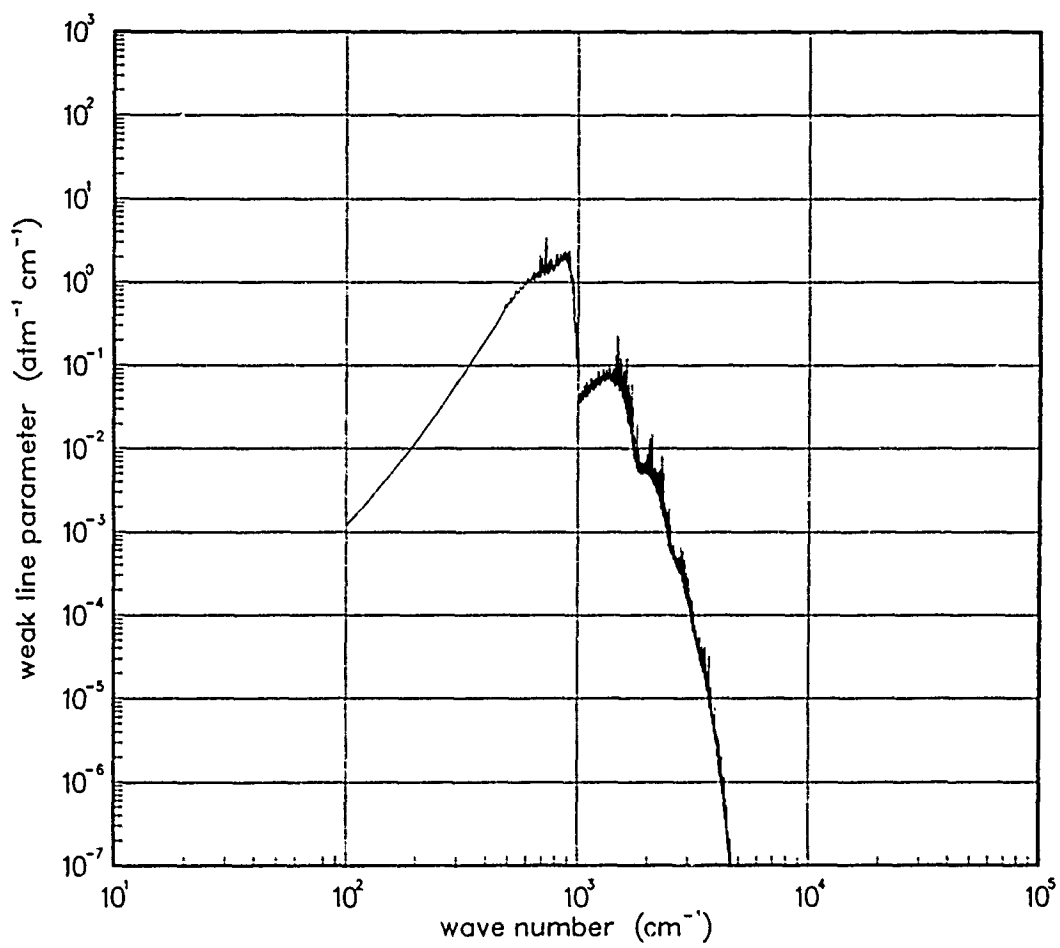


Figure 381. Weak-line parameter for LiO at 7000°K.

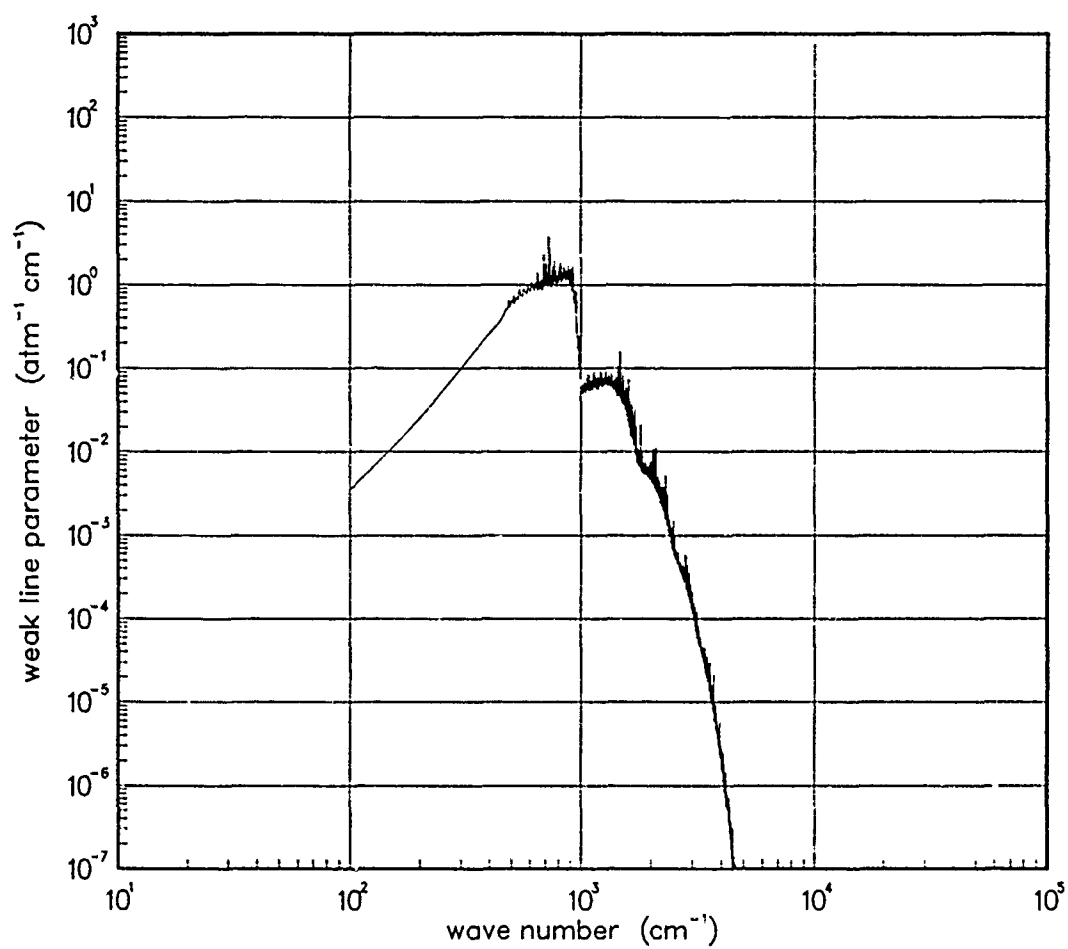


Figure 382. Weak-line parameter for LiO at 10000°K.

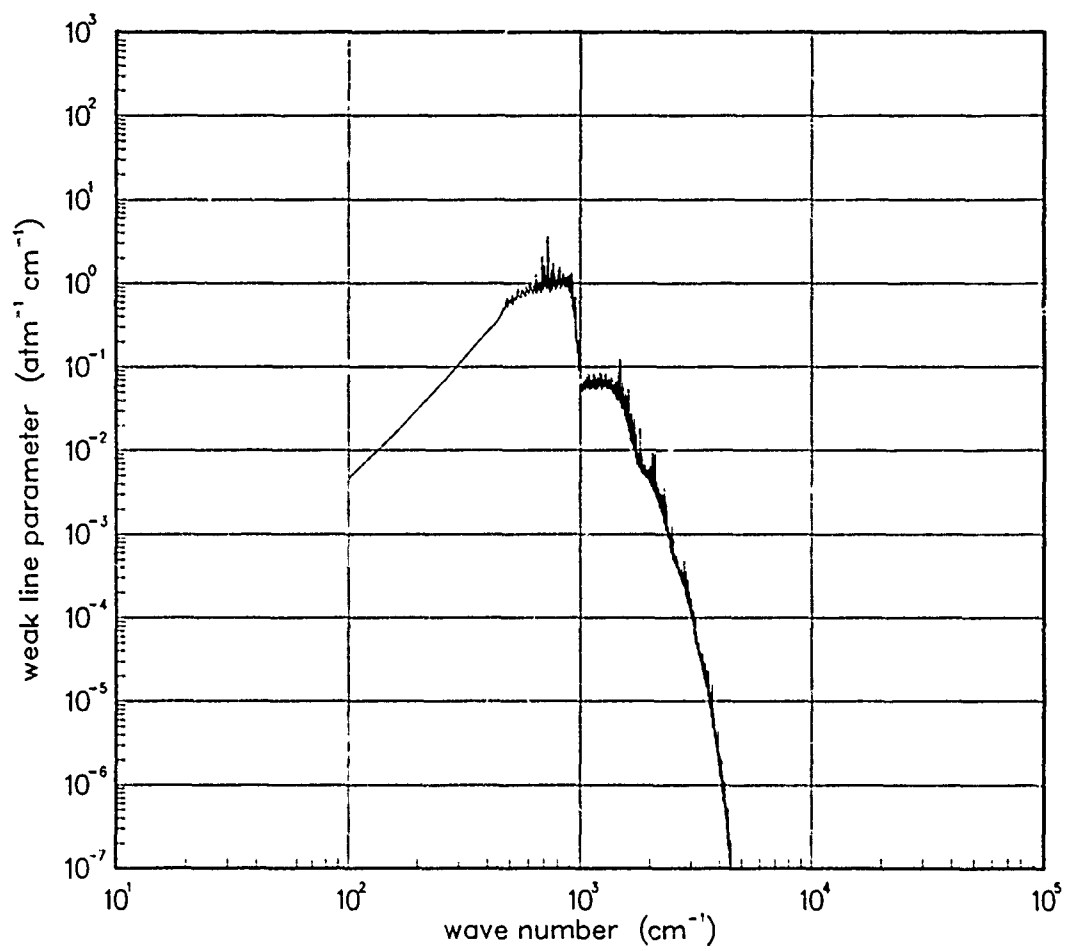


Figure 383. Weak-line parameter for LiO at 12000°K.

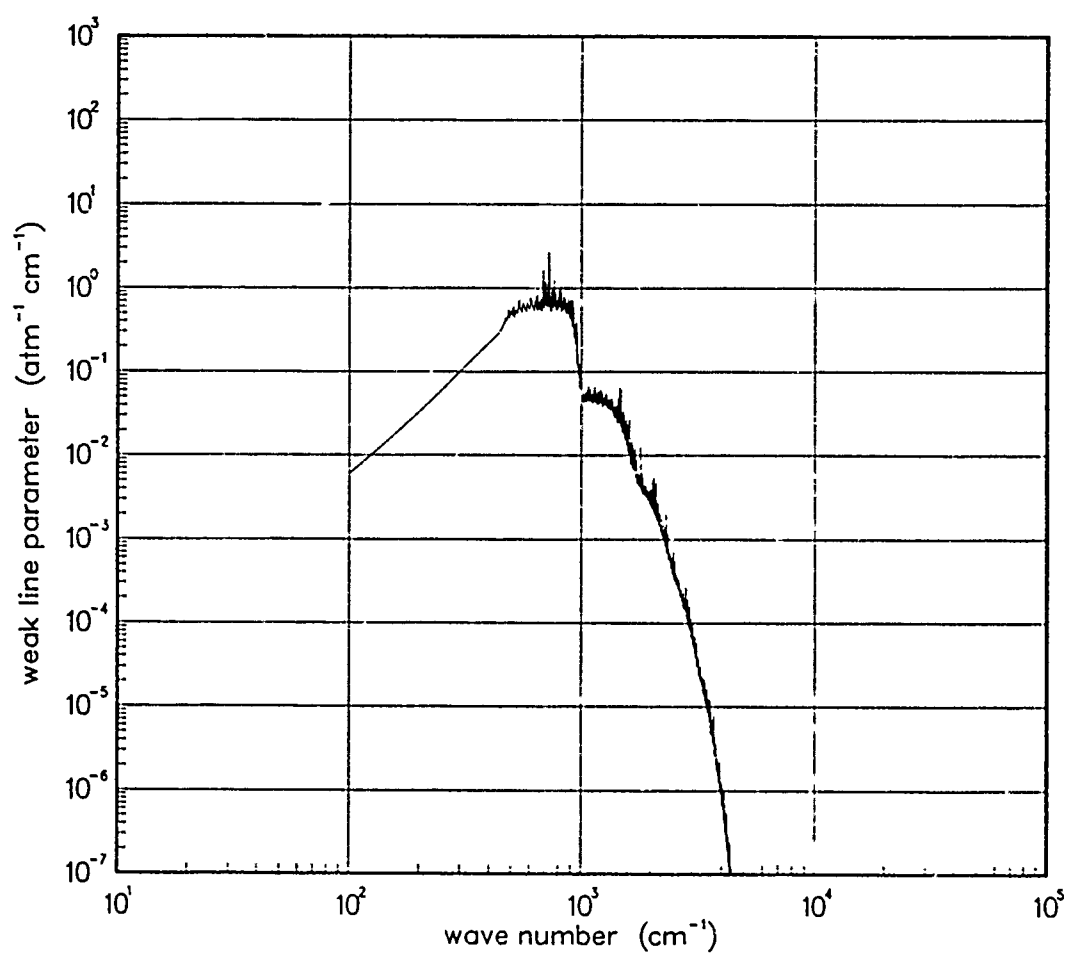


Figure 384. Weak-line parameter for LiO at 18000°K.

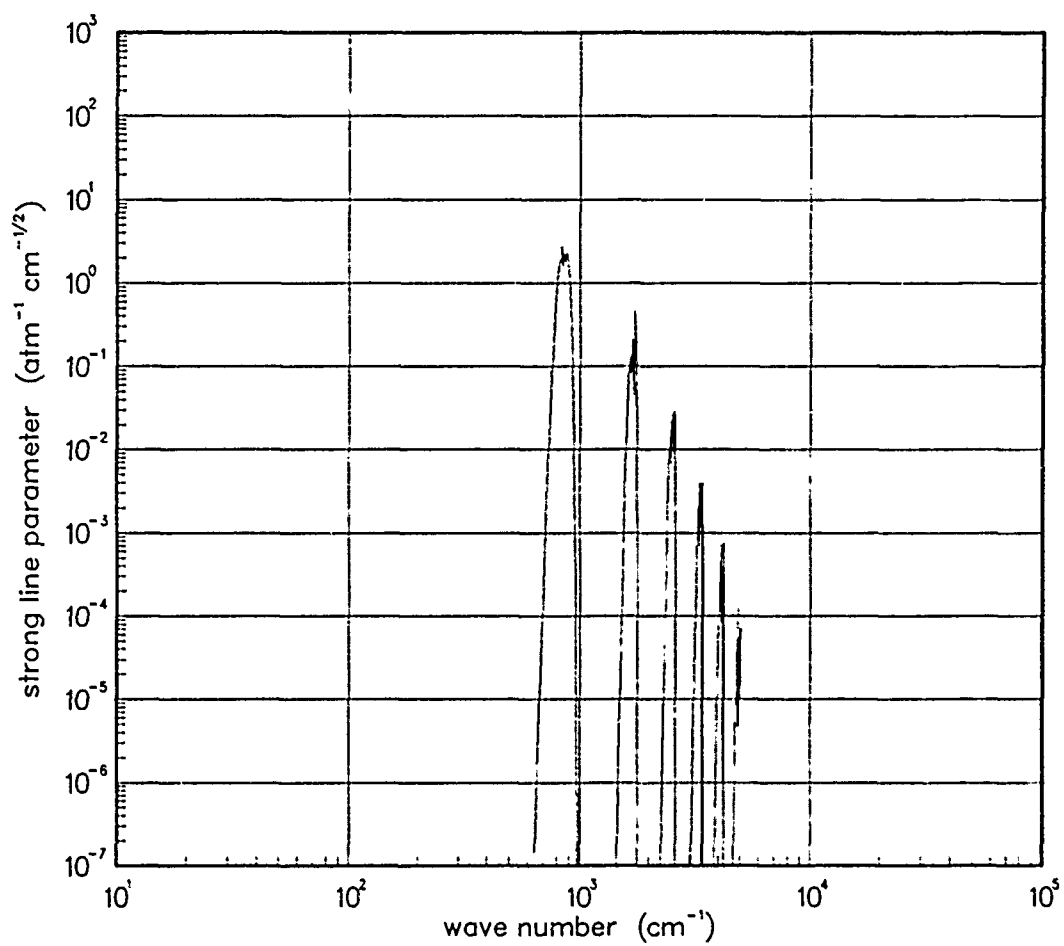


Figure 385. Strong-line parameter for LiO at 200°K.

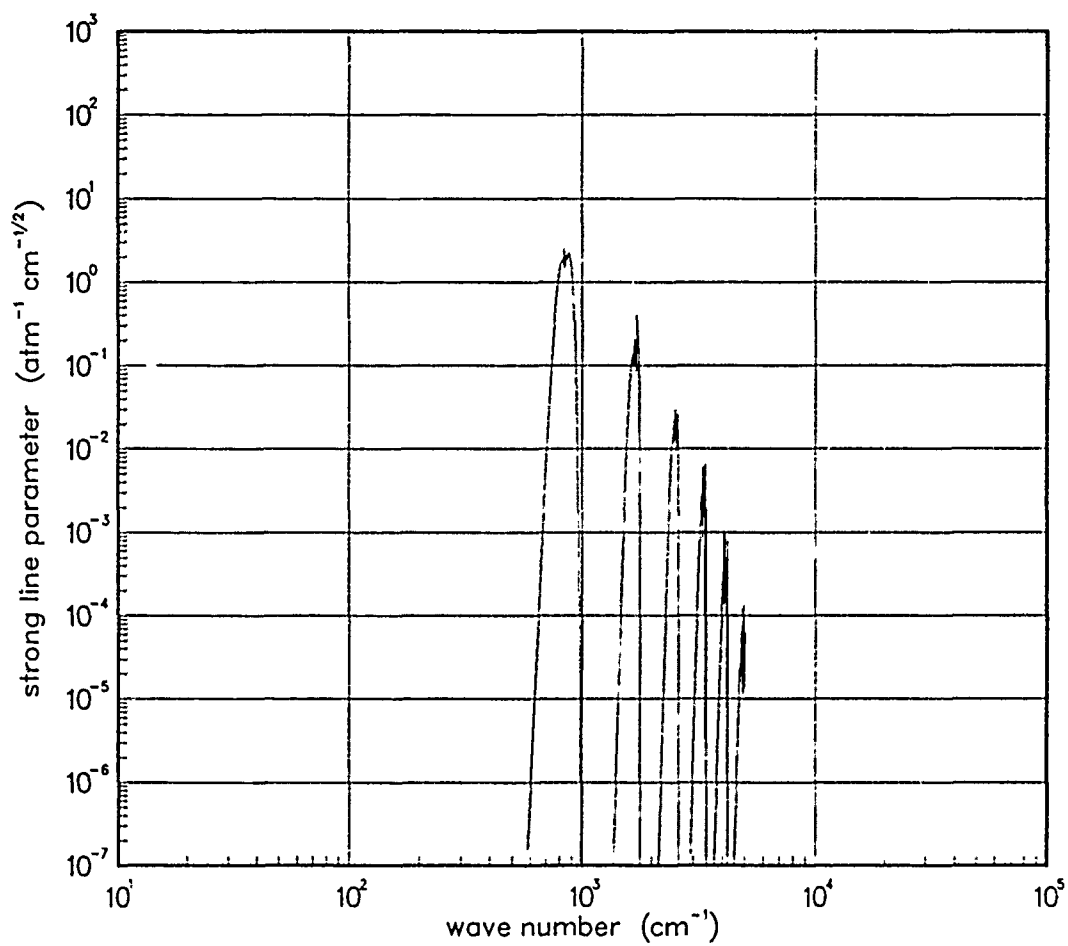


Figure 386. Strong-line parameter for LiO at 300°K.

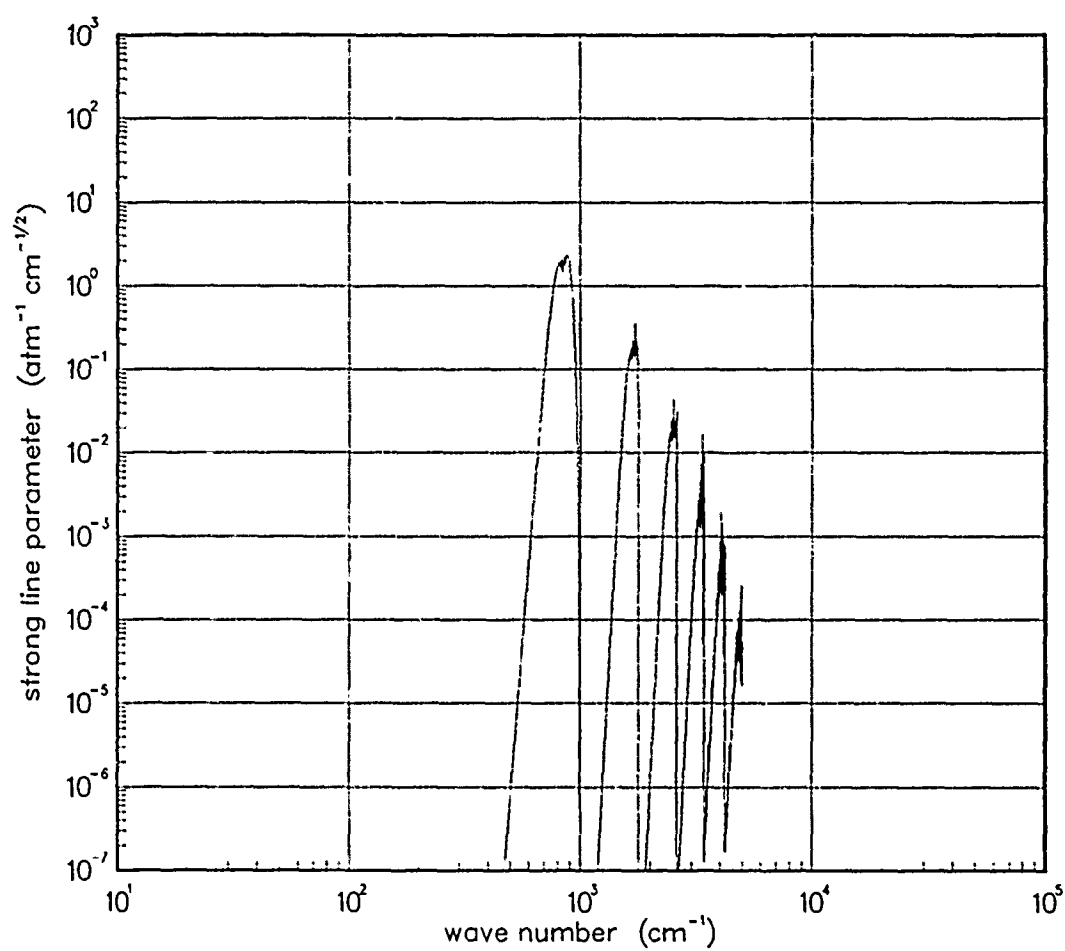


Figure 387. Strong-line parameter for LiO at 500°K.

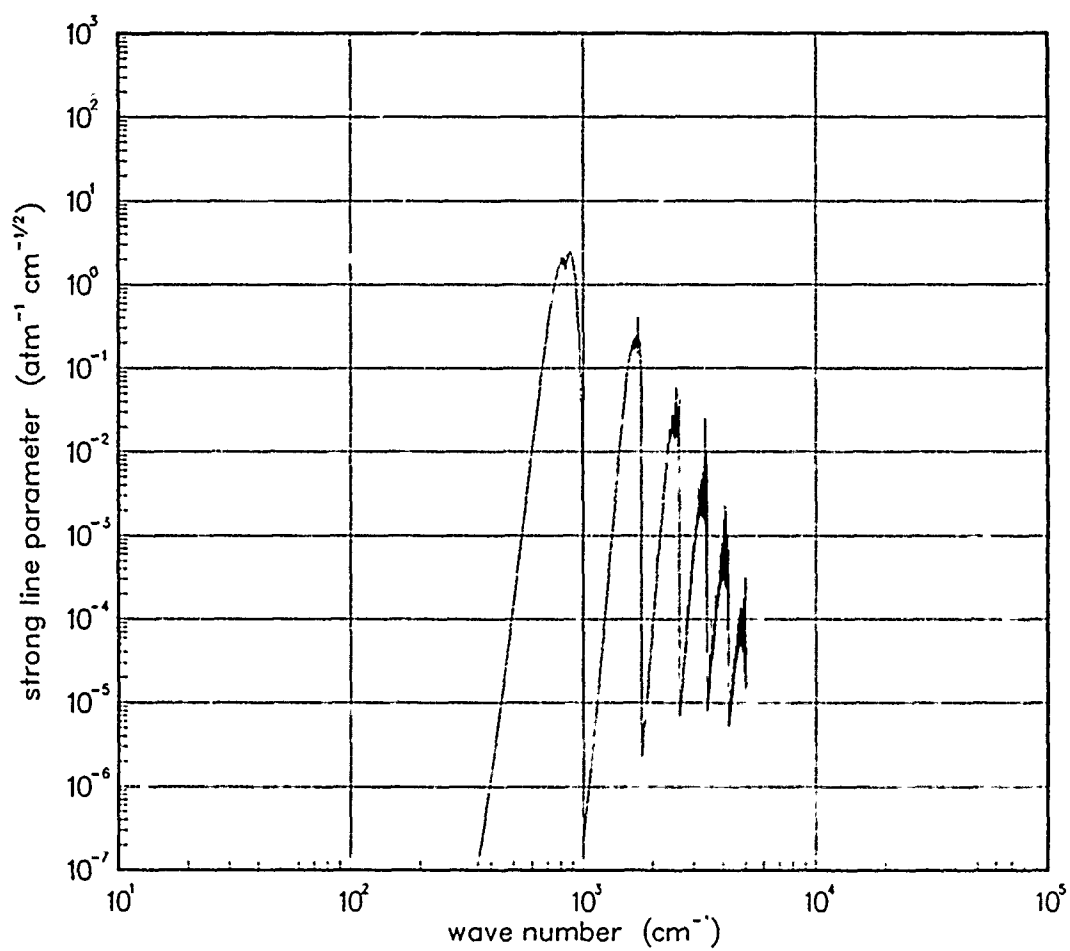


Figure 388. Strong-line parameter for LiO at 750°K.

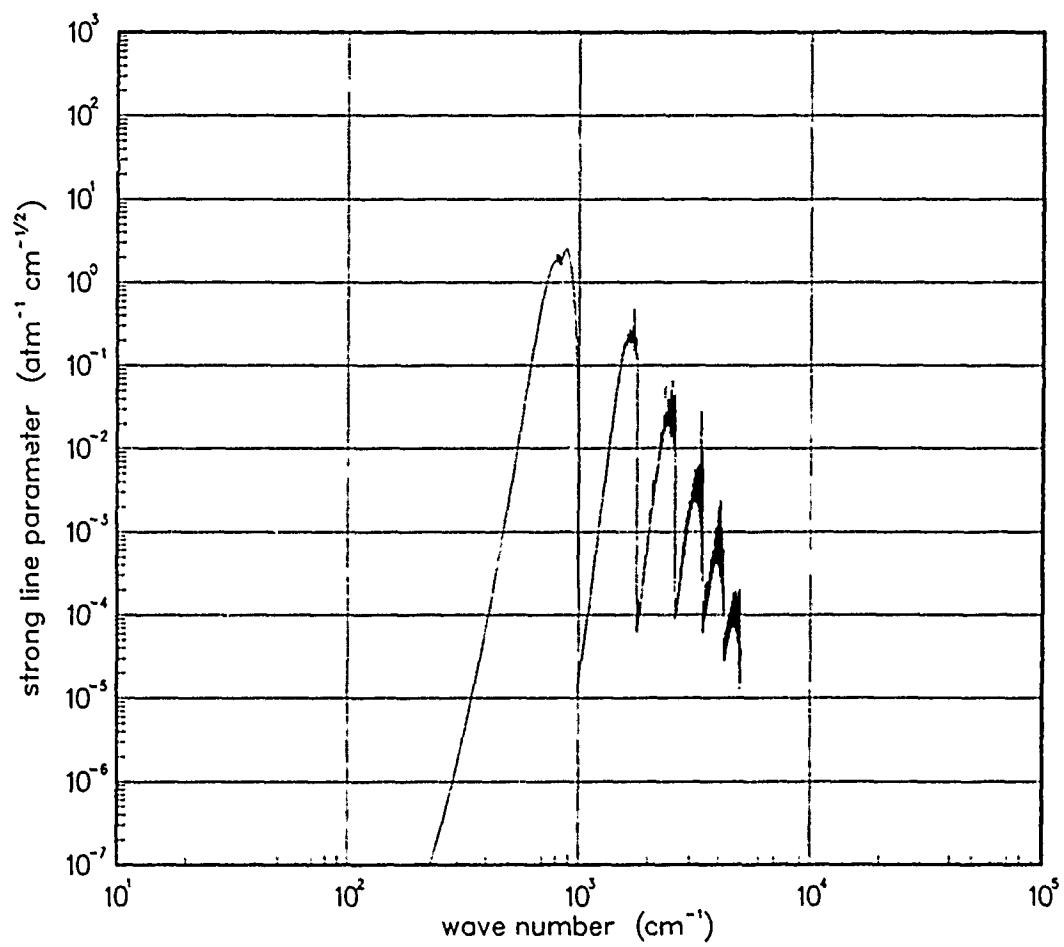


Figure 389. Strong-line parameter for LiO at 1000°K.

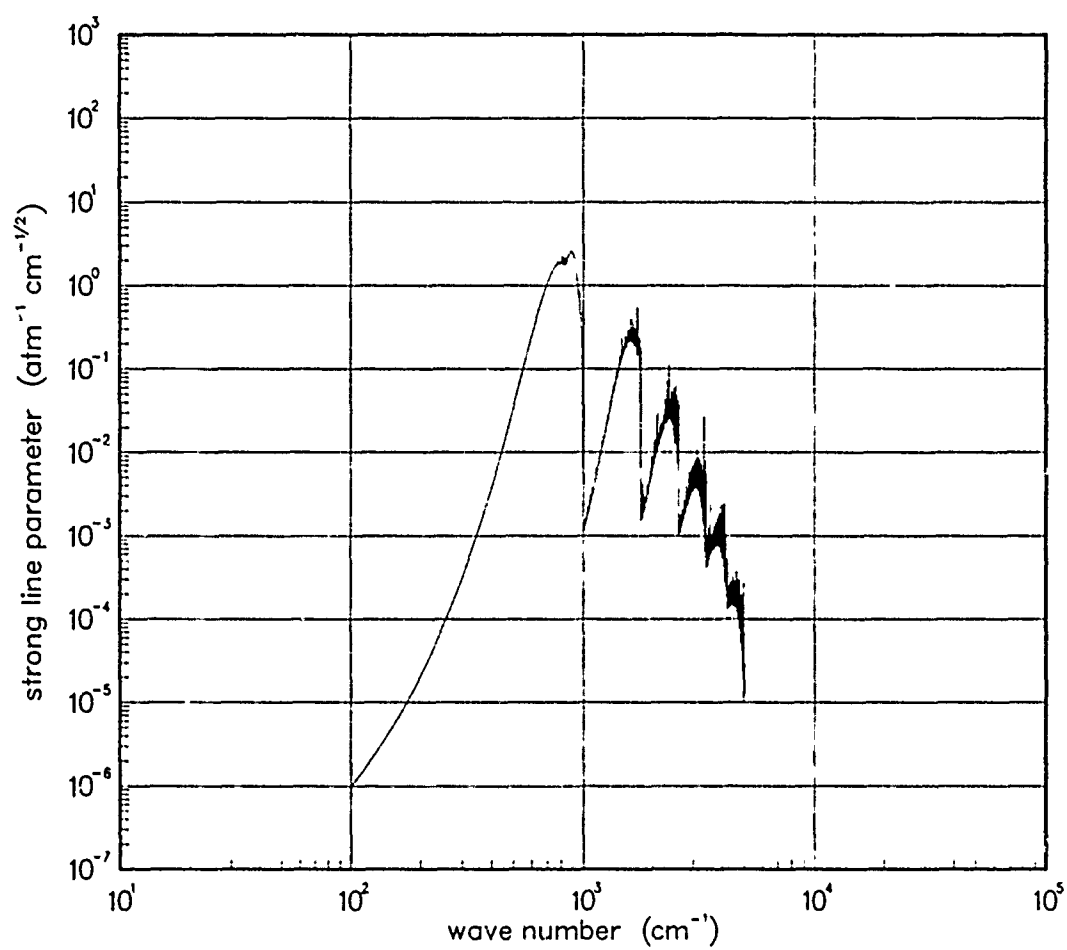


Figure 390. Strong-line parameter for LiO at 1500°K.

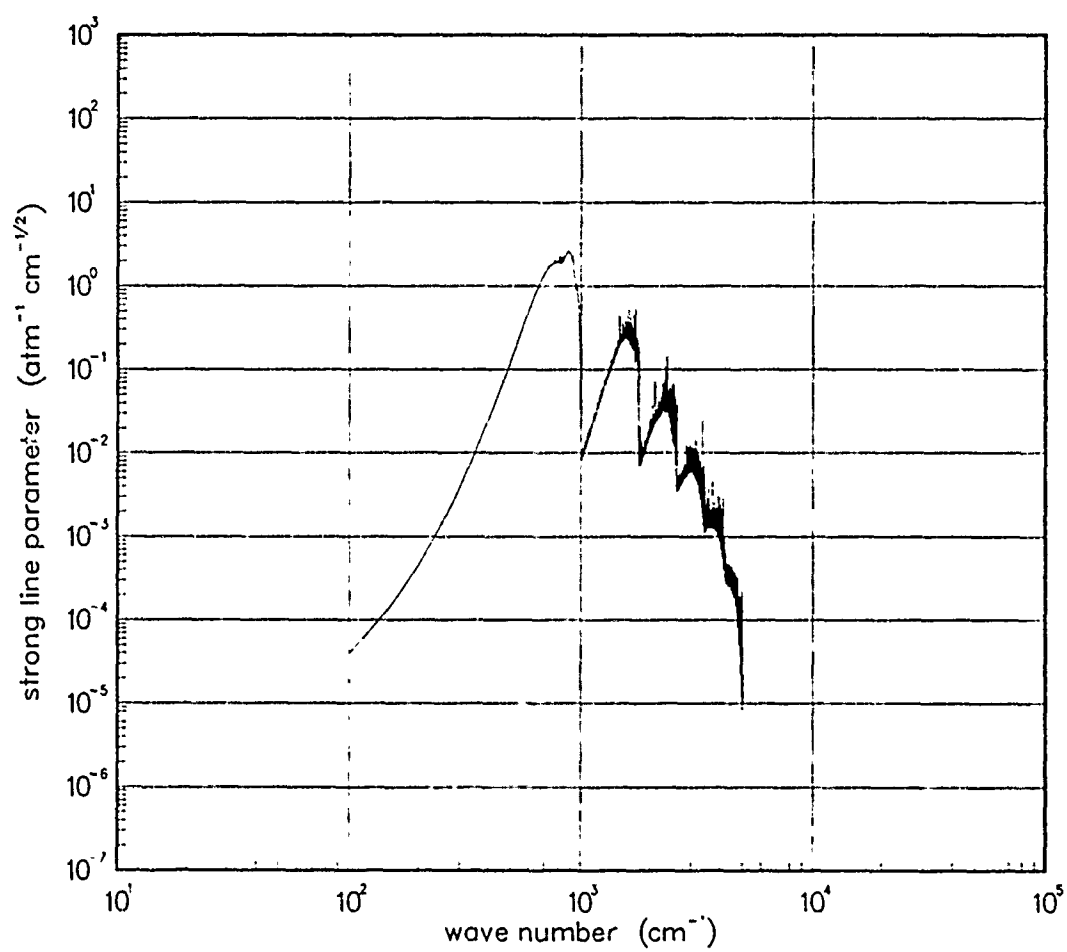


Figure 391. Strong-line parameter for LiO at 2000°K.

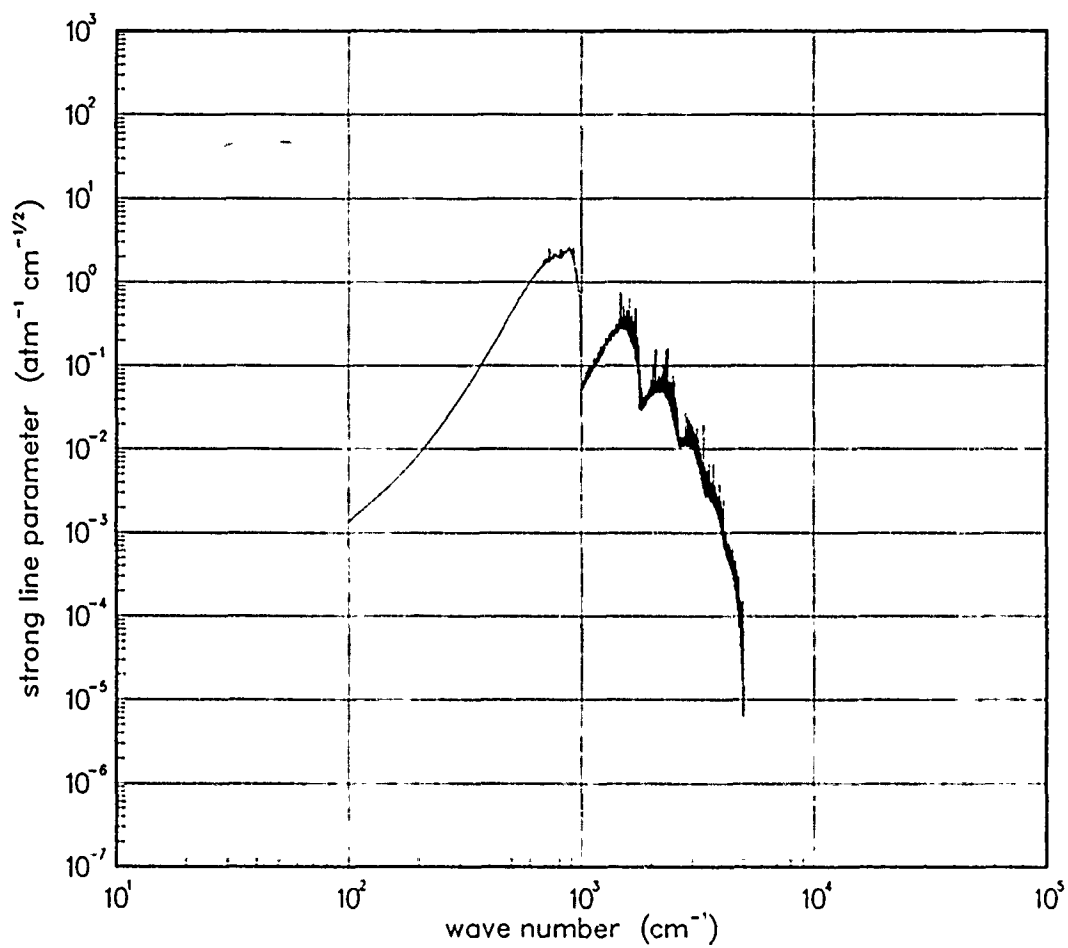


Figure 392. Strong-line parameter for LiO at 3000°K.

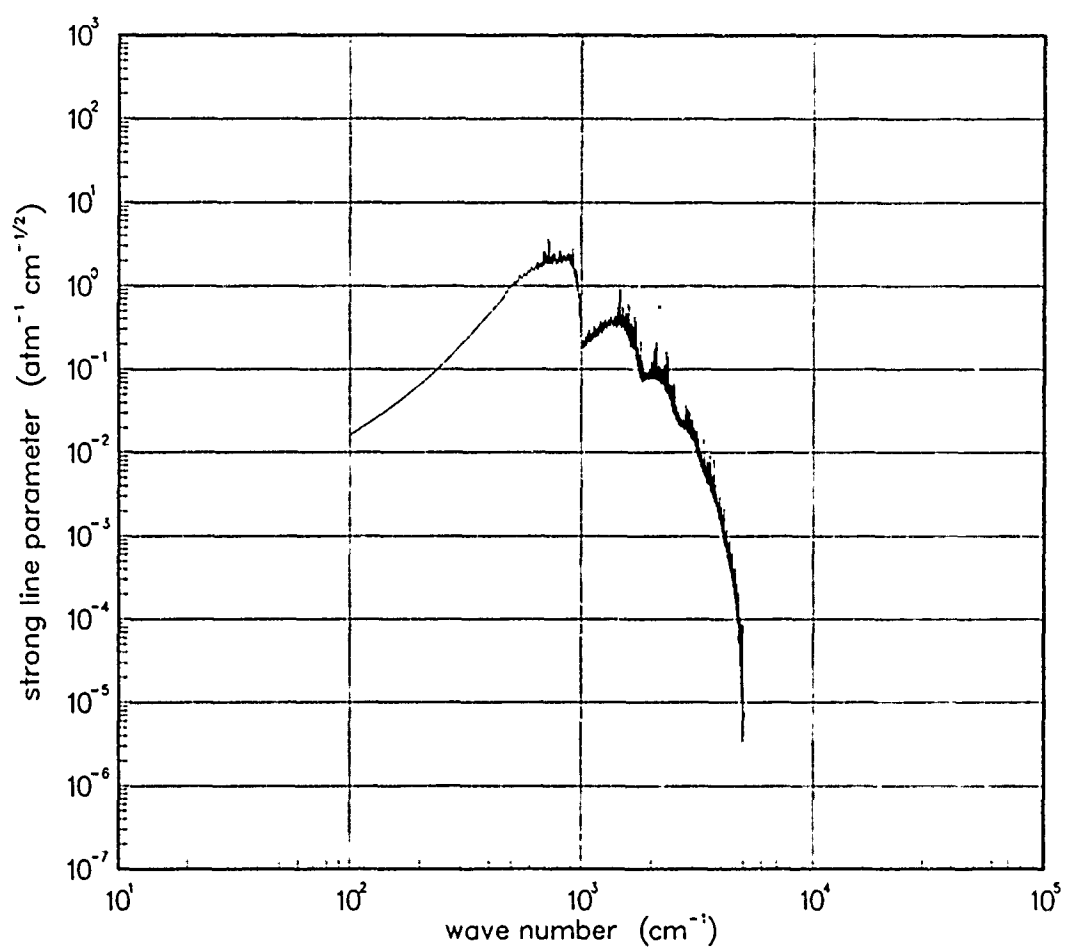


Figure 393. Strong-line parameter for LiO at 5000°K.

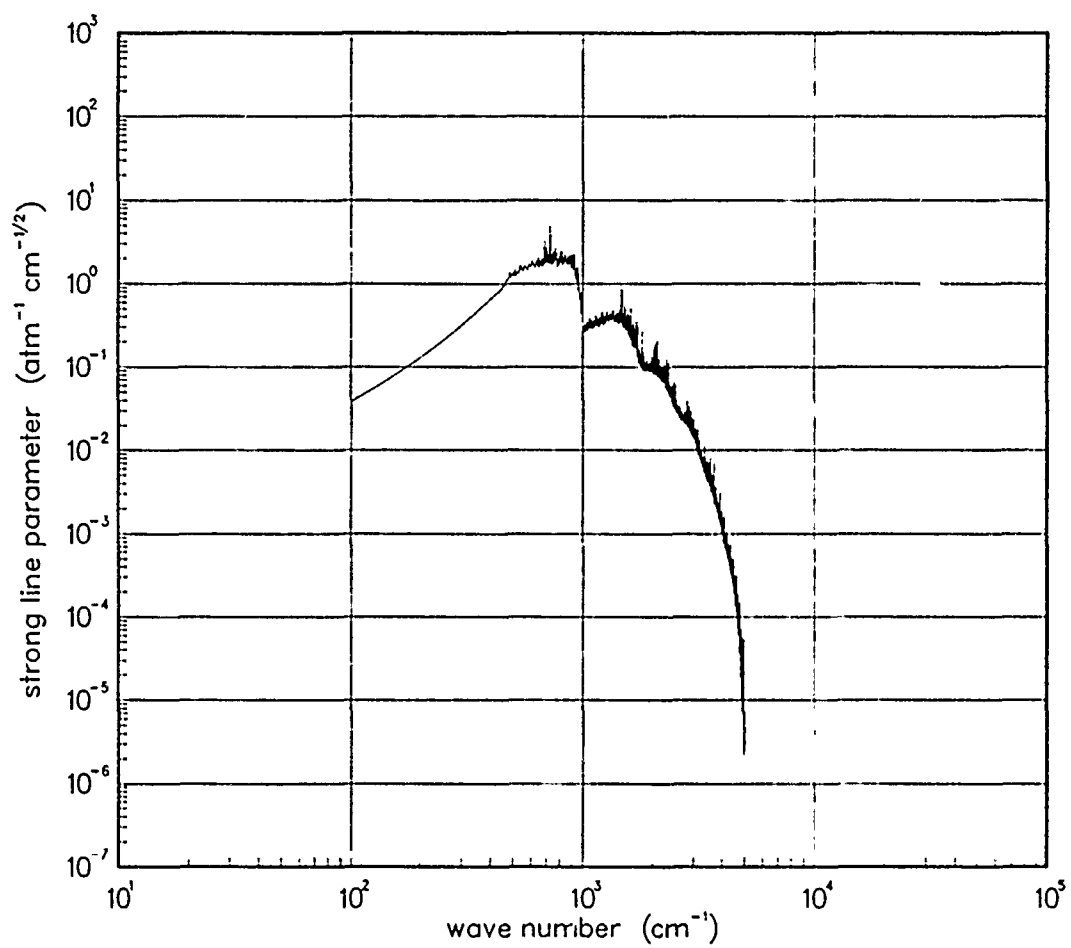


Figure 394. Strong-line parameter for LiO at 7000°K.

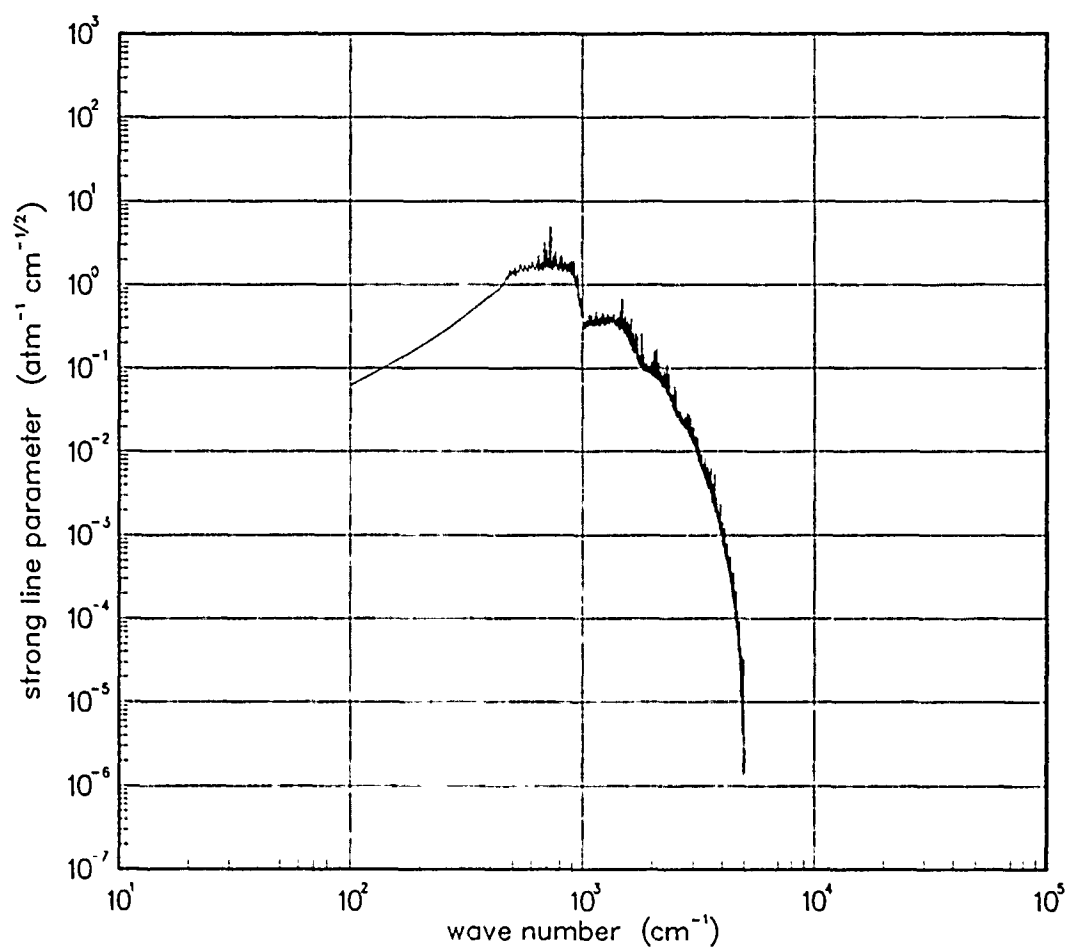


Figure 395. Strong-line parameter for LiO at 10000°K.

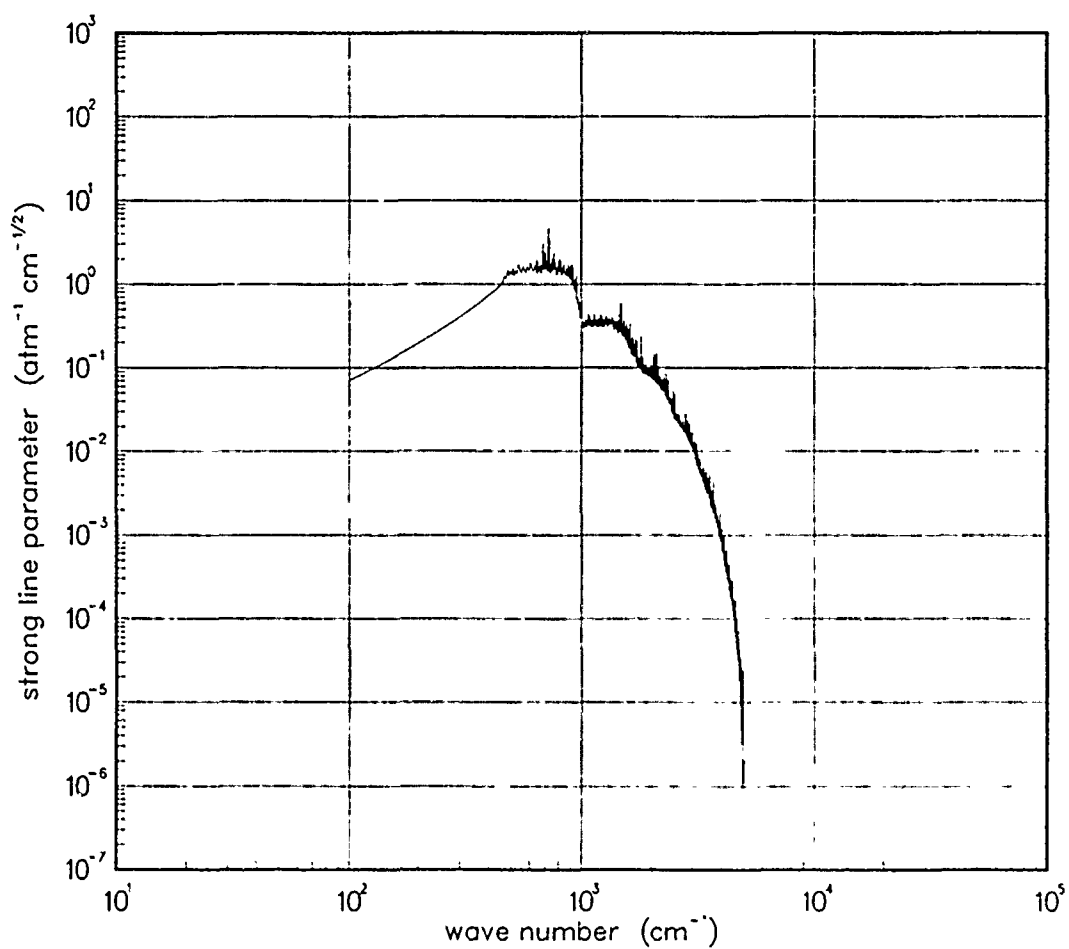


Figure 396. Strong-line parameter for LiO at 12000°K.

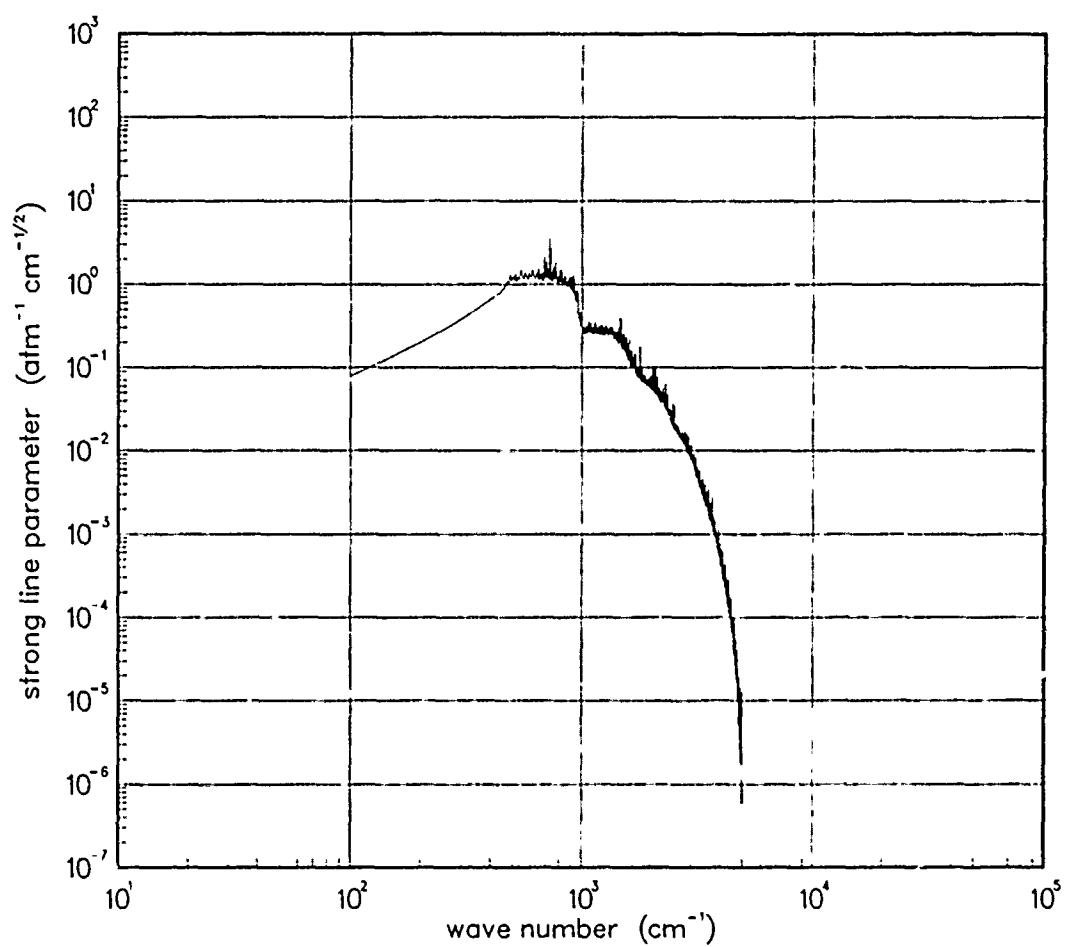


Figure 397. Strong-line parameter for LiO at 18000°K.

6.5. MAGNESIUM OXIDE (MgO).

Table 11. Spectroscopic data for MgO.

X $^1\Sigma$

$$\begin{array}{ll} \omega_e = 785.06^* & \omega_e x_e = 5.18^* \\ \alpha_e = 0.0050^* & B_e = 0.57430^* \end{array}$$

$$S_{10} = 440.^{\dagger}$$

$$\gamma_t(300^\circ\text{K}) = 0.04^{\ddagger}$$

X $^1\Pi$

$$\begin{array}{lll} \omega_e = 664.4^* & \omega_e x_e = 3.9^* & E_e = 3563.30^* \\ \alpha_e = 0.0040^* & B_e = 0.505^* & \end{array}$$

$$S_{10} = 440.^{\dagger}$$

$$\gamma_t(300^\circ\text{K}) = 0.04^{\ddagger}$$

Data Source:

*B. Rosen, ed., Spectroscopic Data Relative to Diatomic Molecules, Pergamon Press, New York (1970).

[†]M. Yoshimine, J. Phys. Soc. Japan 25, 1100 (1968).

[‡]Estimate.

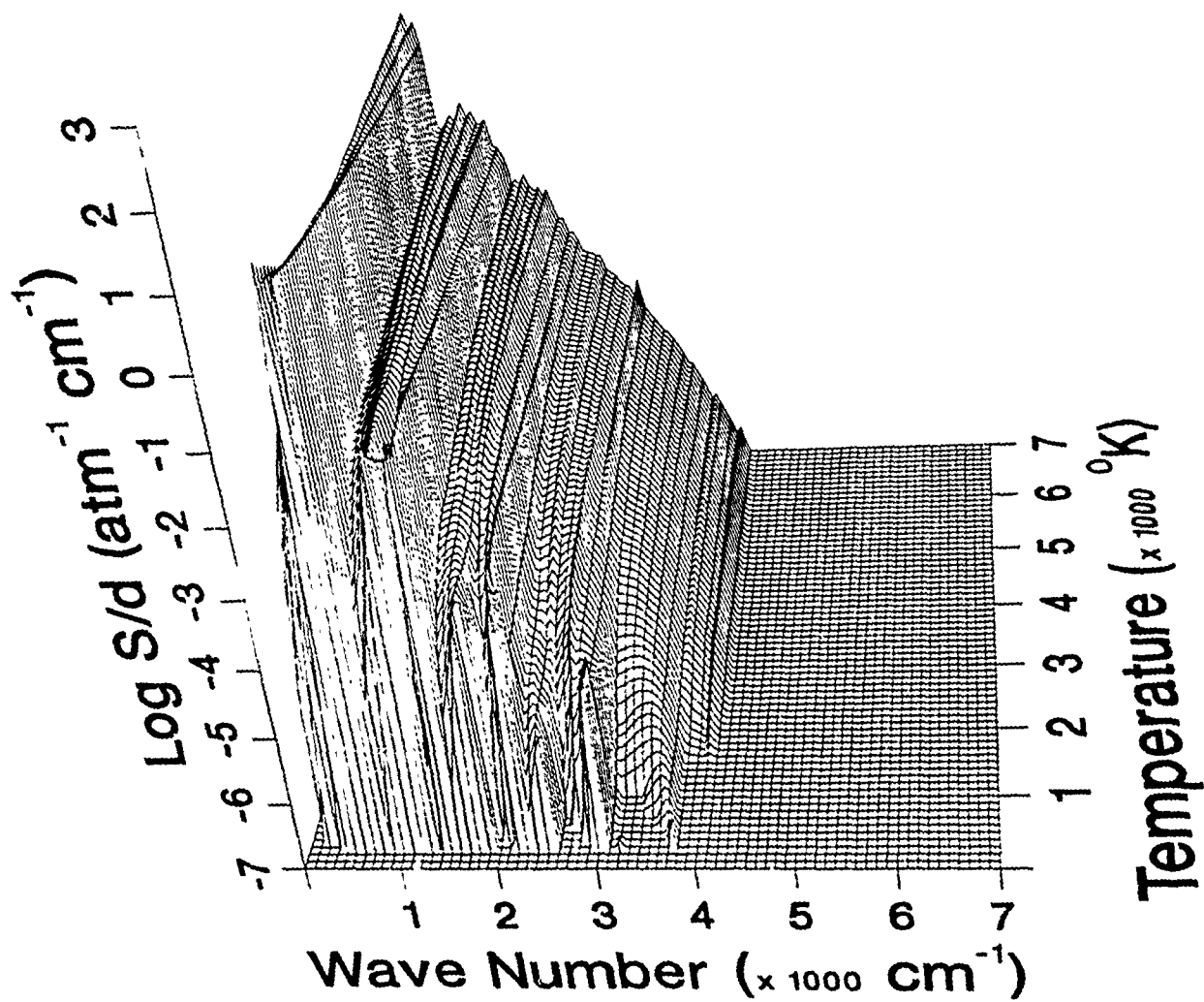


Figure 398. Weak-line parameter for MgO.

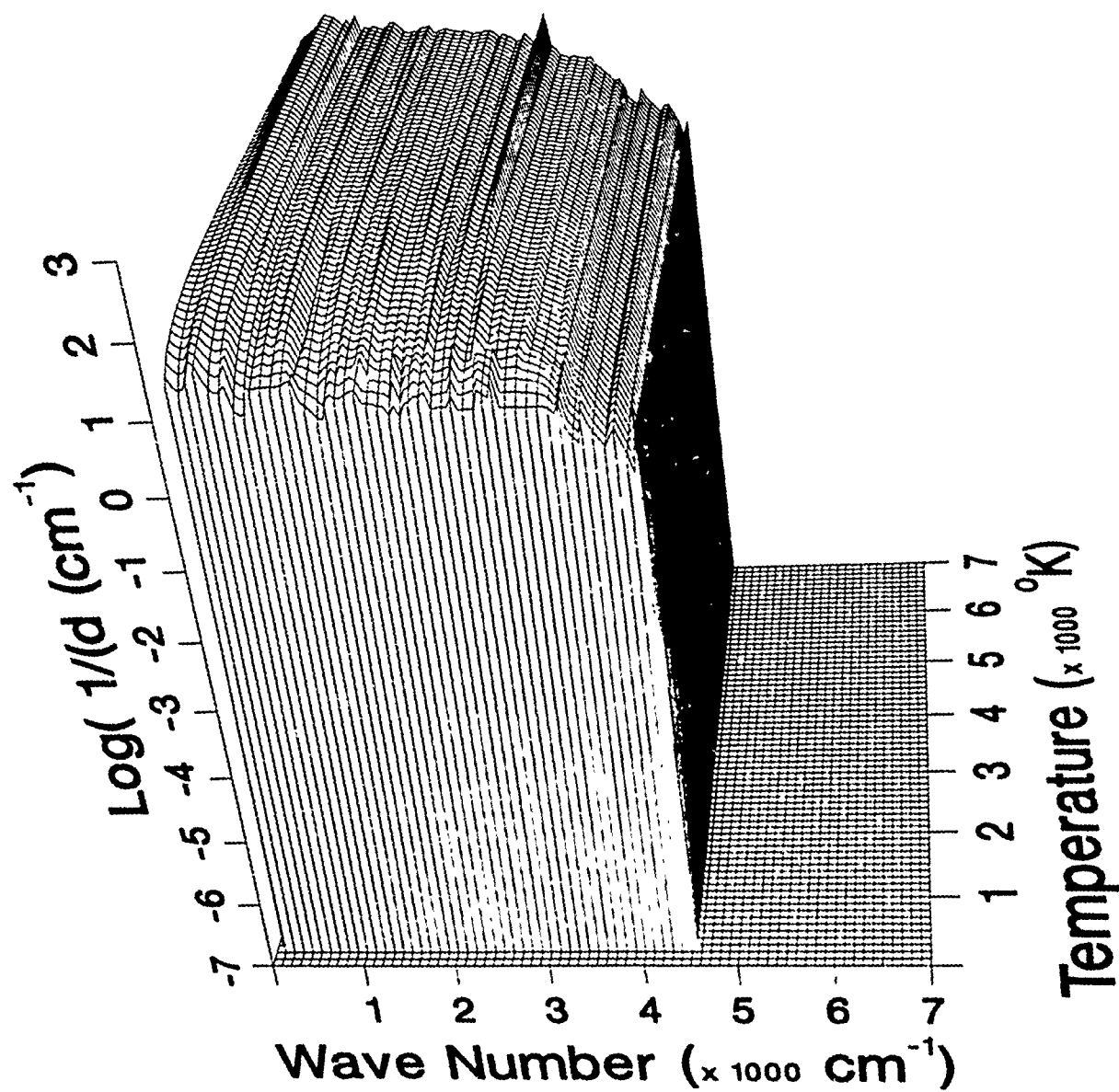


Figure 399. Inverse line spacing for MgO.

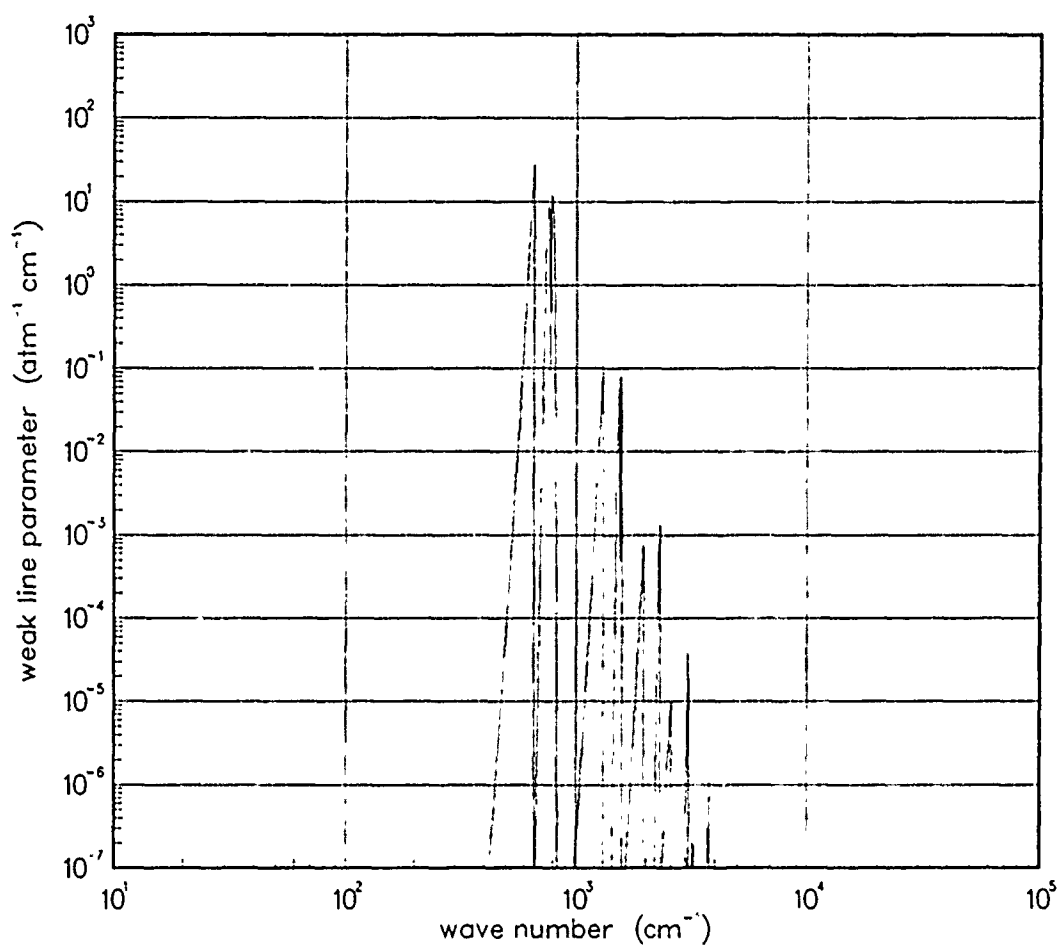


Figure 400. Weak-line parameter for MgO at 200°K.

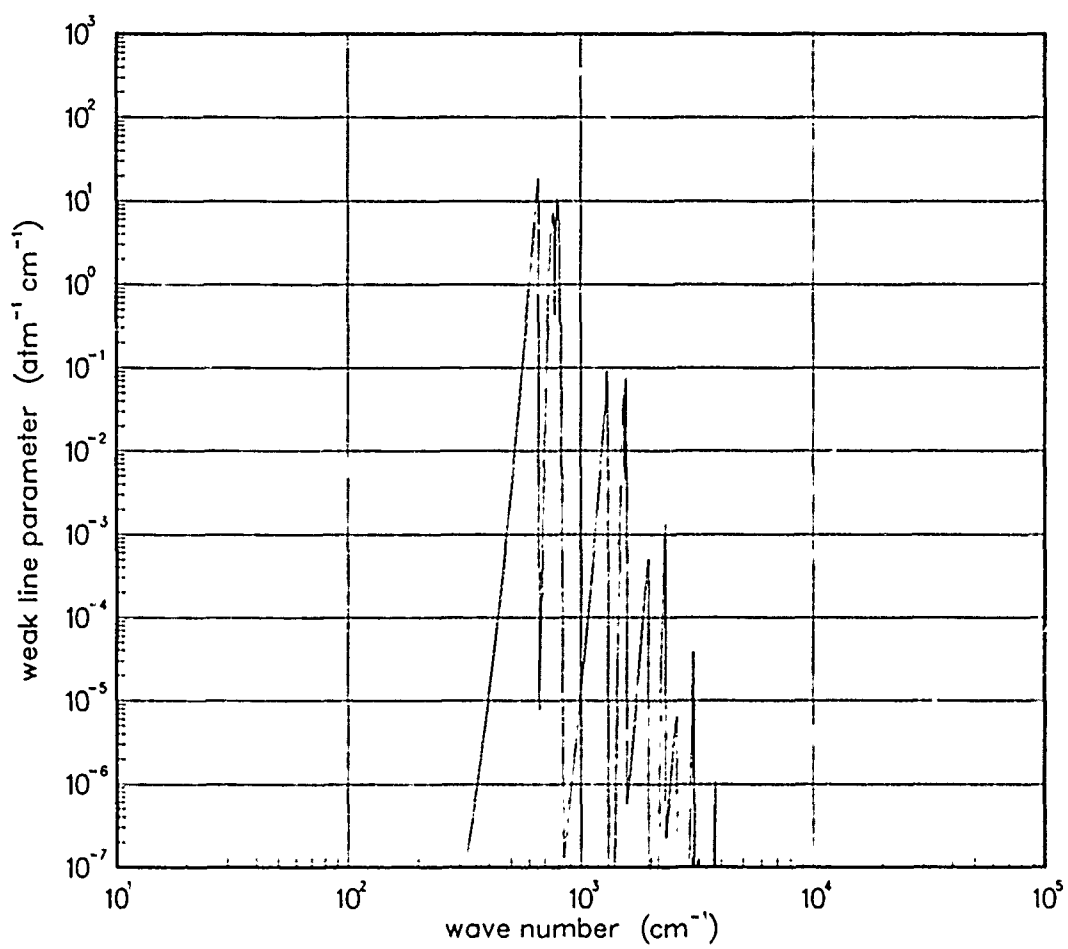


Figure 401. Weak-line parameter for MgO at 300°K.

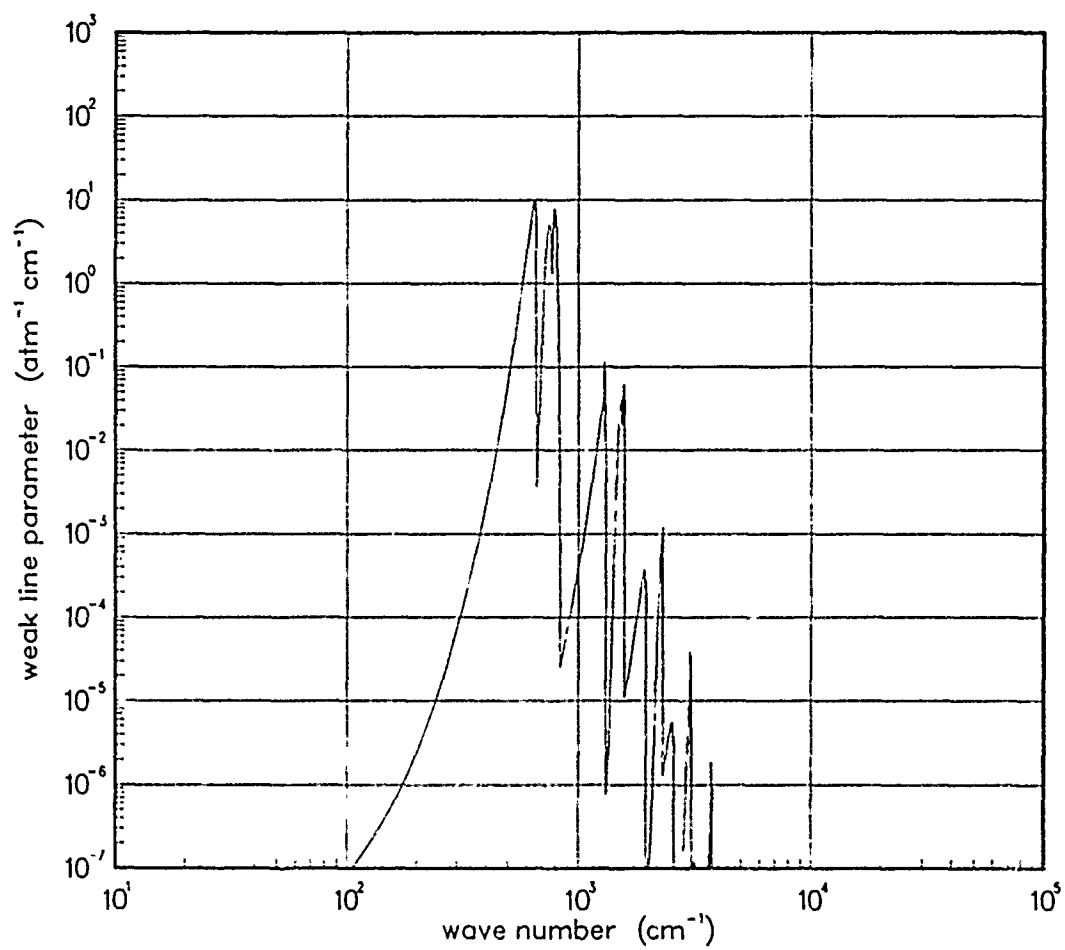


Figure 402. Weak-line parameter for MgO at 500°K.

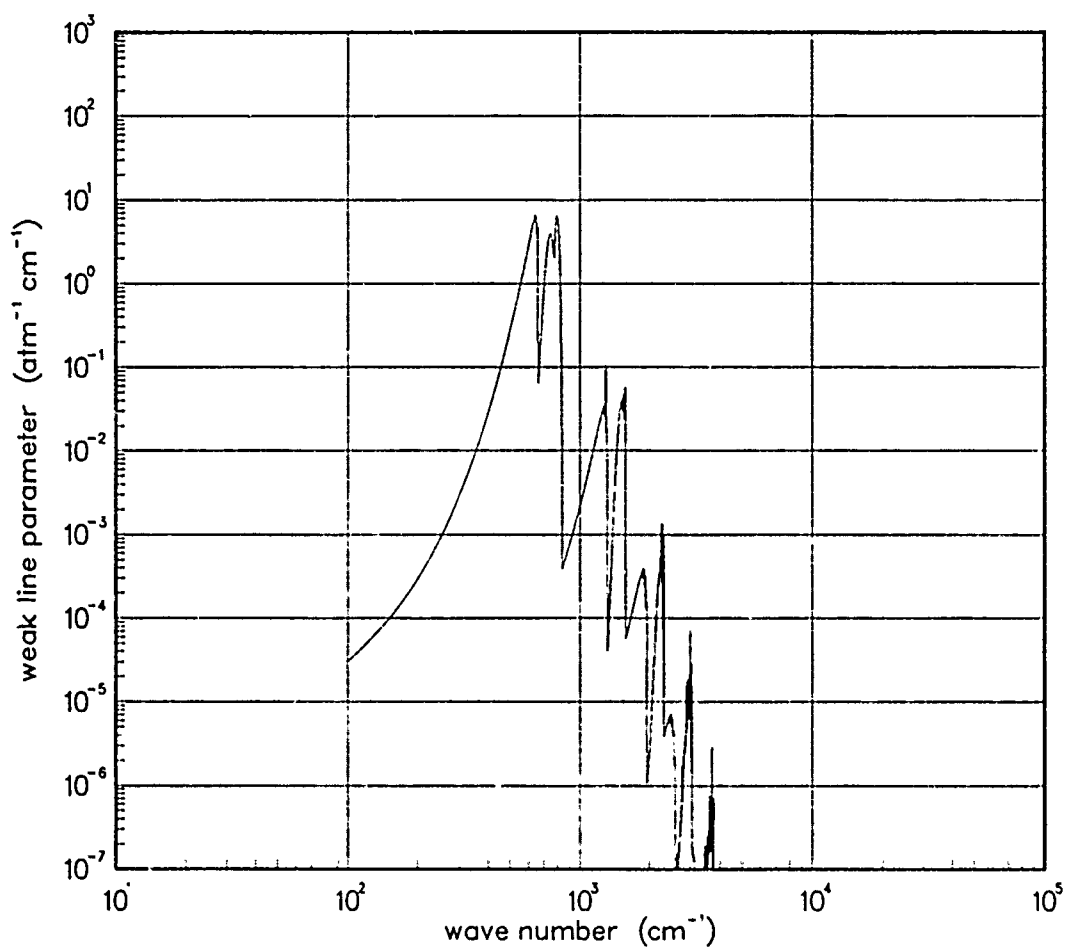


Figure 403. Weak-line parameter for MgO at ~50°K.

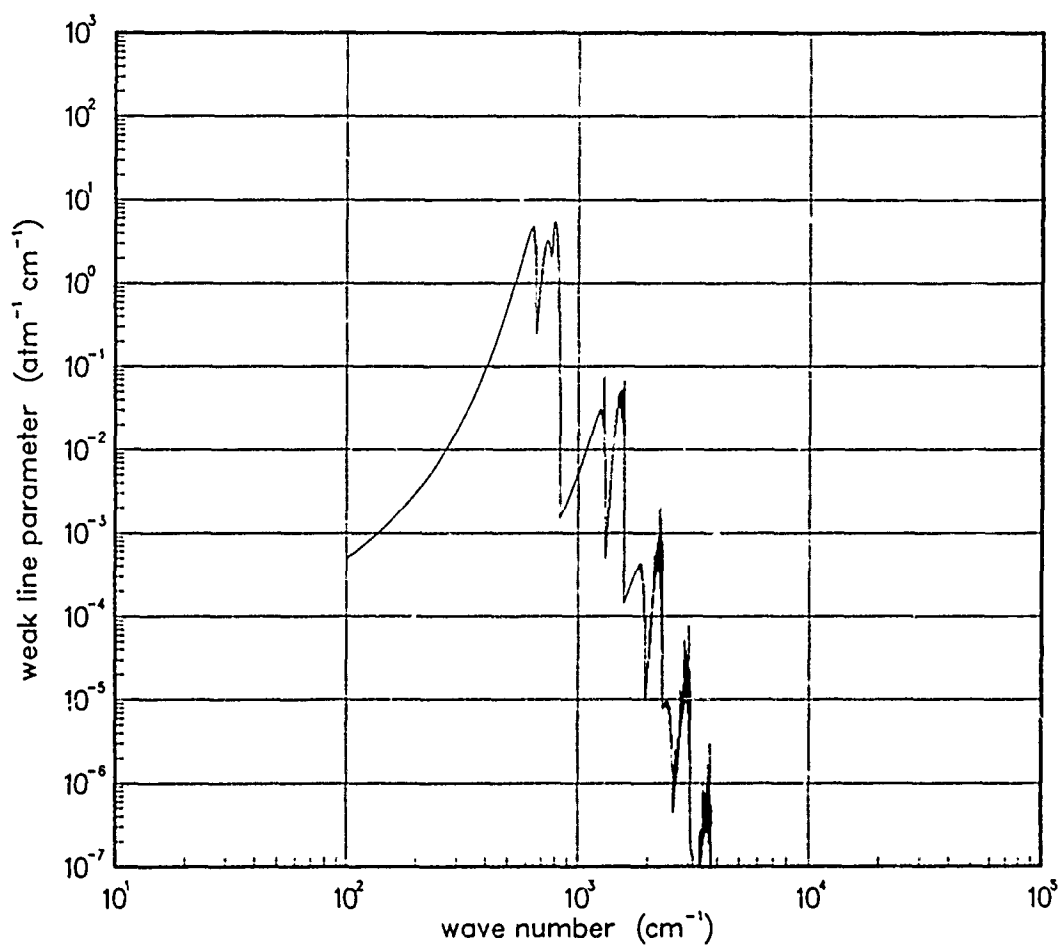


Figure 404. Weak-line parameter for MgO at 1000°K.

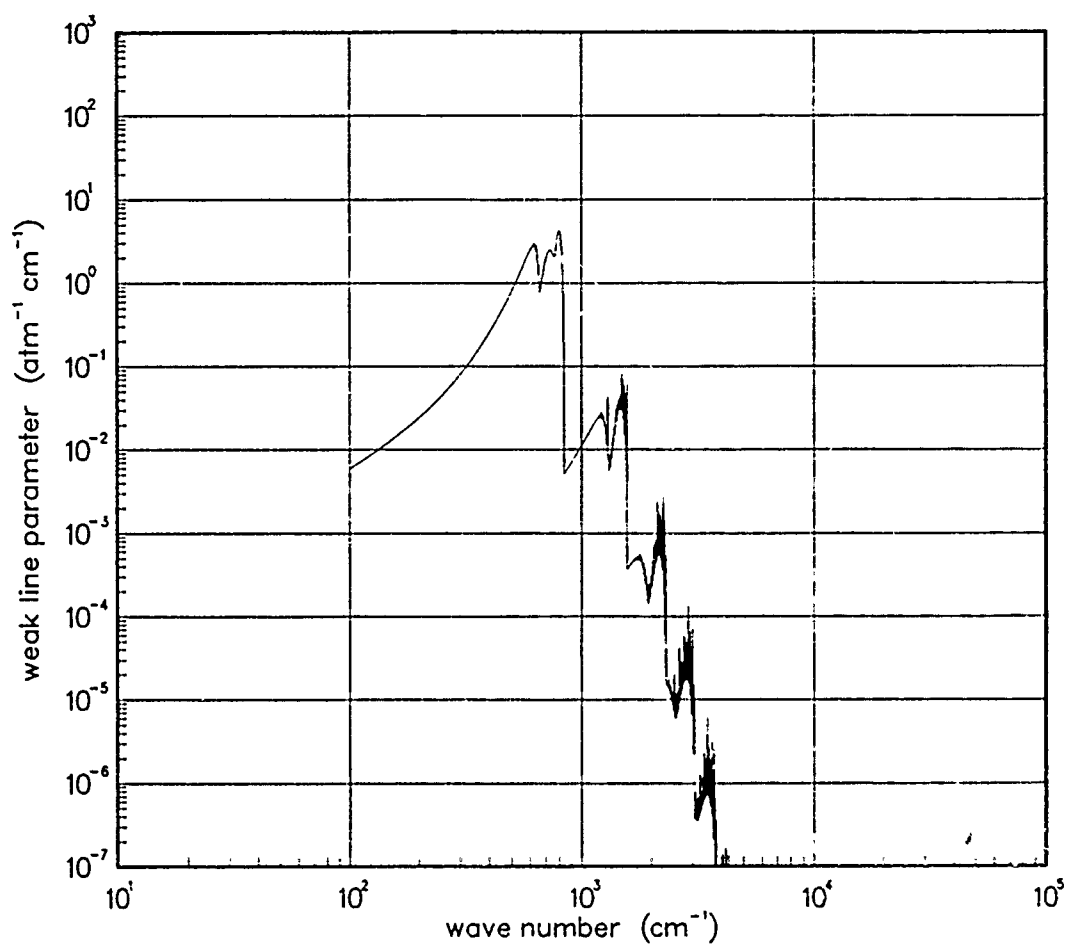


Figure 405. Weak-line parameter for MgO at 1500°K.

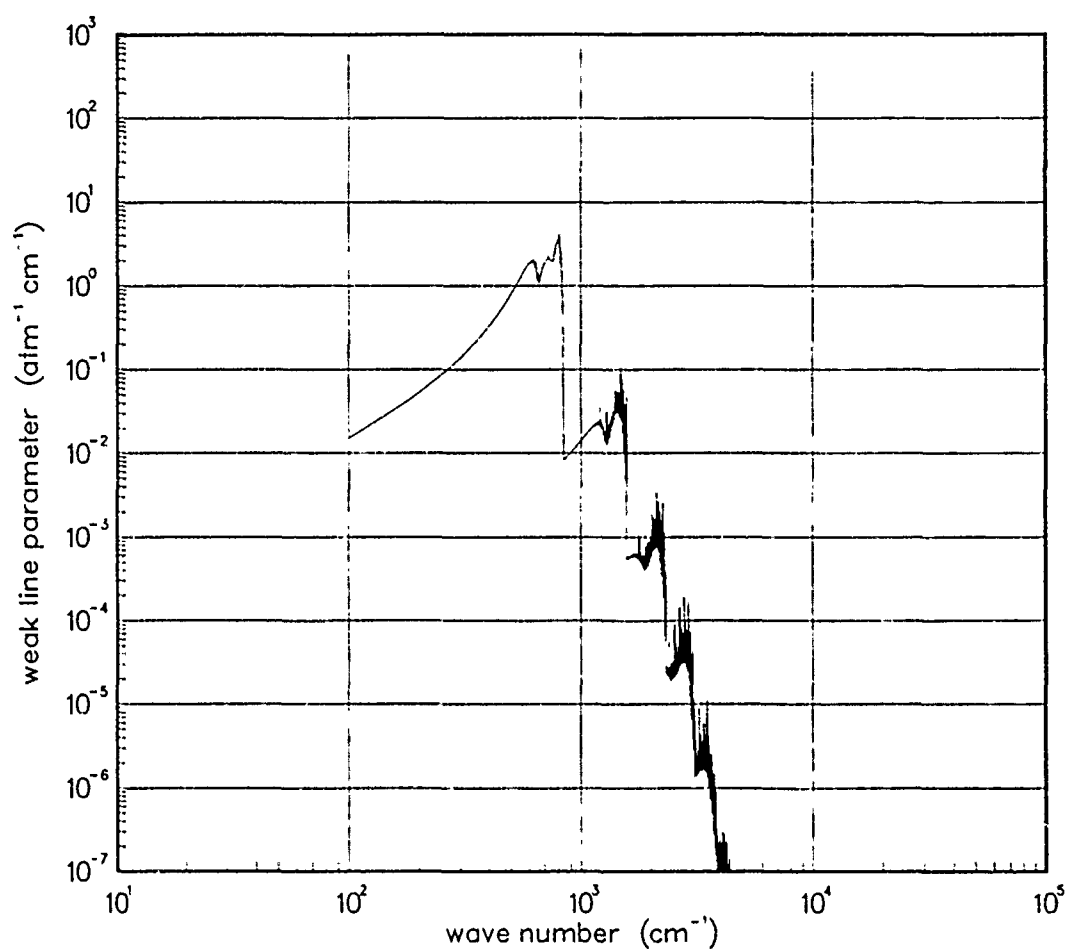


Figure 406. Weak-line parameter for MgO at 2000°K.

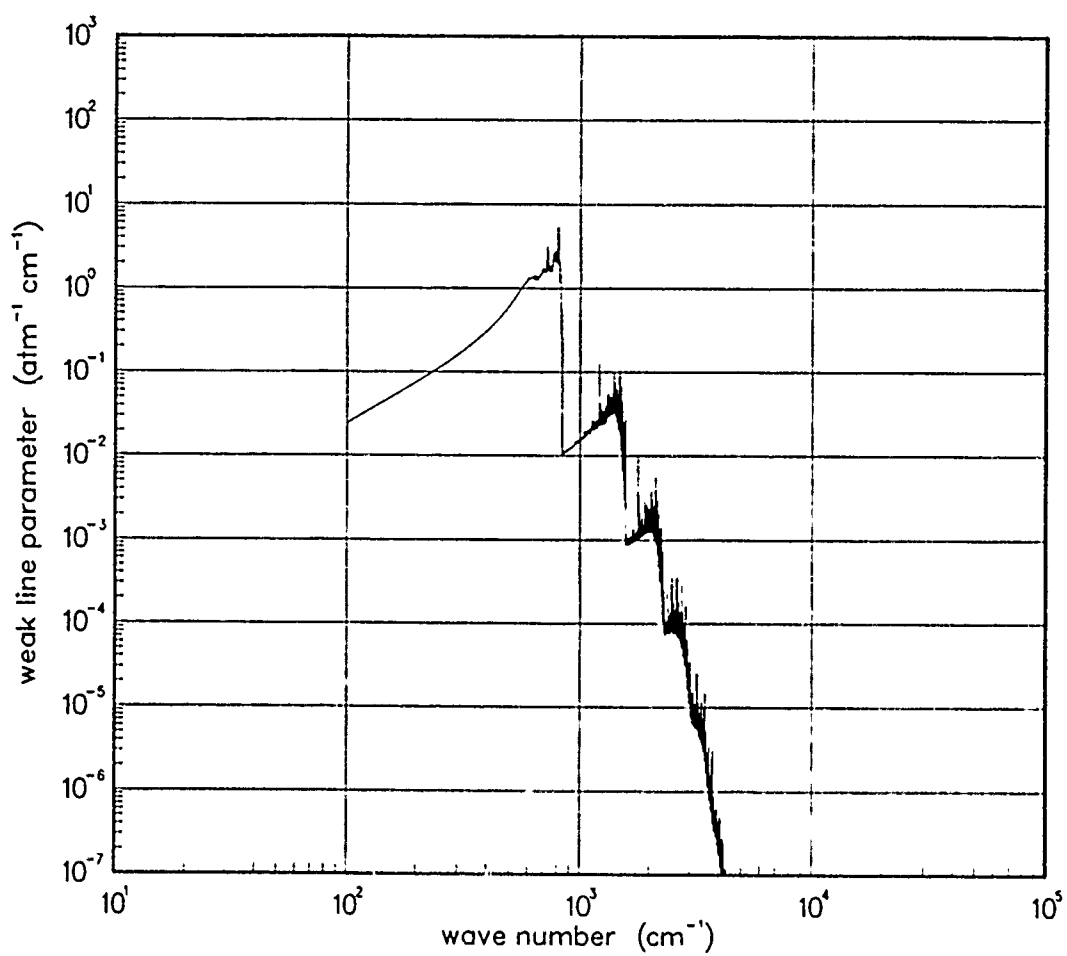


Figure 407. Weak-line parameter for MgO at 3000°K.

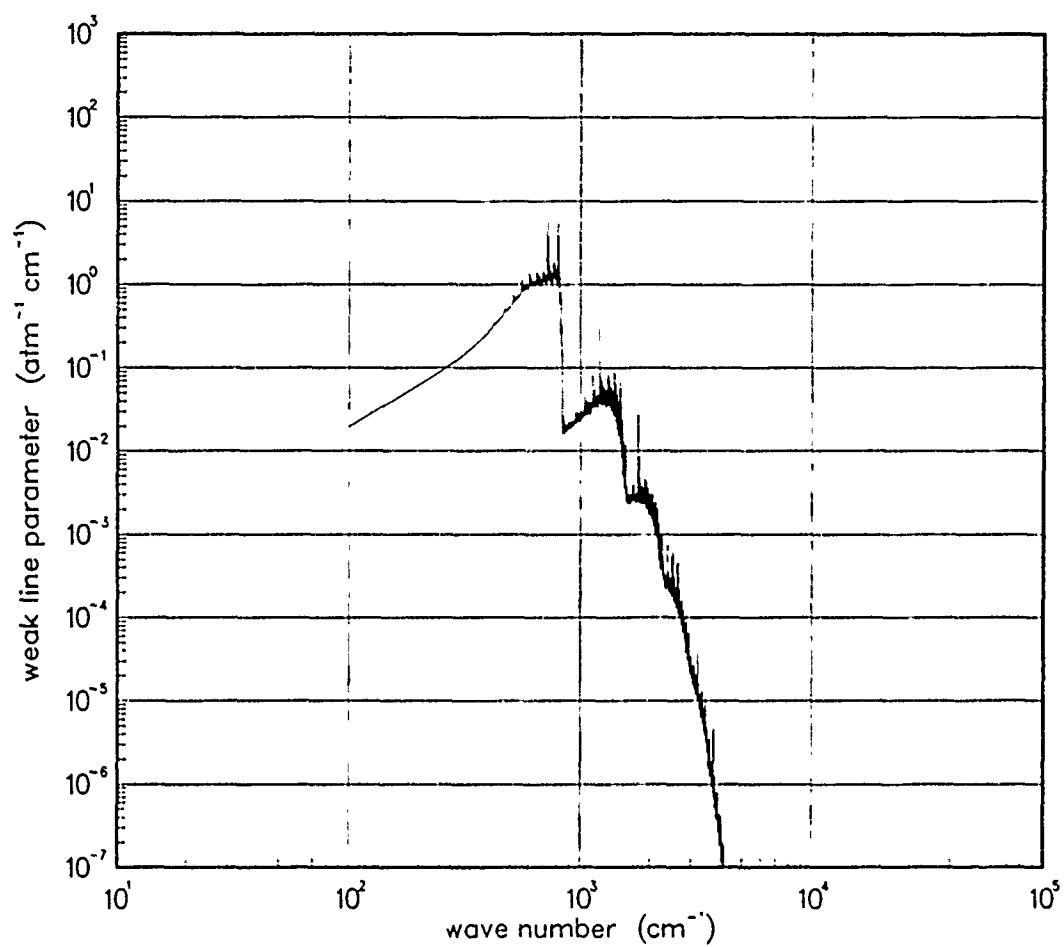


Figure 408. Weak-line parameter for MgO at 5000°K.

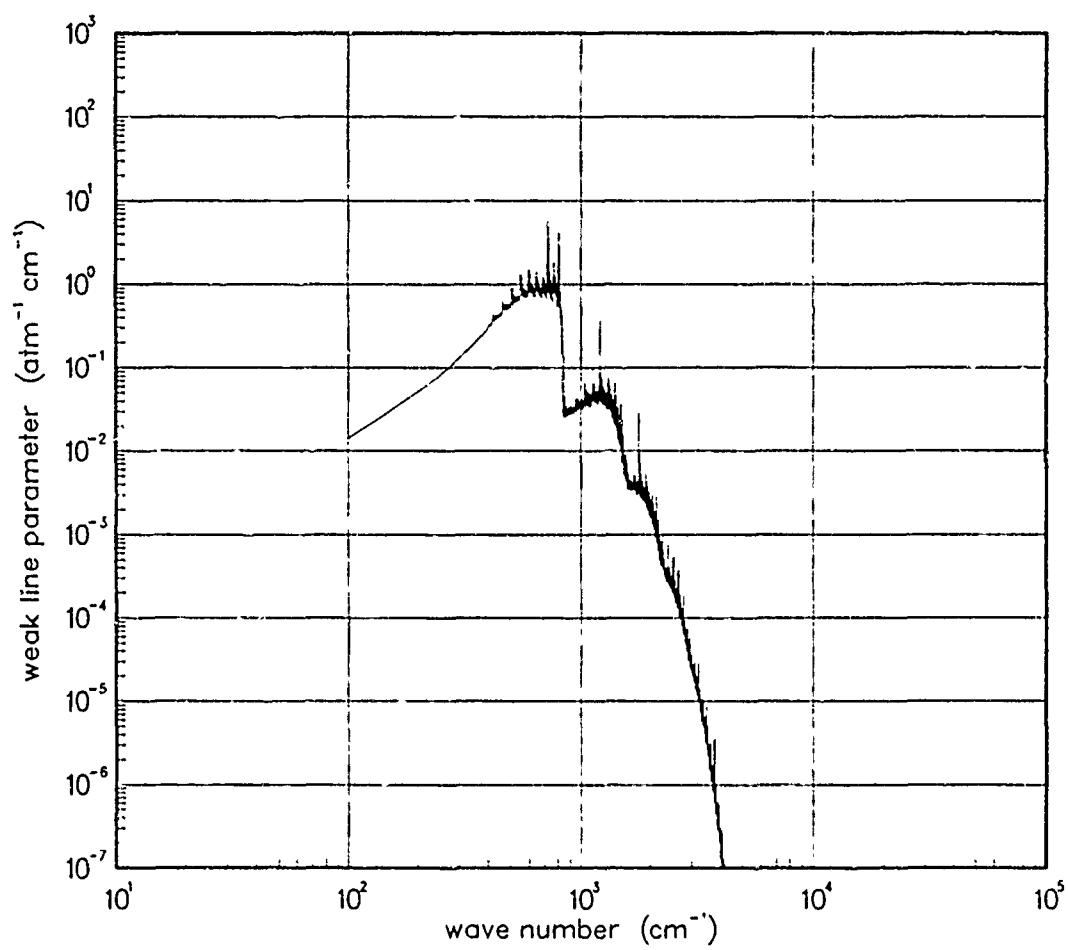


Figure 409. Weak-line parameter for MgO at 7000°K.

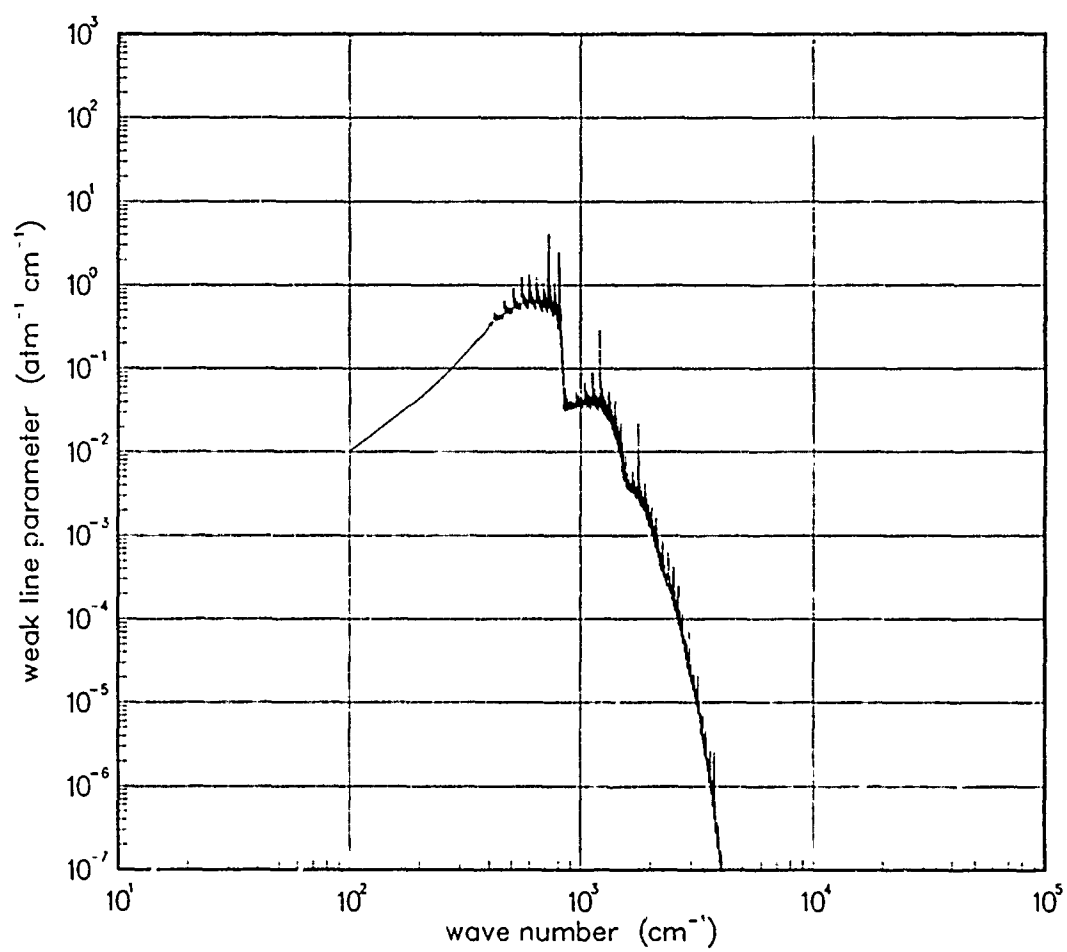


Figure 410. Weak-line parameter for MgO at 10000°K.

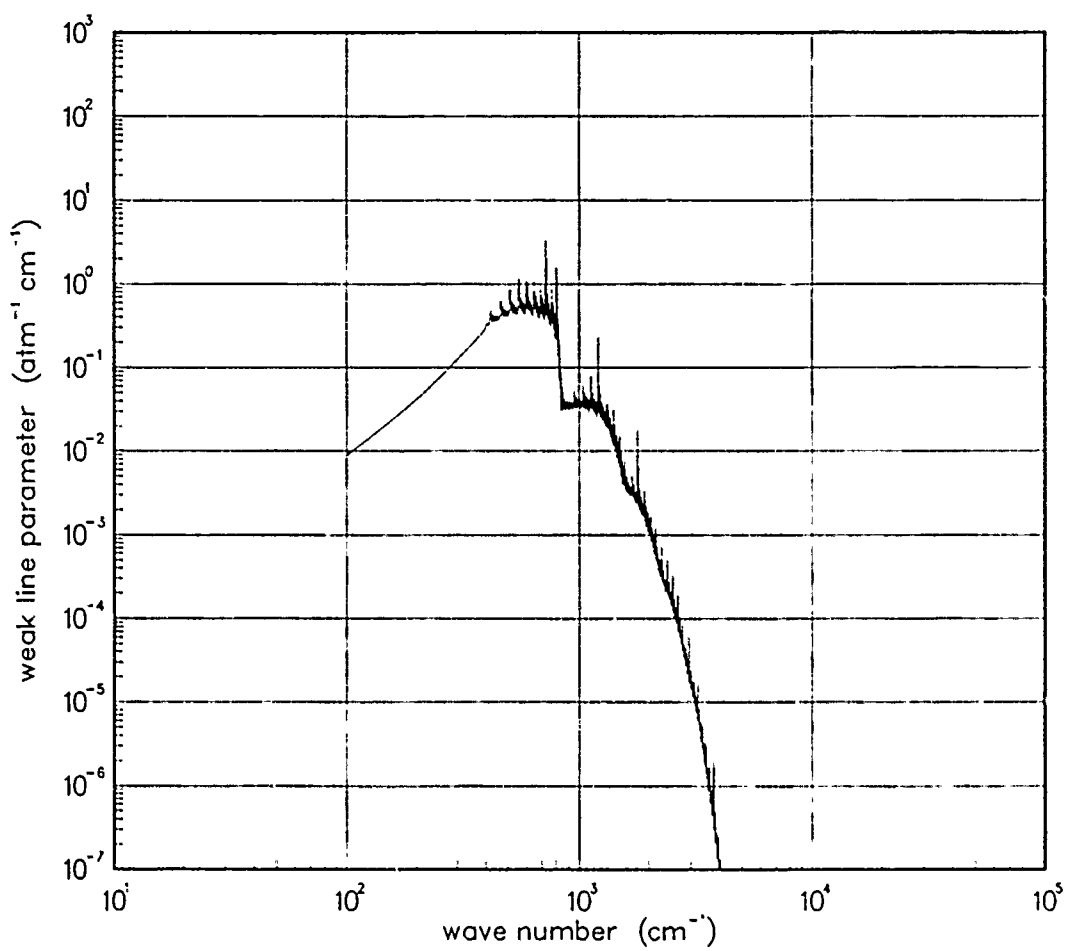


Figure 411. Weak-line parameter for MgO at 12000°K.

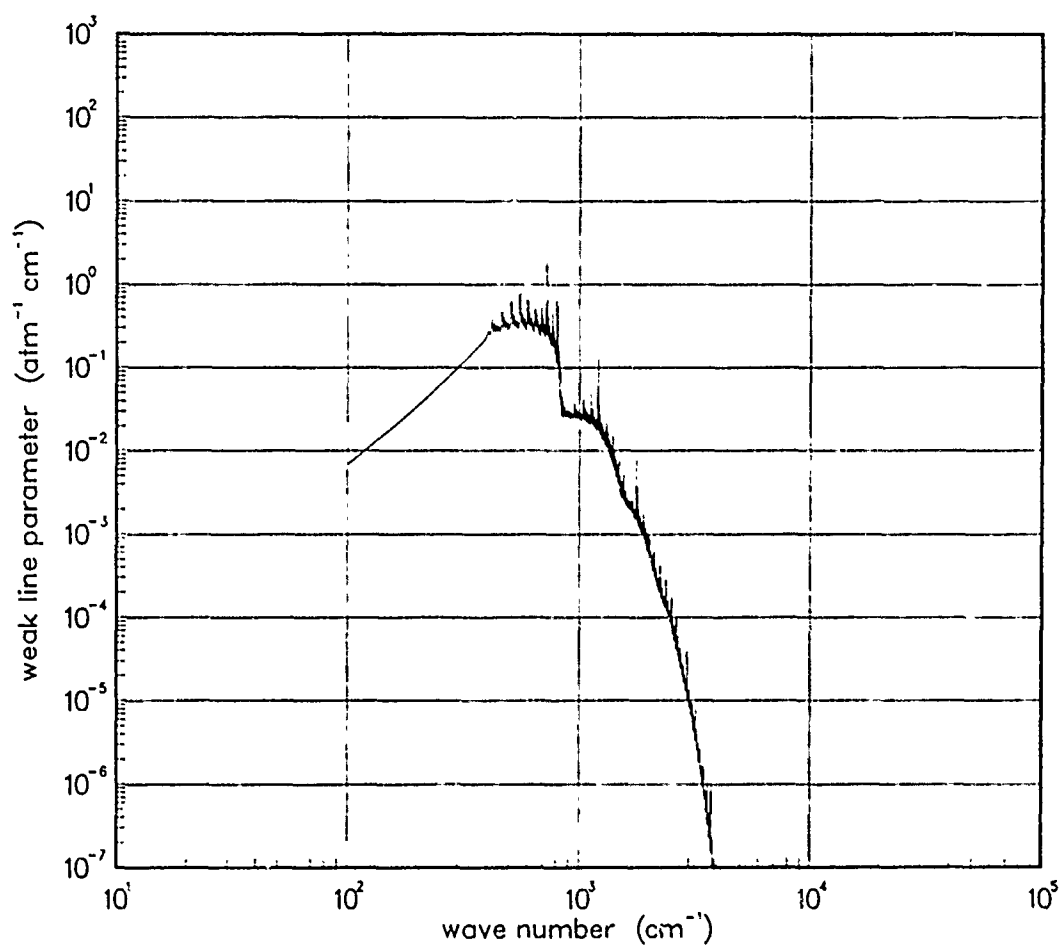


Figure 412. Weak-line parameter for MgO at 18000°K.

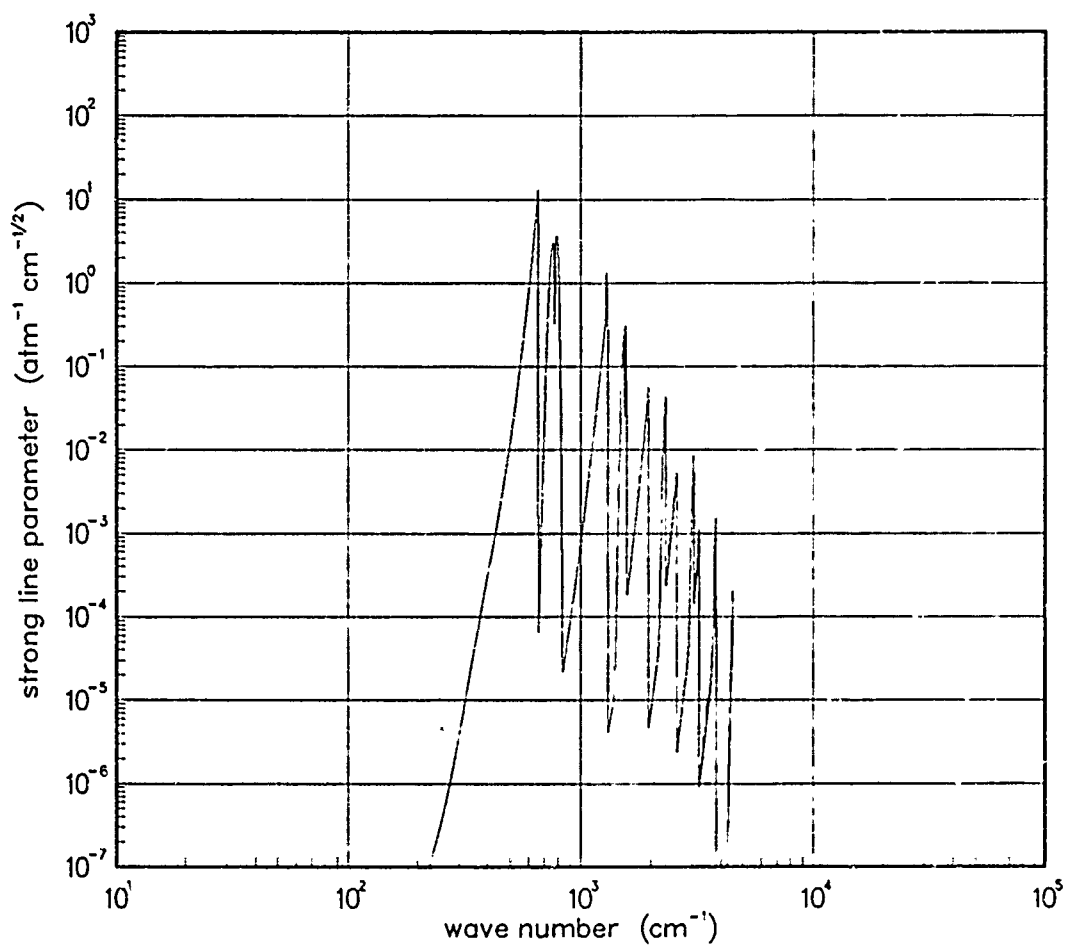


Figure 413. Strong-line parameter for MgO at 200°K.

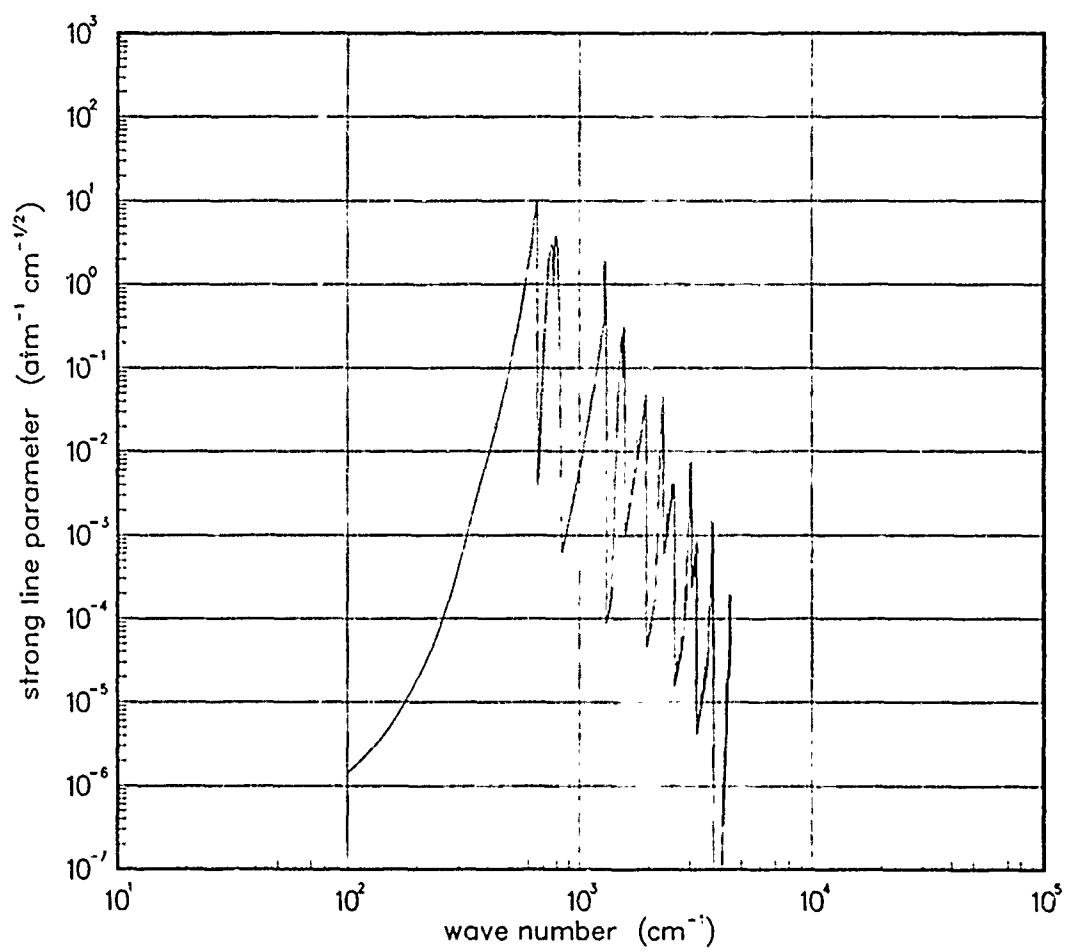


Figure 414. Strong-line parameter for MgO at 300°K.

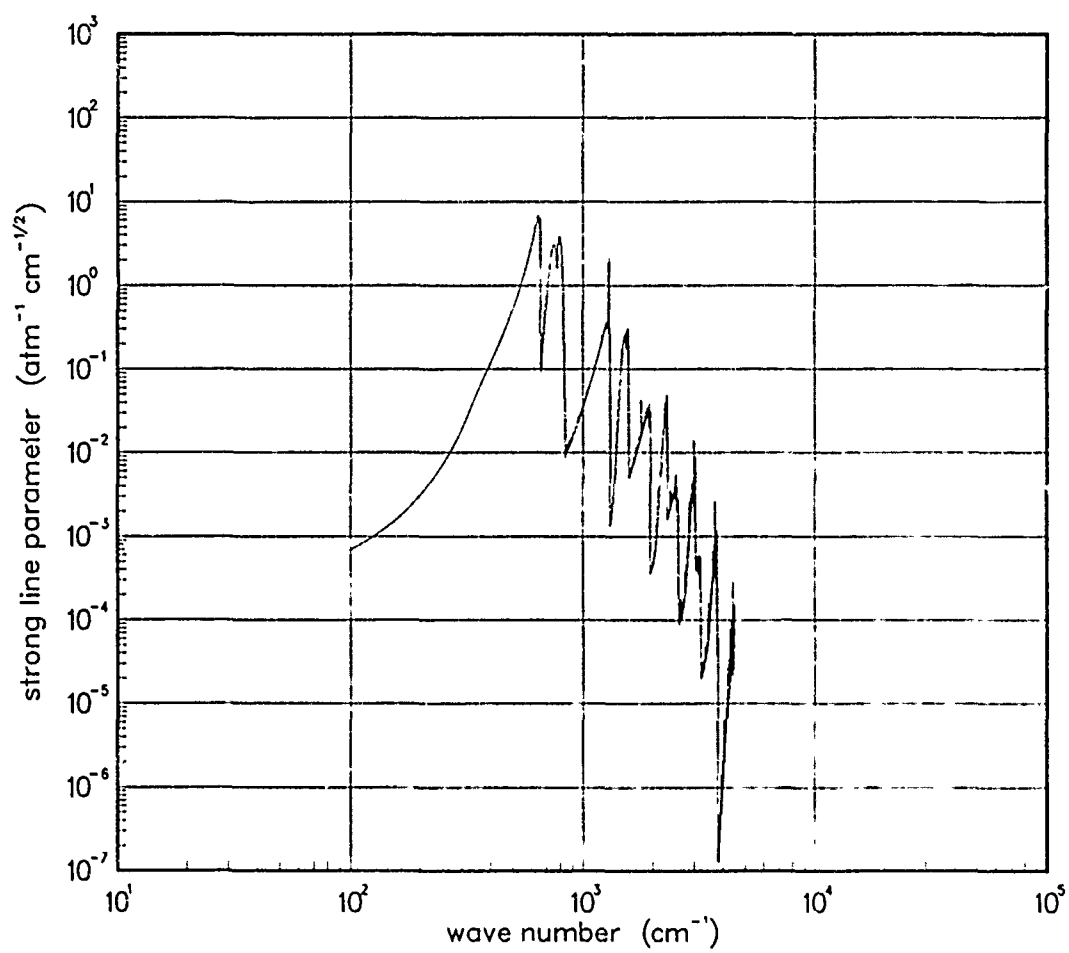


Figure 415. Strong-line parameter for MgO at 500°K.

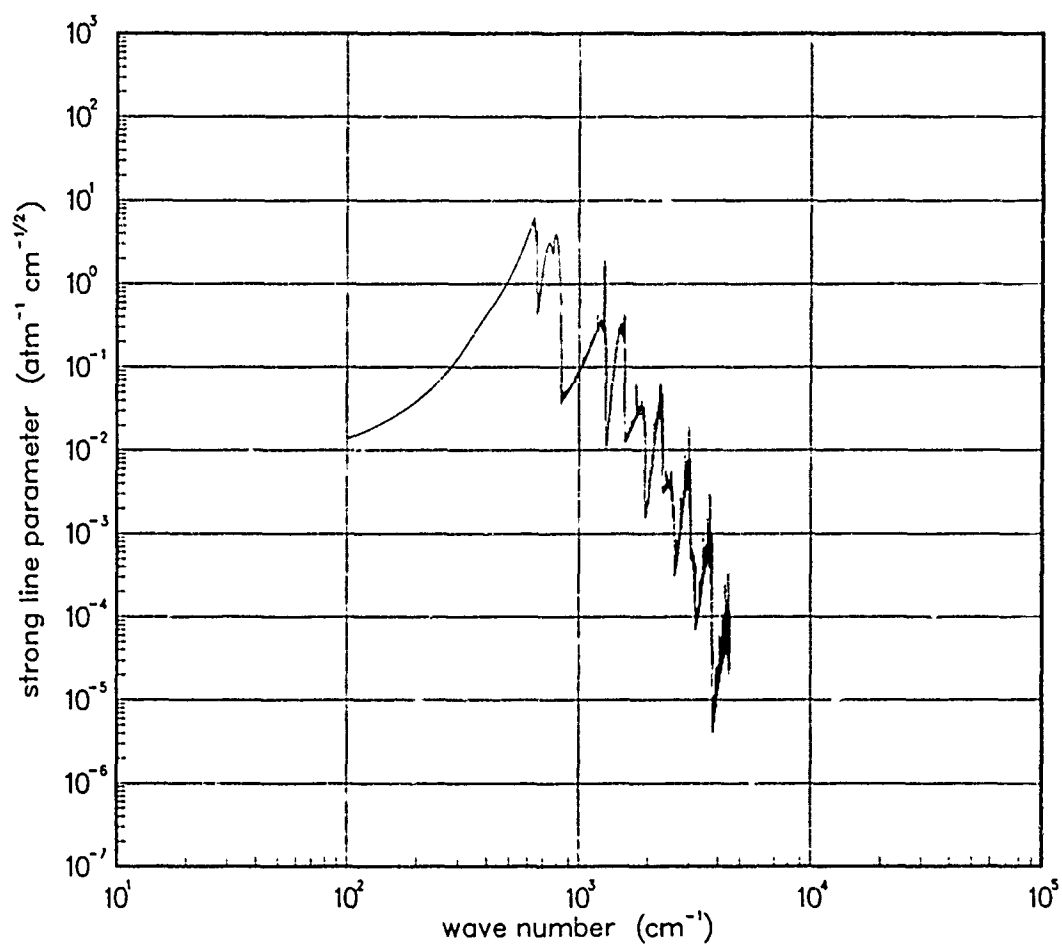


Figure 416. Strong-line parameter for MgO at 750°K.

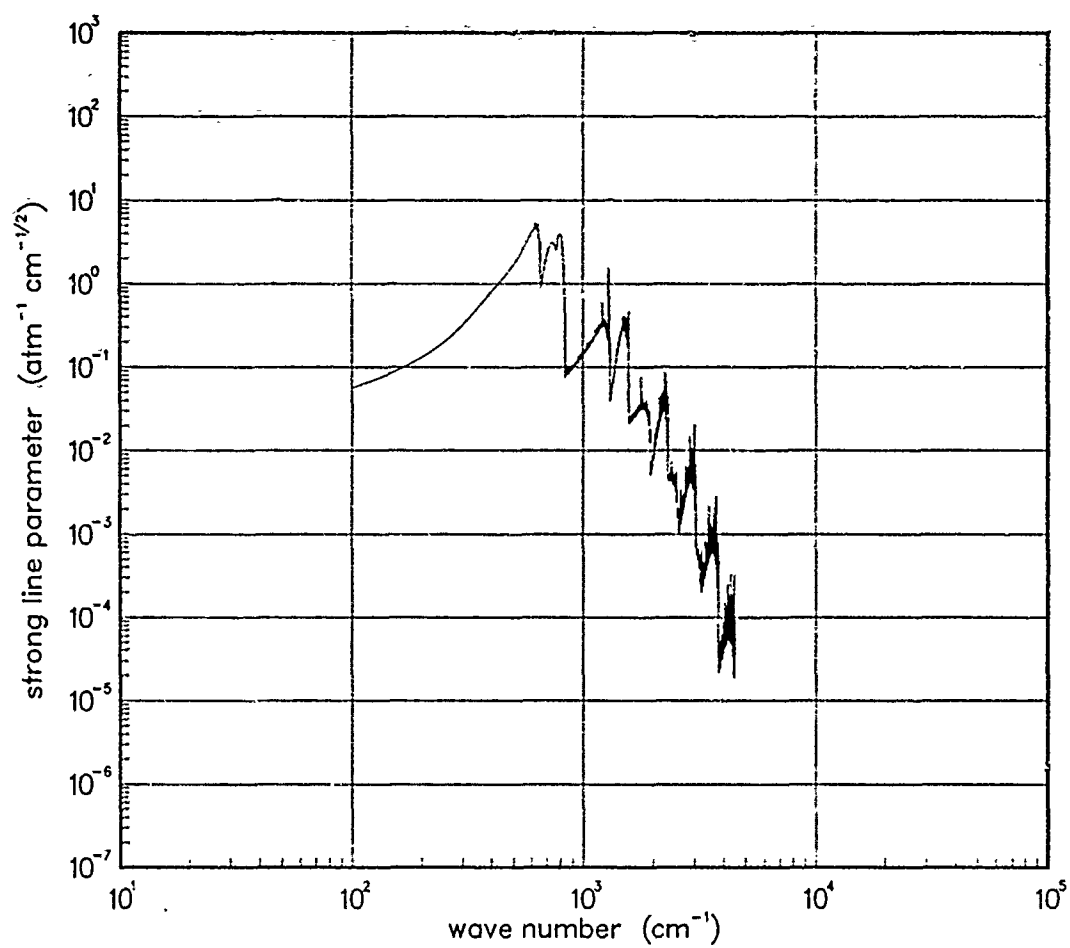


Figure 417. Strong-line parameter for MgO at 1000°K.

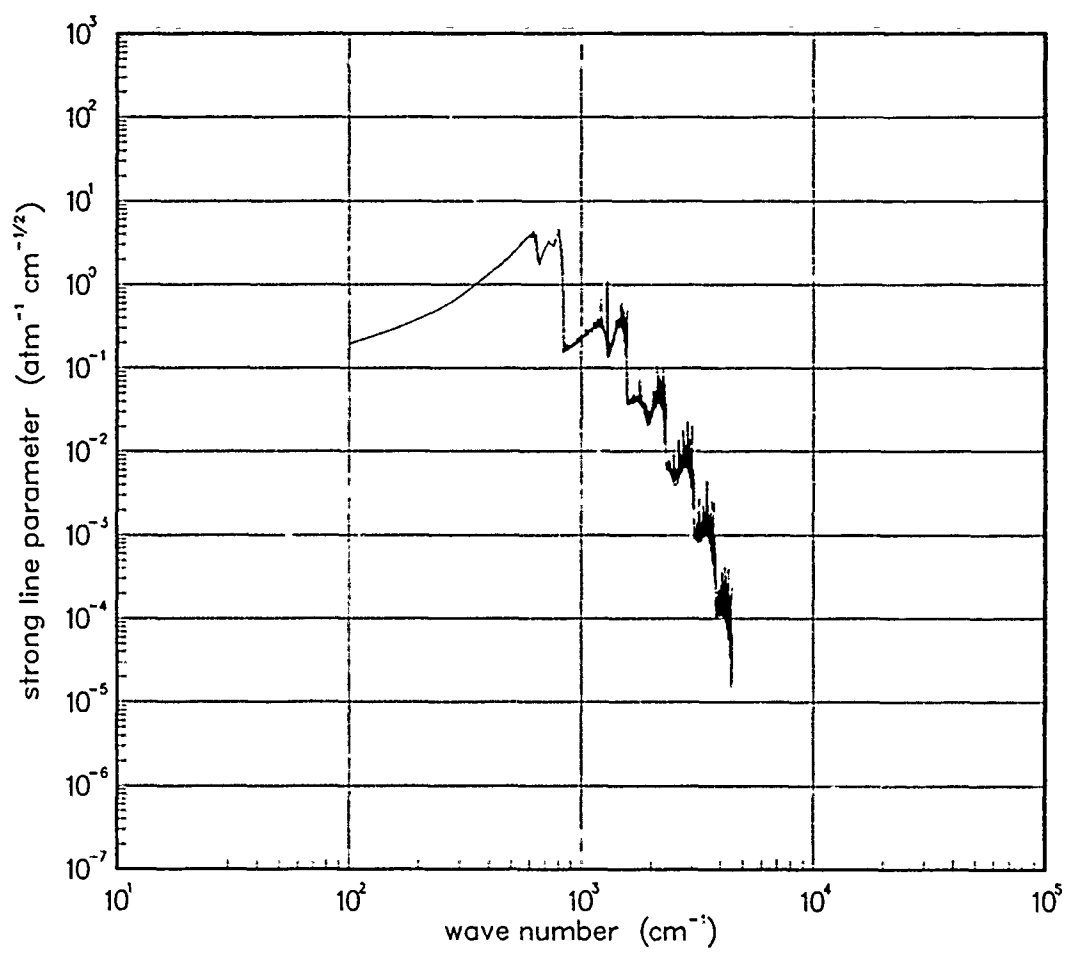


Figure 418. Strong-line parameter for MgO at 1500°K.

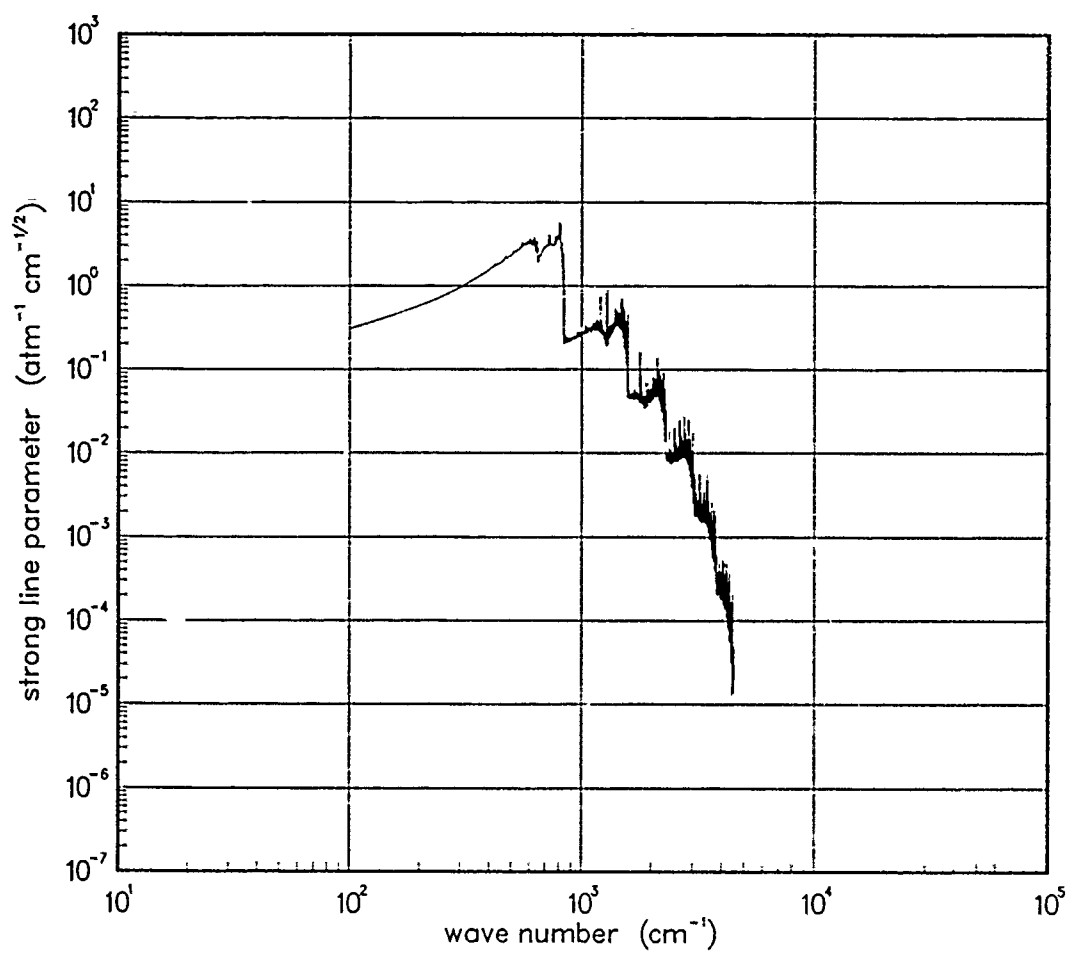


Figure 419. Strong-line parameter for MgO at 2000°K.

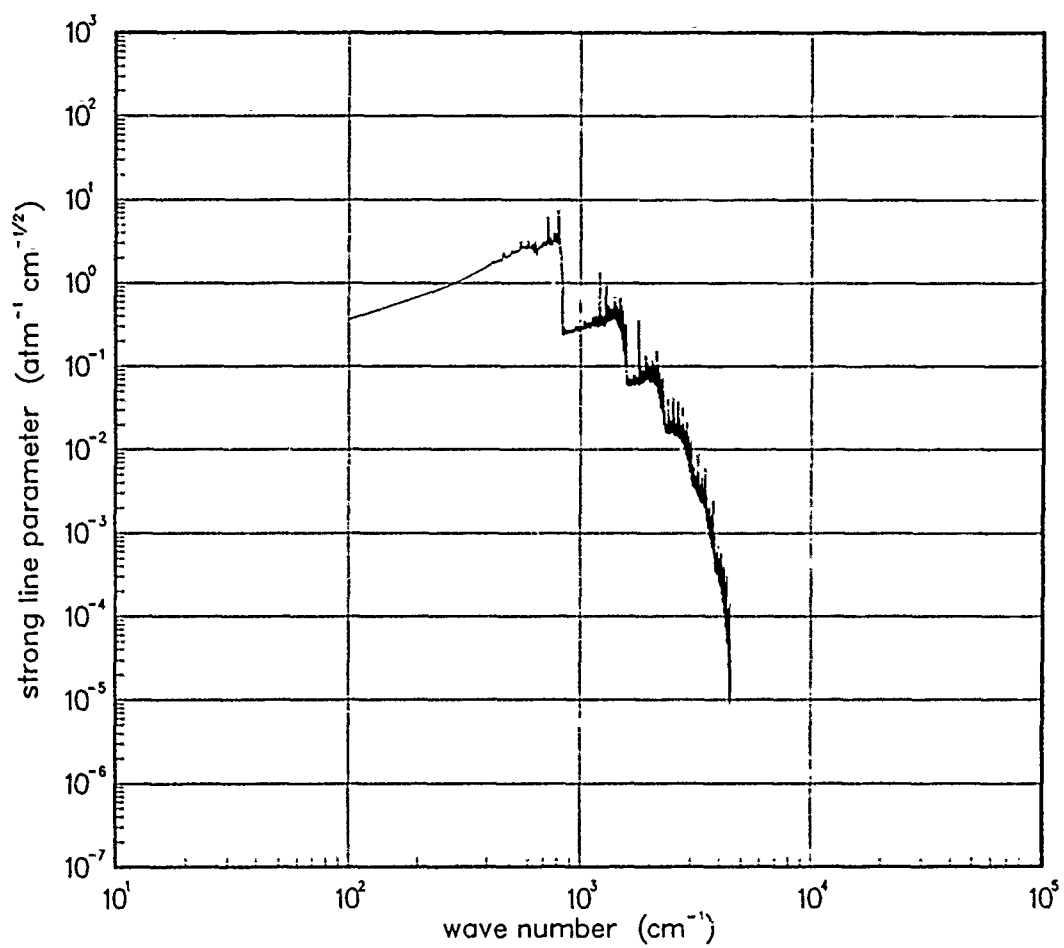


Figure 420. Strong-line parameter for MgO at 3000°K.

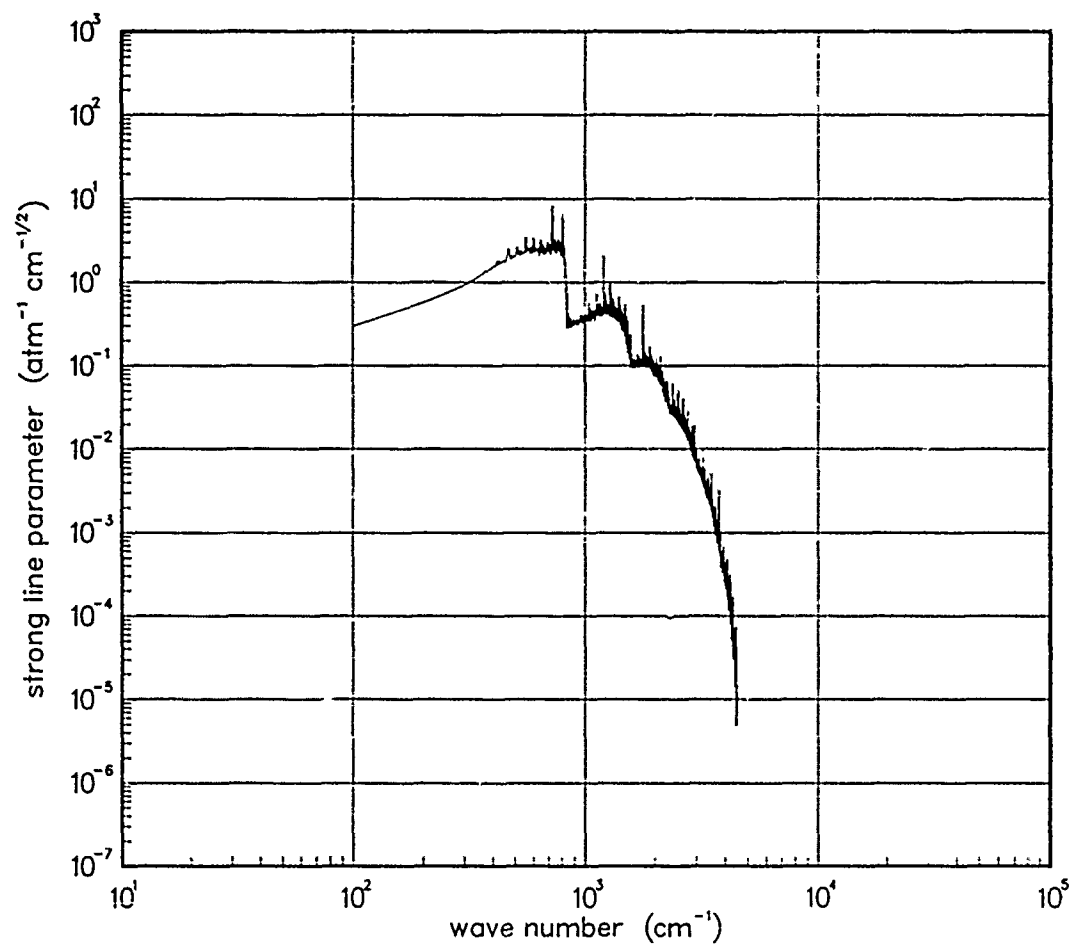


Figure 421. Strong-line parameter for MgO at 5000°K.

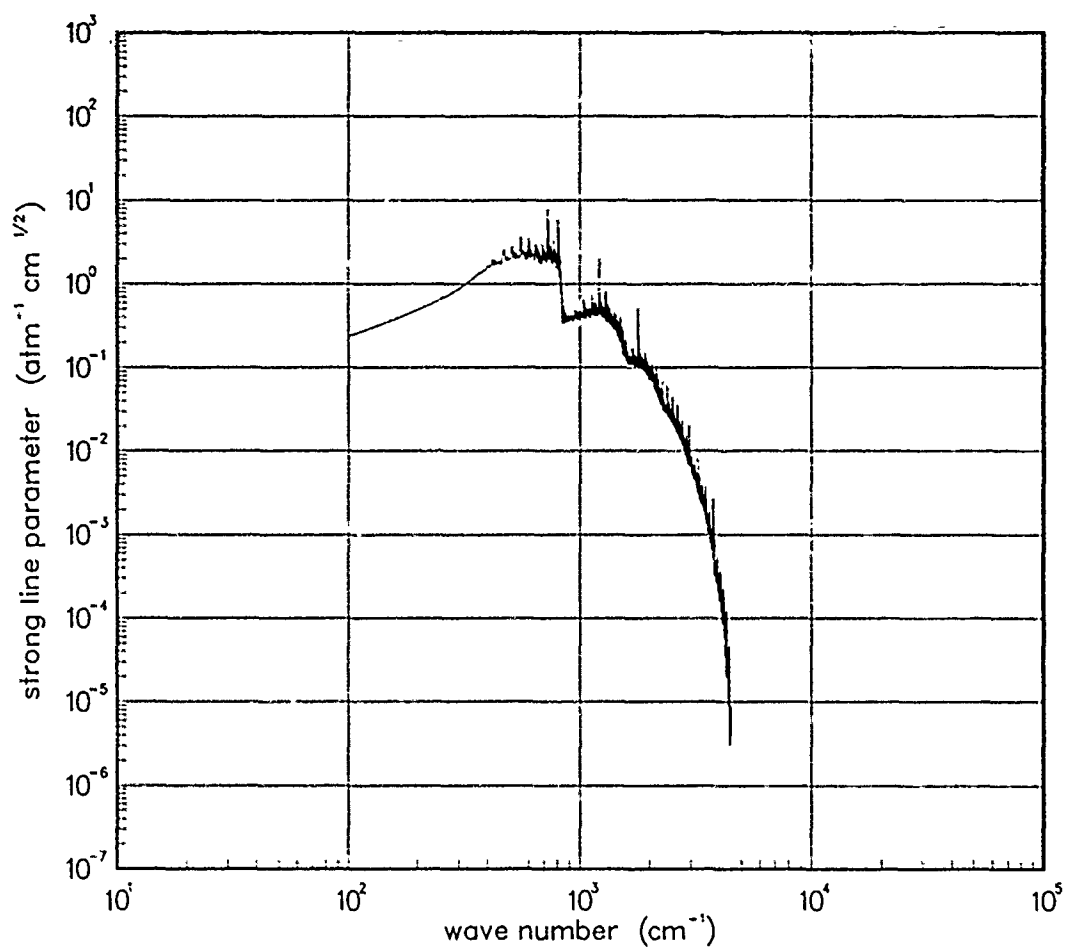


Figure 422. Strong-line parameter for MgO at 7000°K.

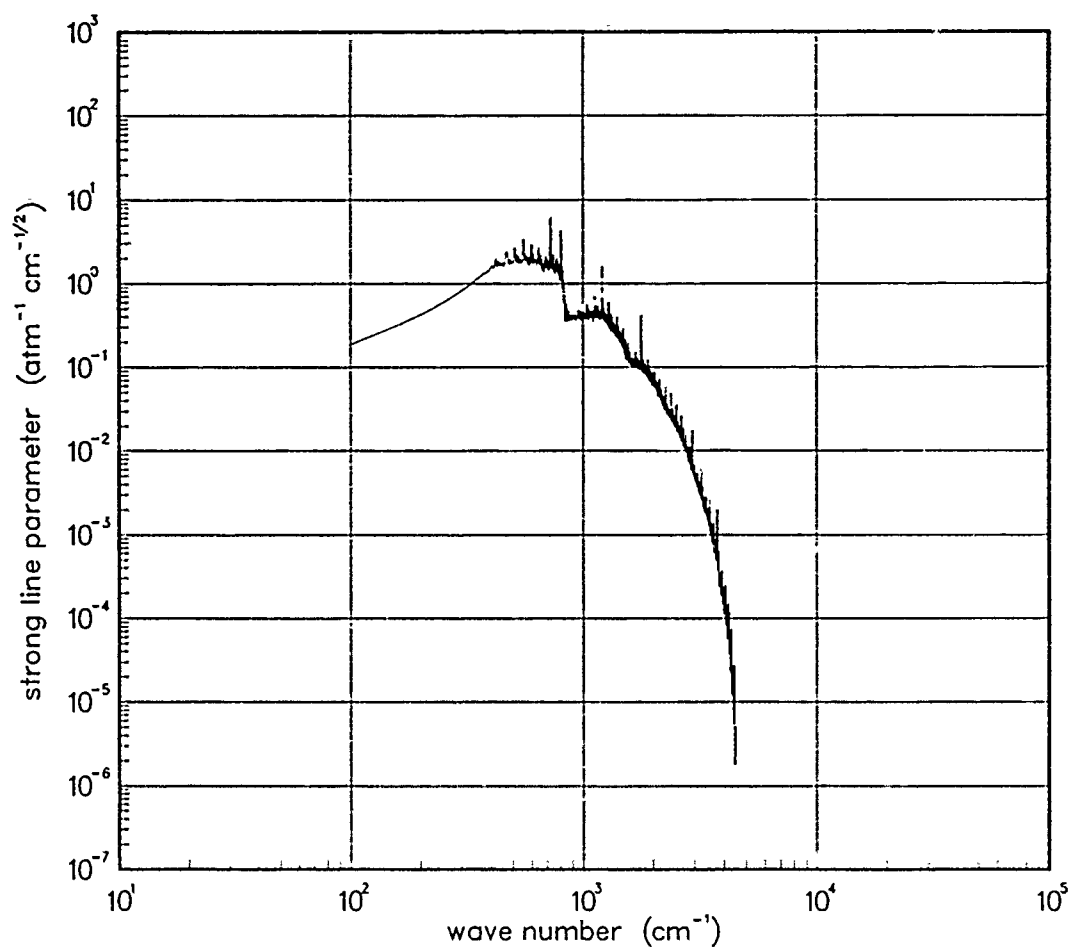


Figure 423. Strong-line parameter for MgO at 10000°K.

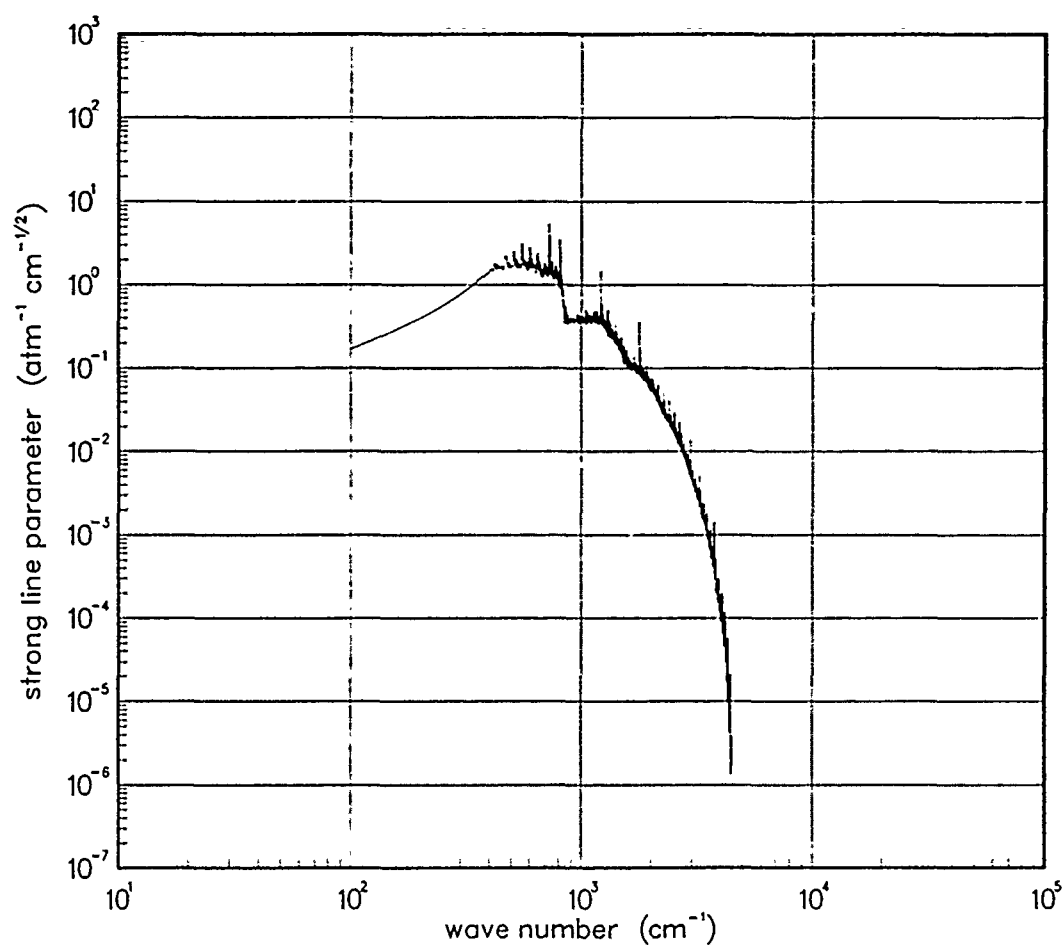


Figure 424. Strong-line parameter for MgO at 12000°K.

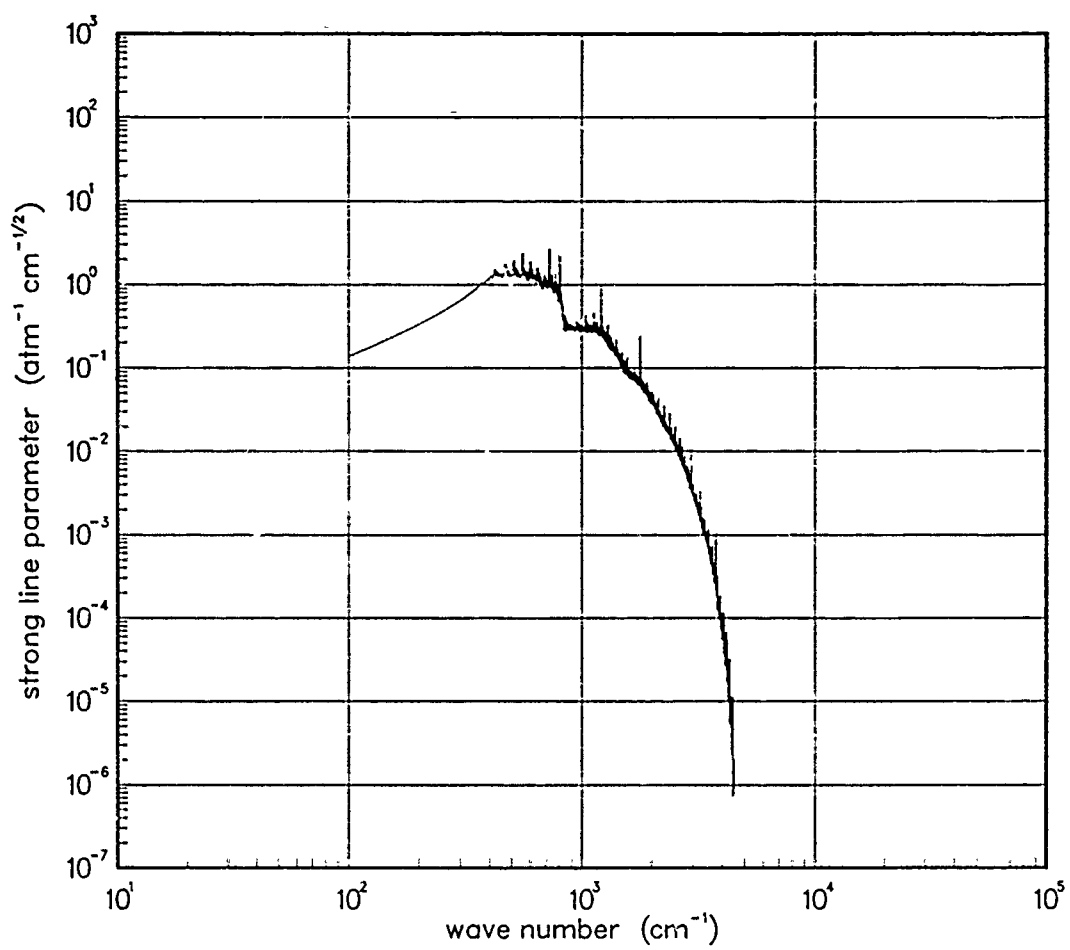


Figure 425. Strong-line parameter for MgO at 18000°K.

6.6 SILICON OXIDE (SiO).

Table 12. Spectroscopic data for SiO.

$X^1\Sigma^+$

$$\begin{array}{ll} \omega_e = 1241.44^* & \omega_e x_e = 5.92^* \\ \alpha_e = .00504^* & B_e = 0.72675^* \end{array}$$

$$S_{10} = 90.6^\dagger \quad S_{20} = .428^\dagger \quad S_{30} = 0.020^\dagger$$

$$\gamma_t(300^\circ\text{K}) = 0.04$$

Data Source:

*B. Rosen, ed., Spectroscopic Data Relative to Diatomic Molecules, Pergamon Press, New York (1970).

†H.H. Michels, Diatomic Oxide Vibrational Band Intensities, United Aircraft Research Laboratories, K921094-4 (May 1971).

‡Fit to the Oscillator Strength data in Note †.

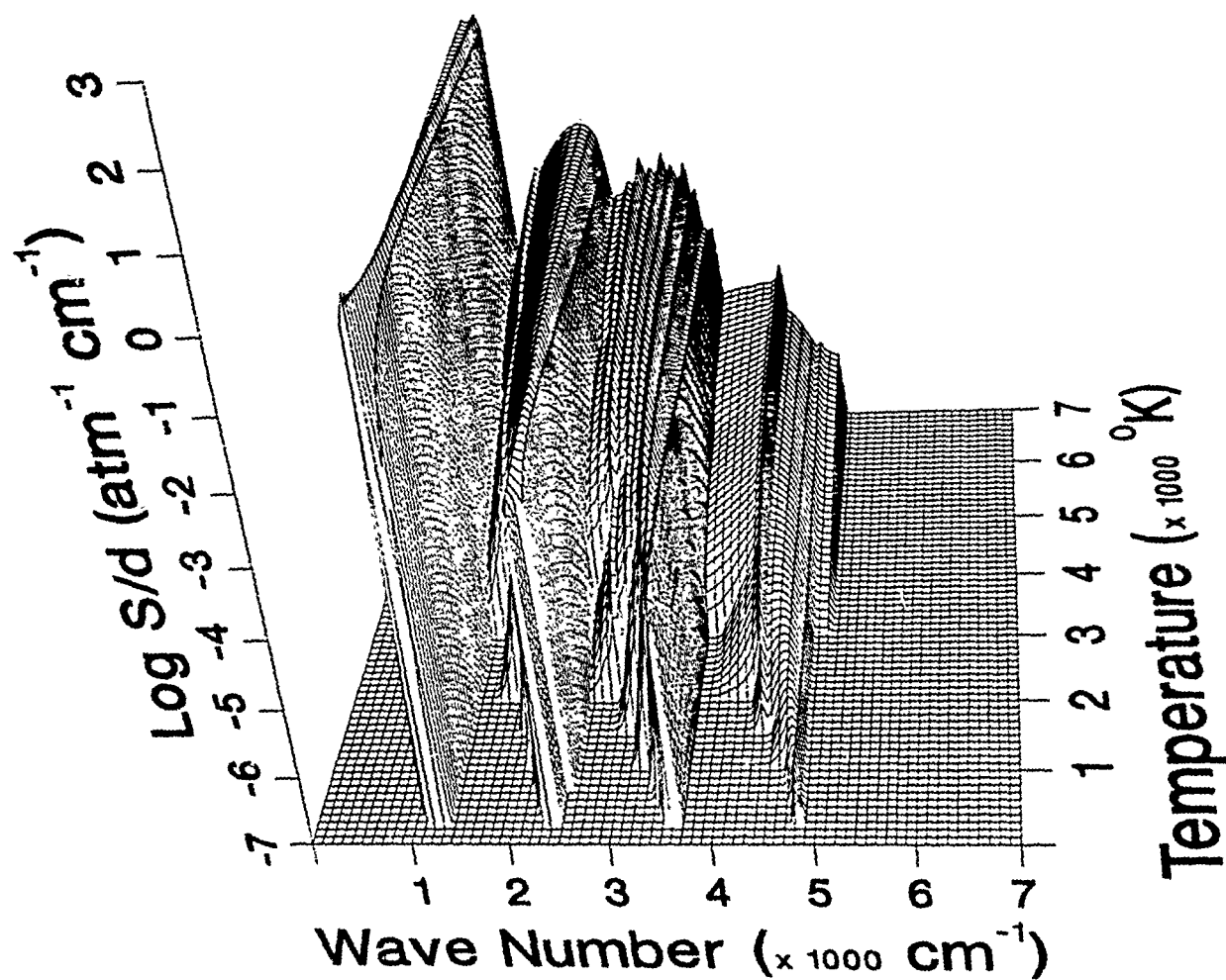


Figure 426. Weak-line parameter for SiO.

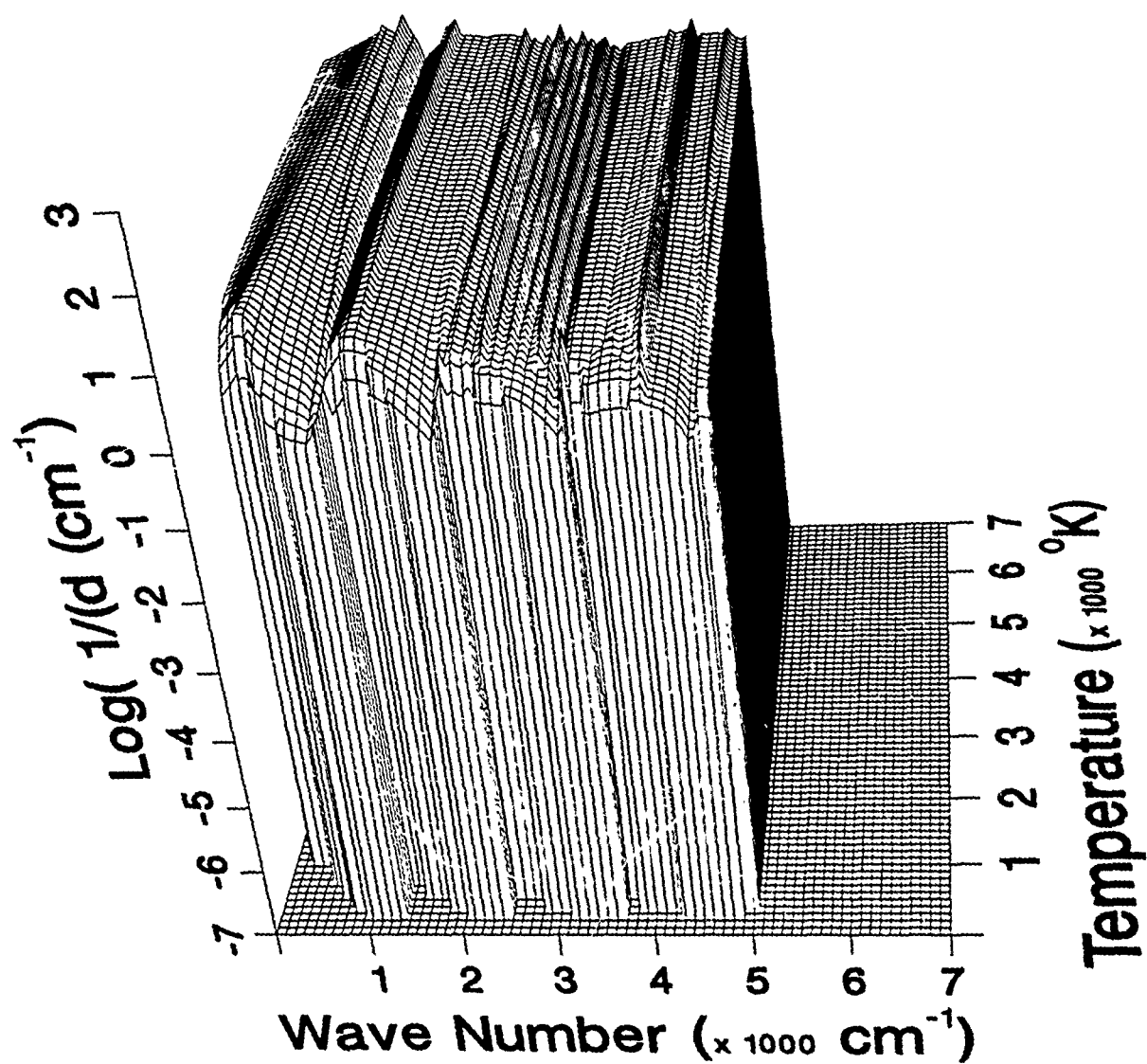


Figure 427. Inverse line spacing for SiO.

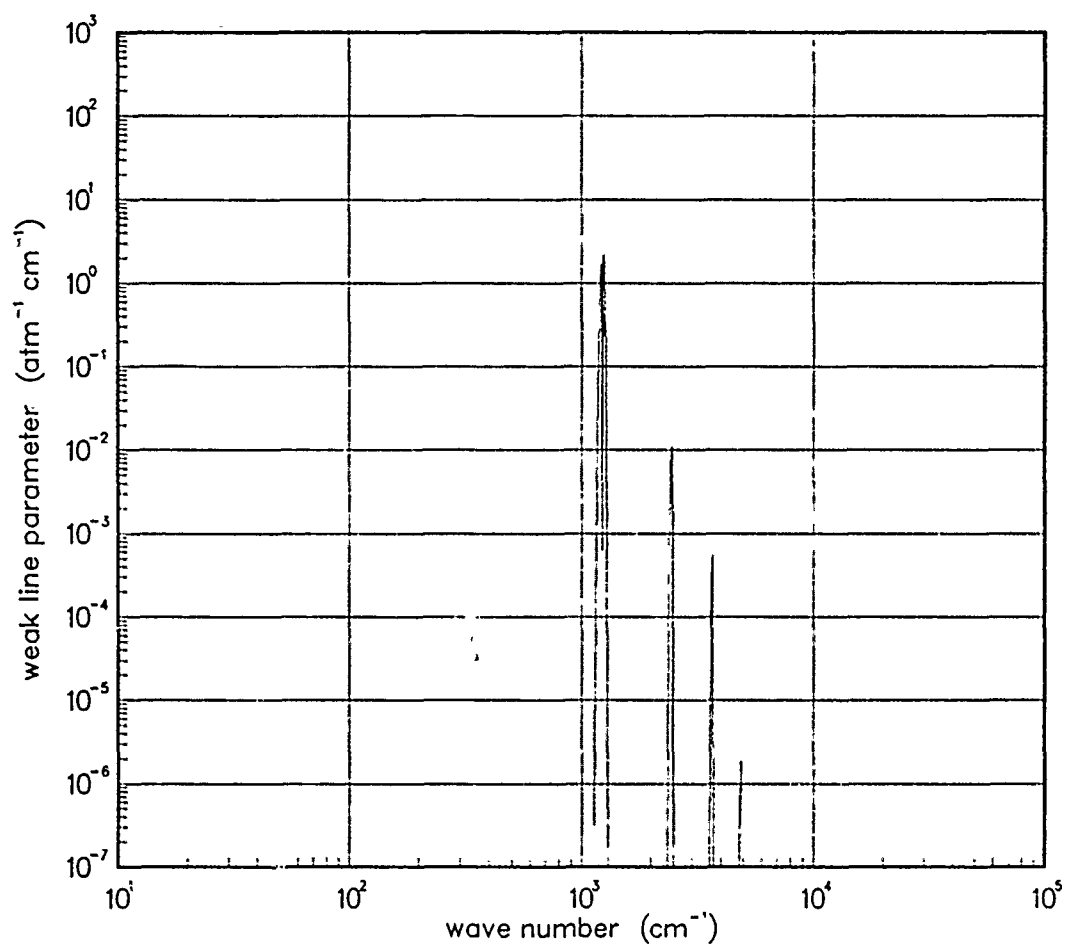


Figure 428. Weak-line parameter for SiO at 200°K.

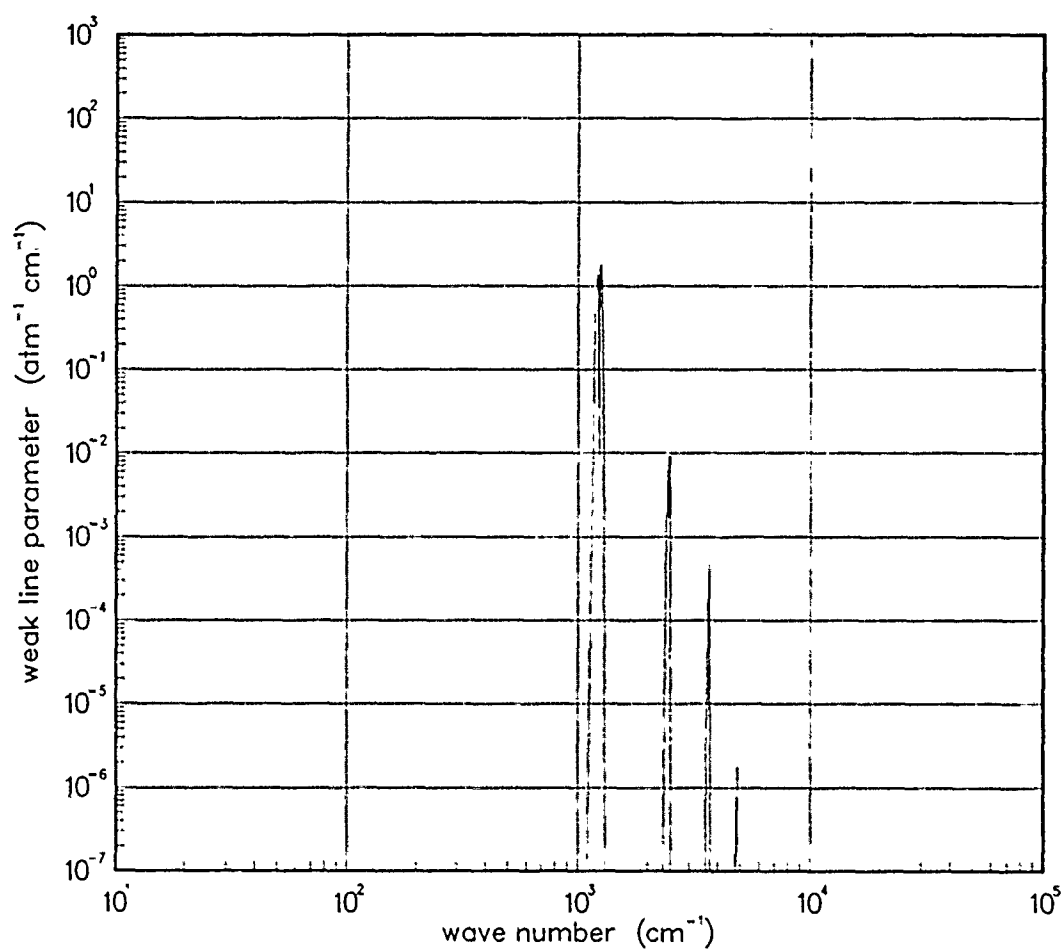


Figure 429. Weak-line parameter for SiO at 300°K.

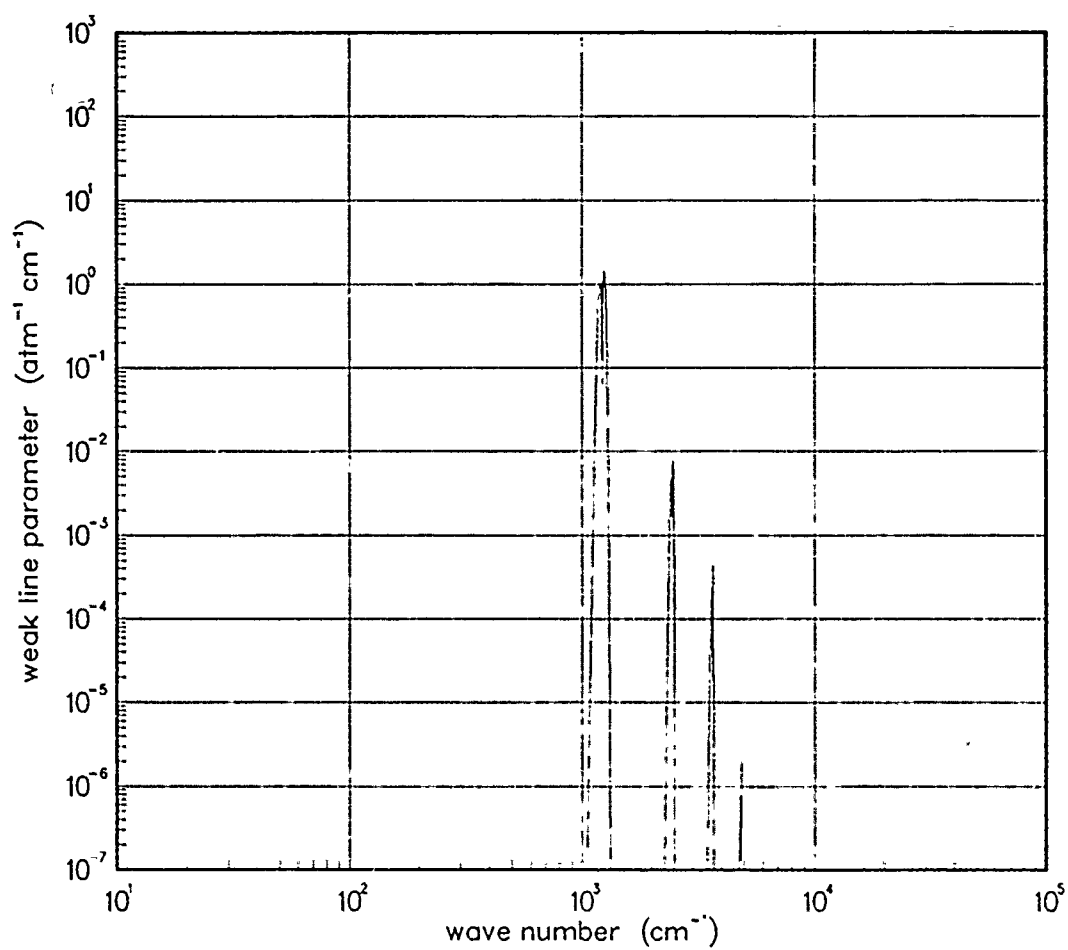


Figure 430. Weak-line parameter for SiO at 500°K.

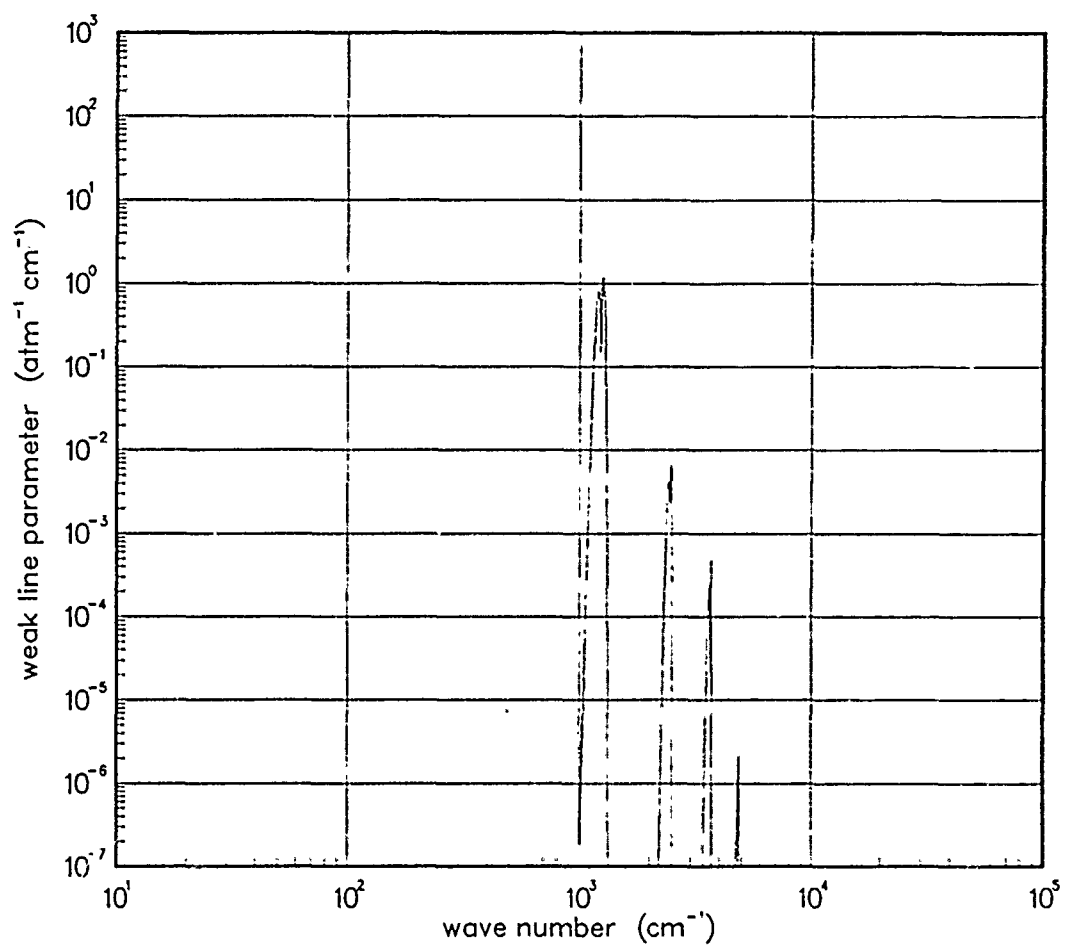


Figure 431. Weak-line parameter for SiO at 750°K.

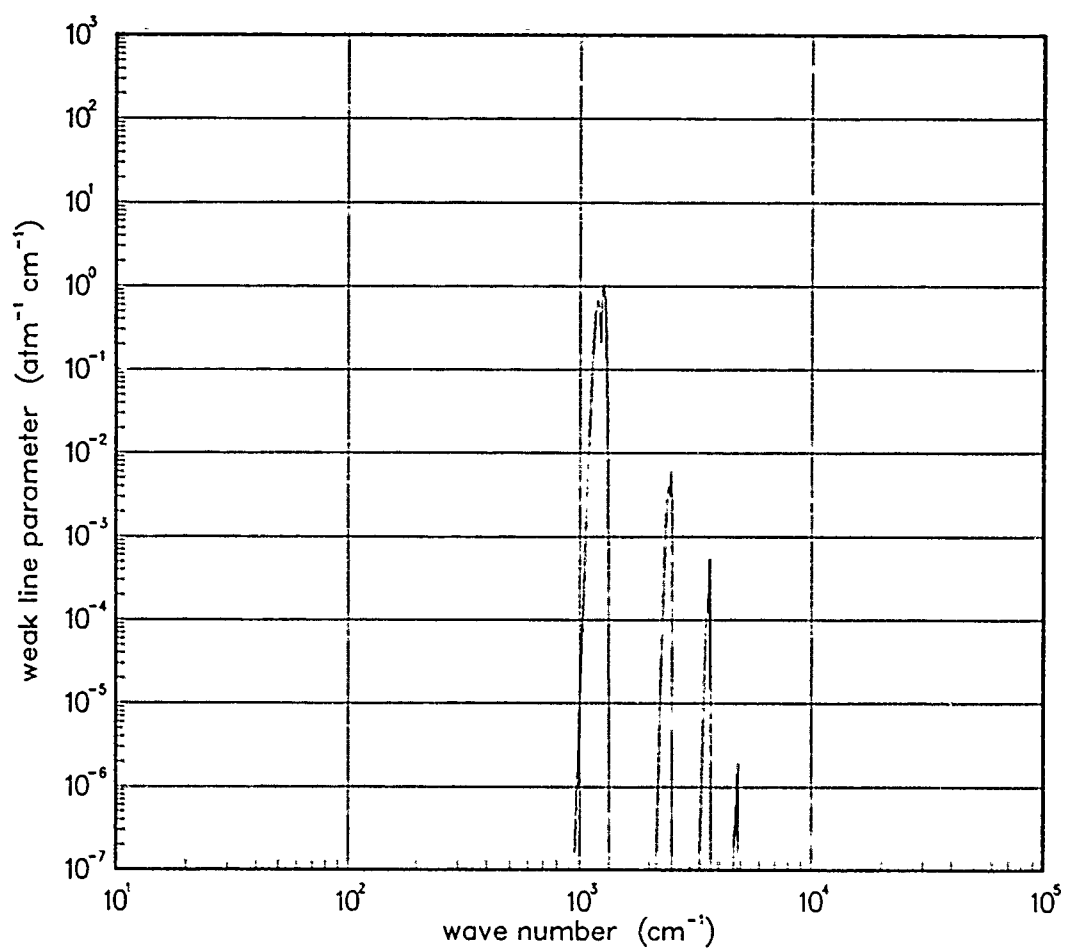


Figure 432. Weak-line parameter for SiO at 1000°K.

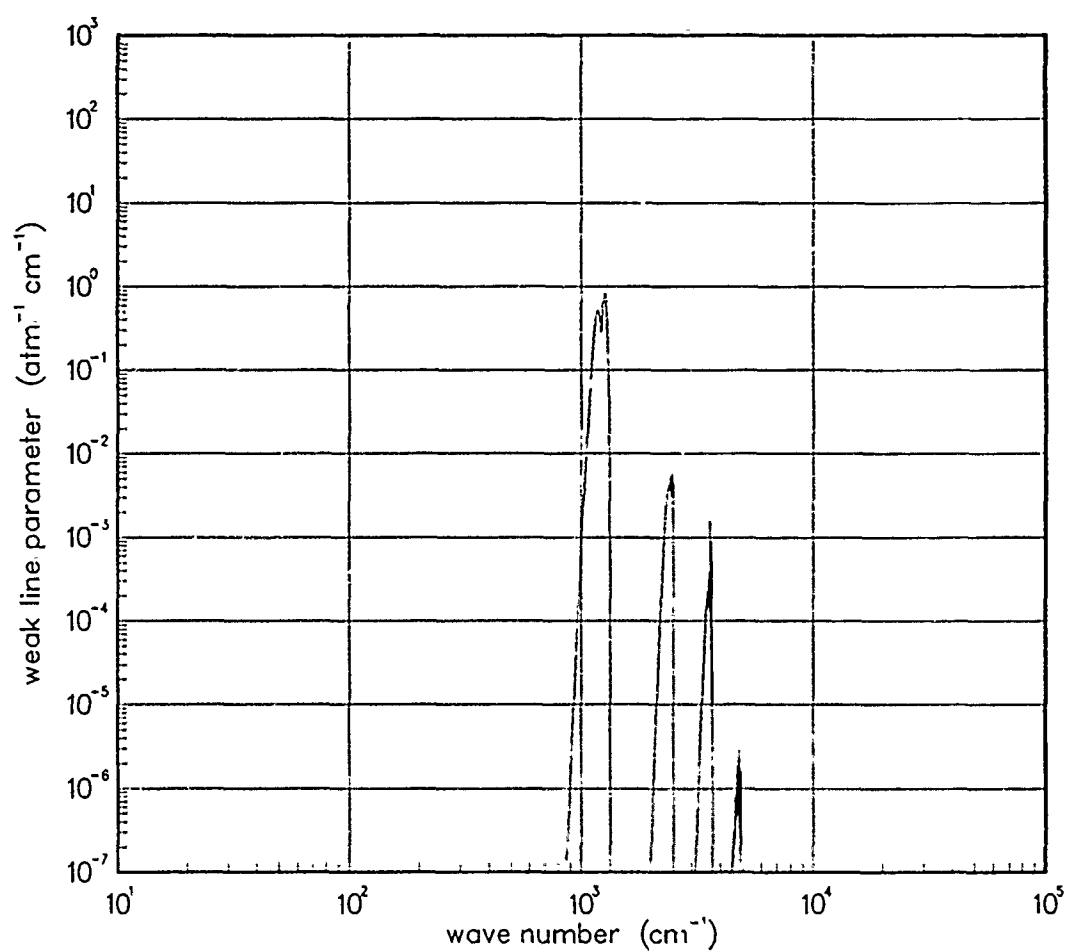


Figure 433. Weak-line parameter for SiO at 1500°K.

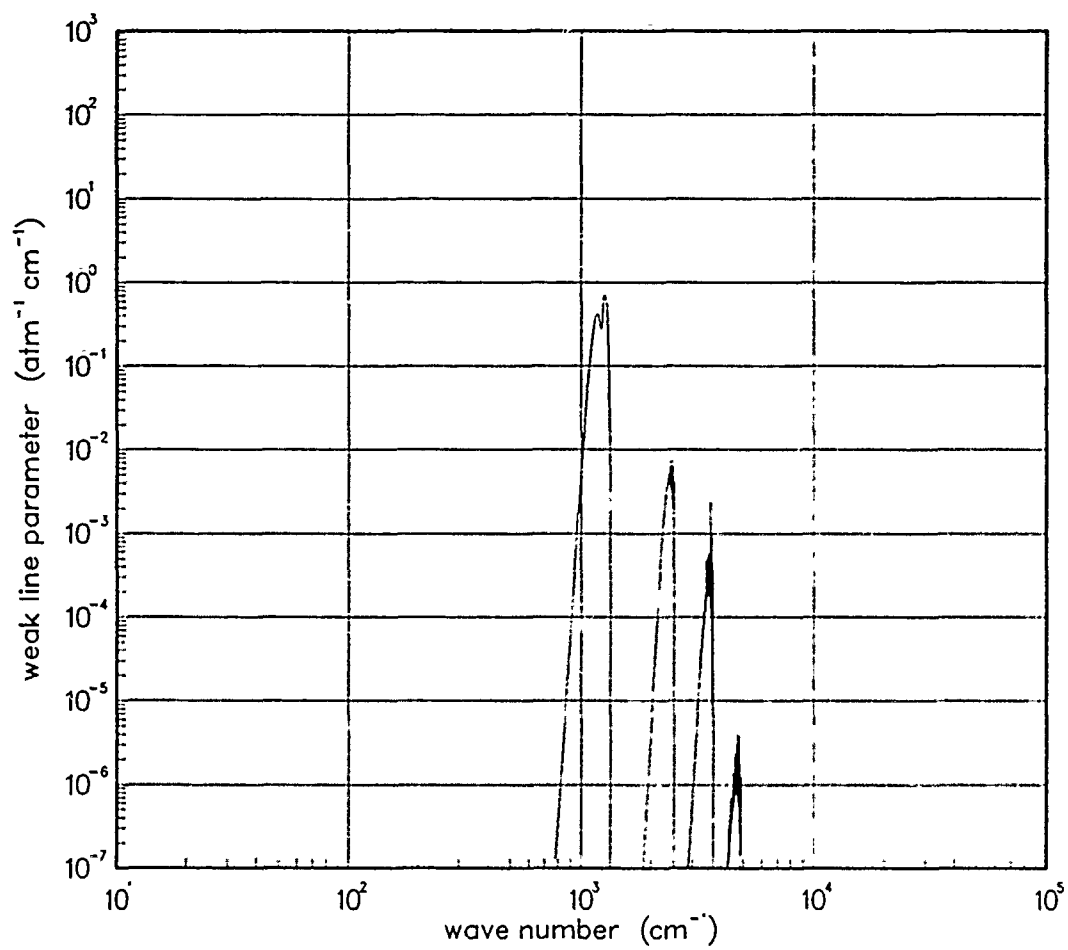


Figure 434. Weak-line parameter for SiO at 2000°K.

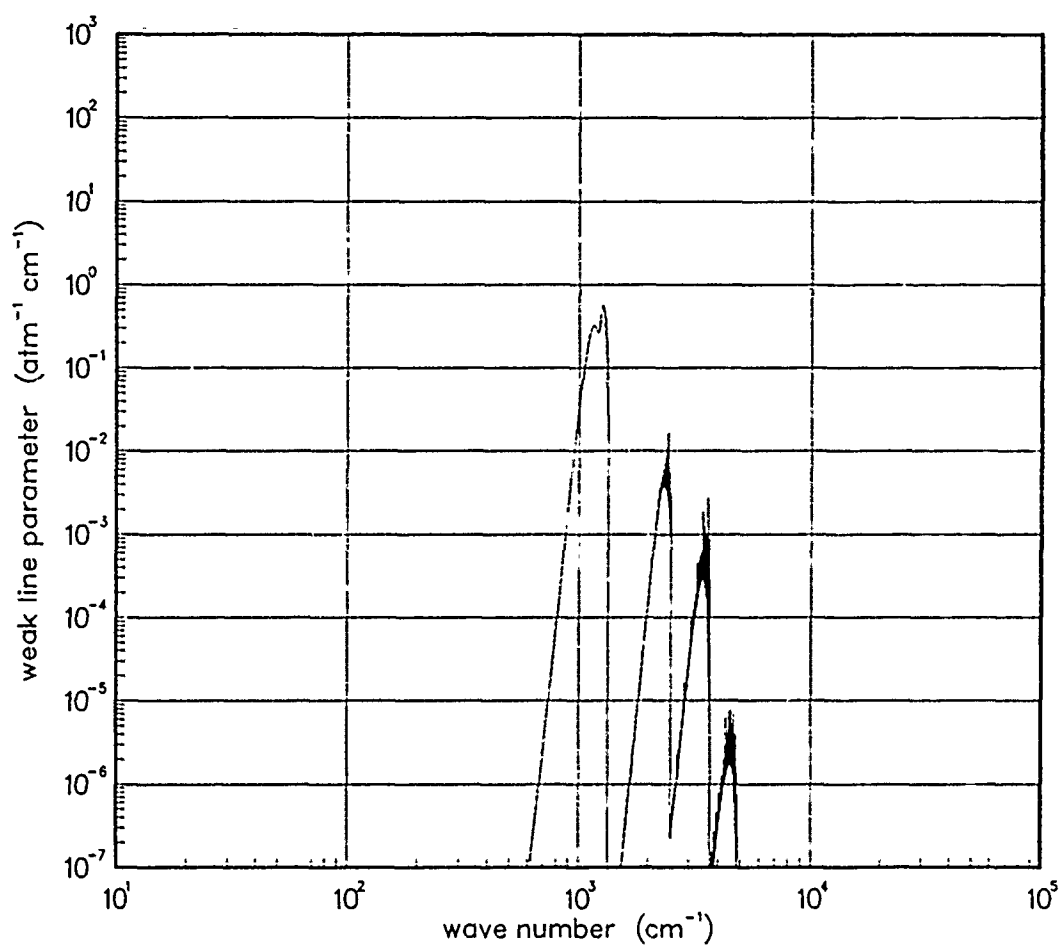


Figure 435. Weak-line parameter for SiO at 3000°K.

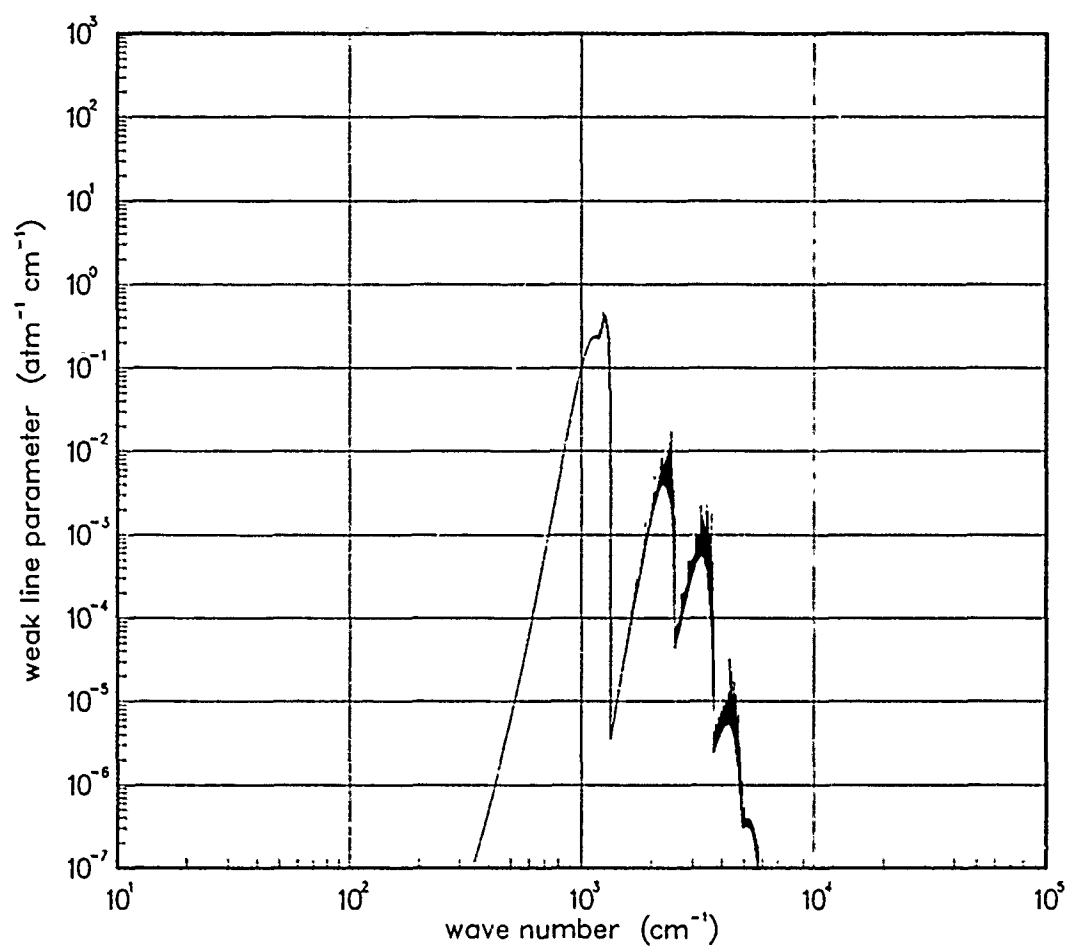


Figure 436. Weak-line parameter for SiO at 5000°K.

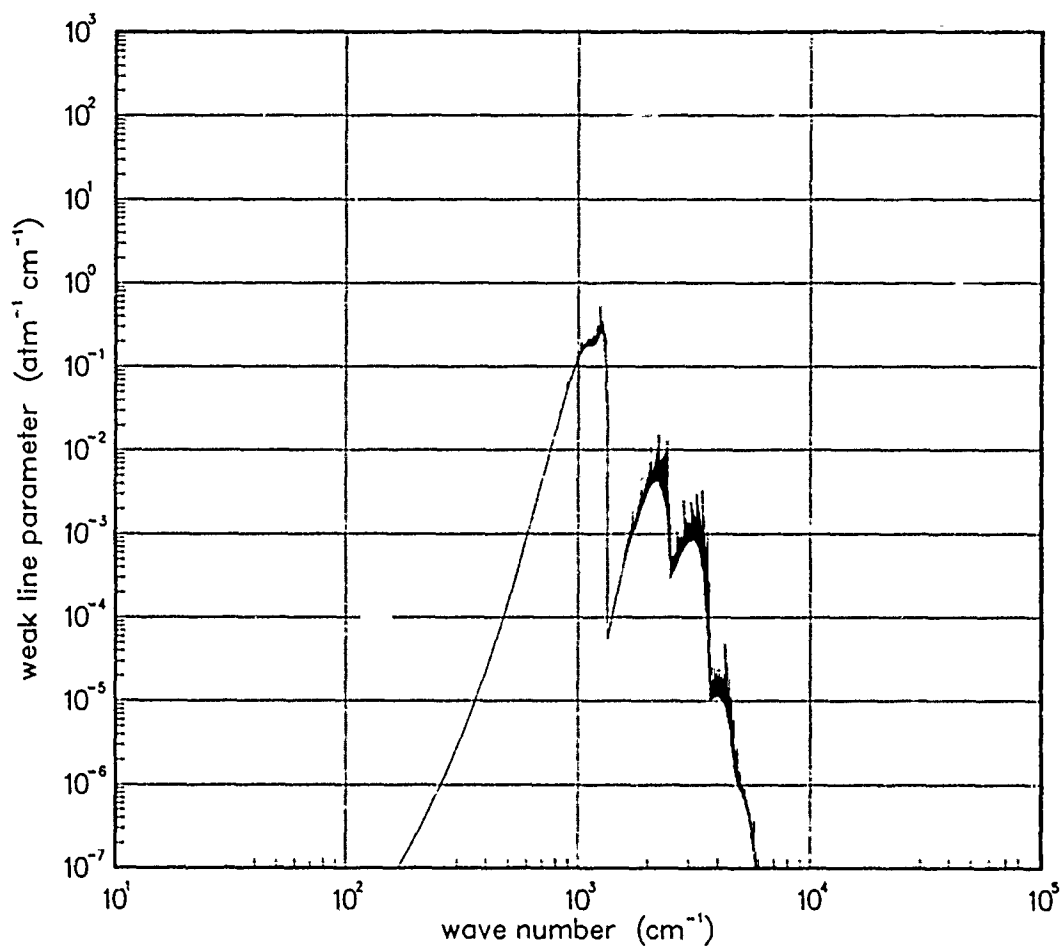


Figure 437. Weak-line parameter for SiO at 7000°K.

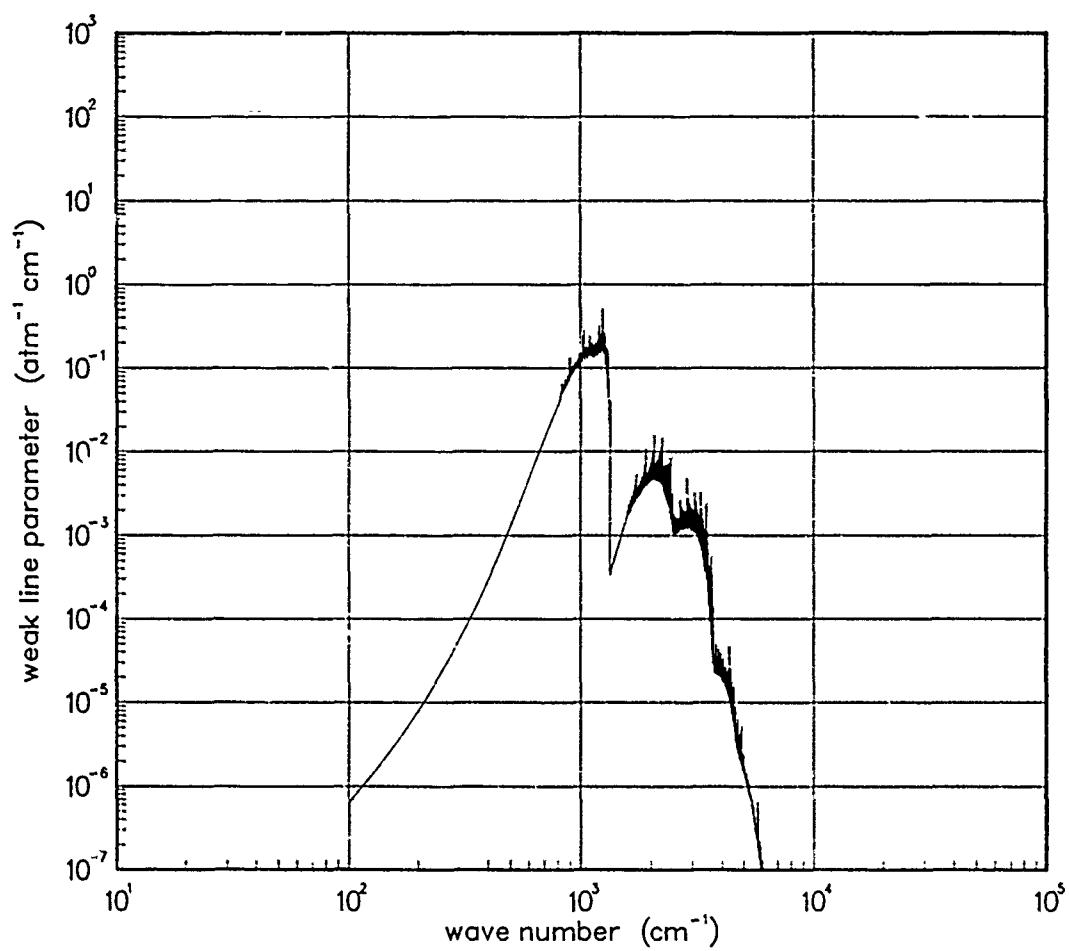


Figure 438. Weak-line parameter for SiO at 10000°K.

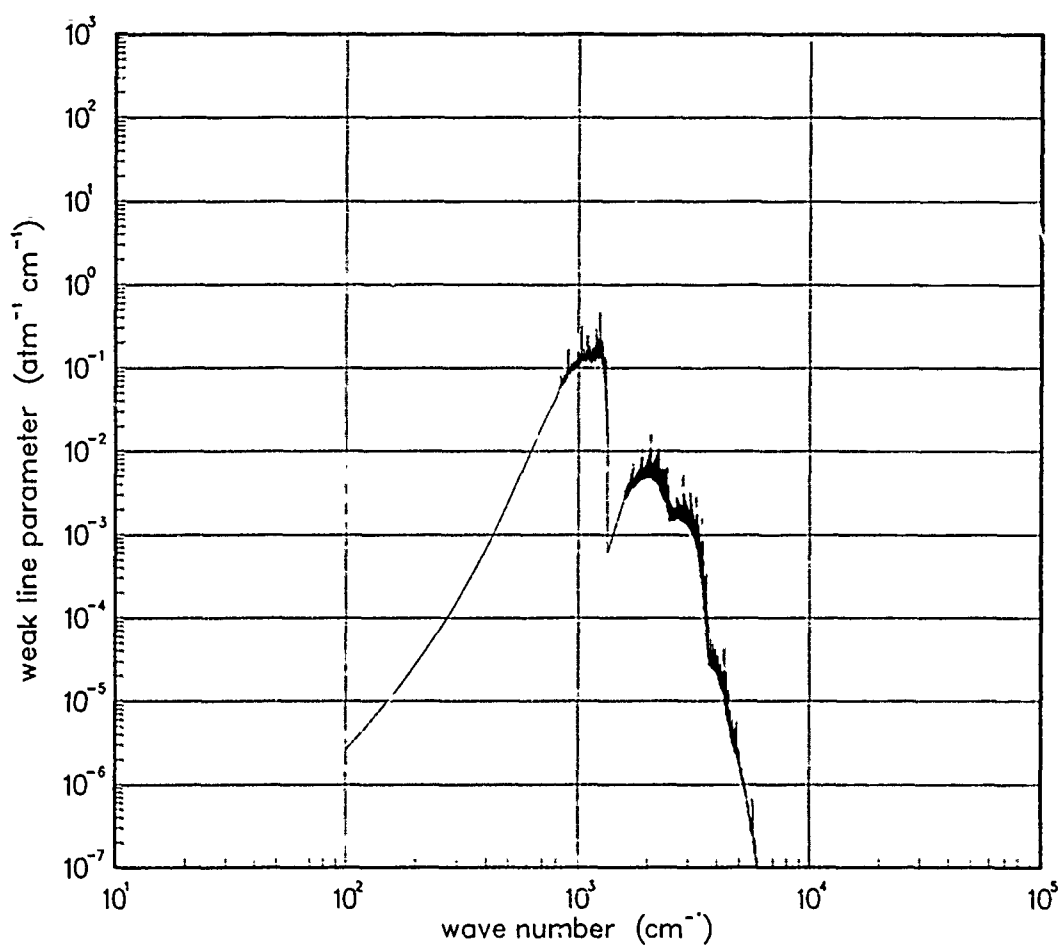


Figure 439. Weak-line parameter for SiO at 12000°K.

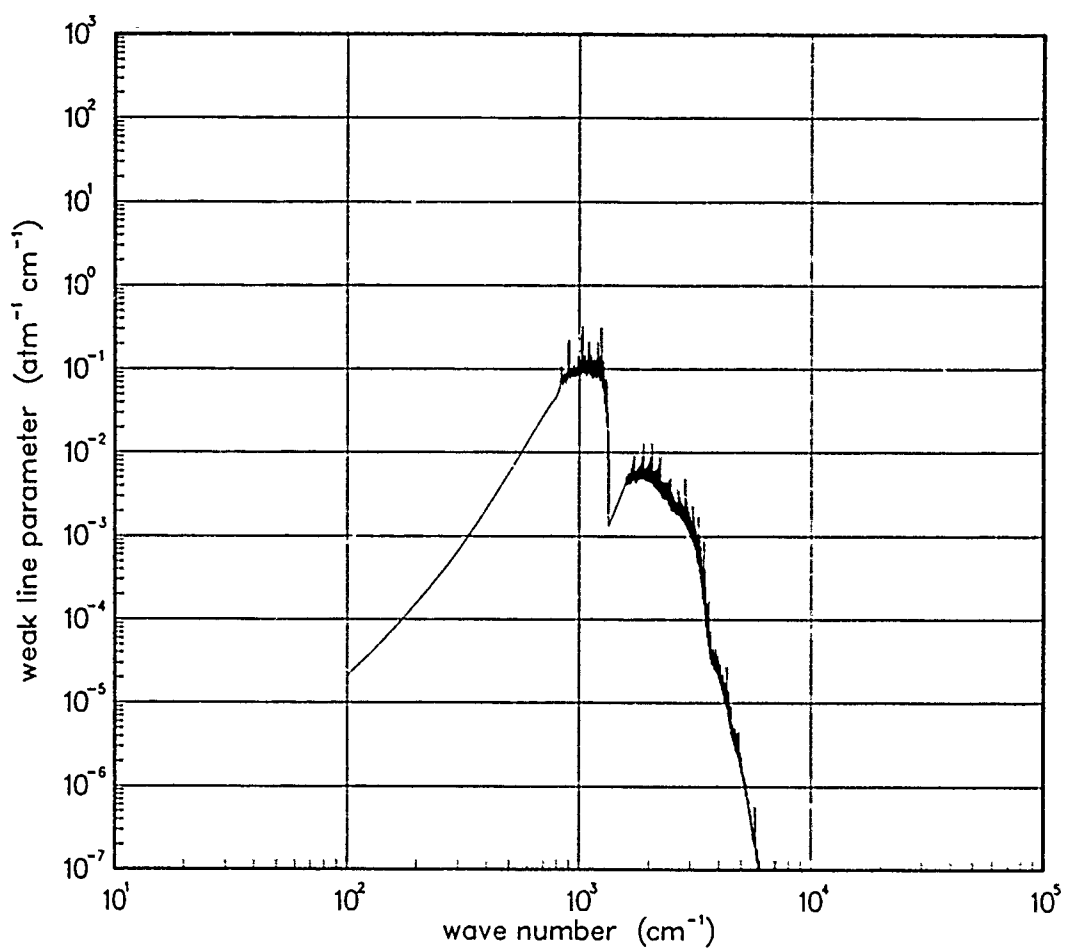


Figure 440. Weak-line parameter for SiO at 18000°K.

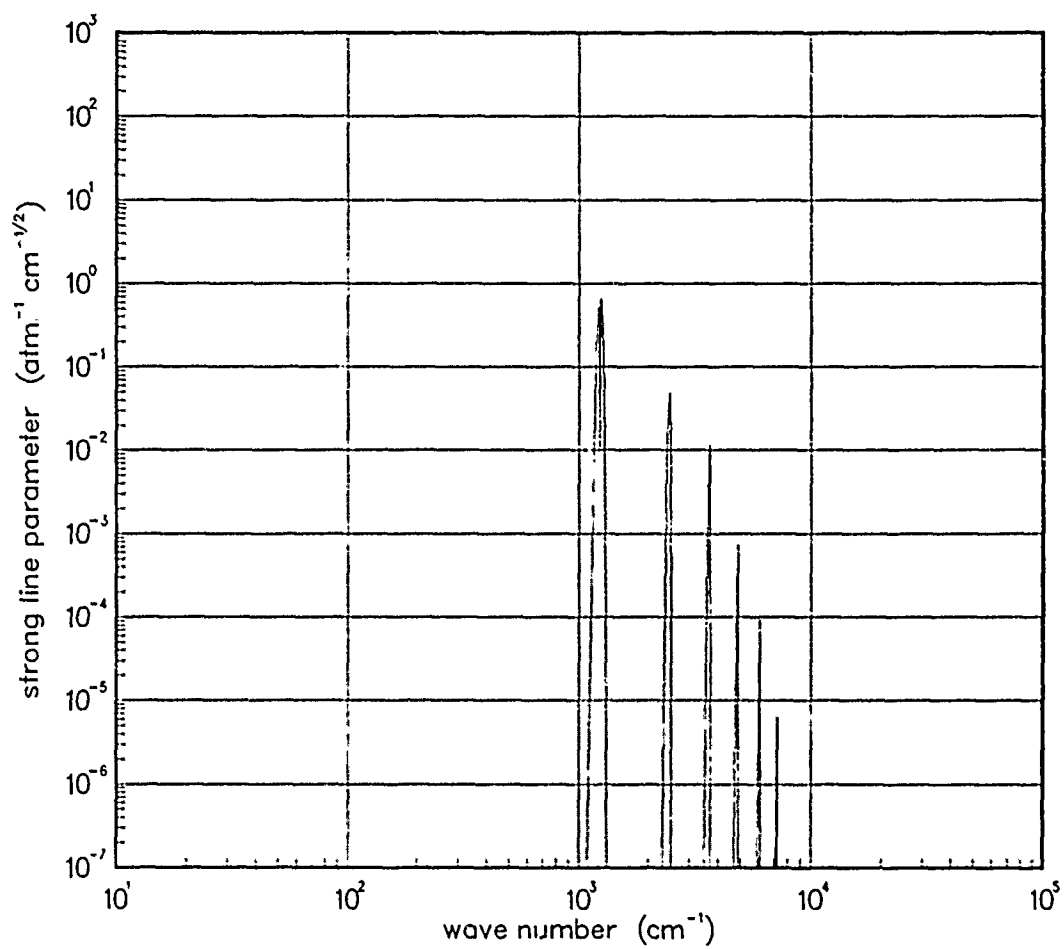


Figure 441. Strong-line parameter for SiO at 200°K.

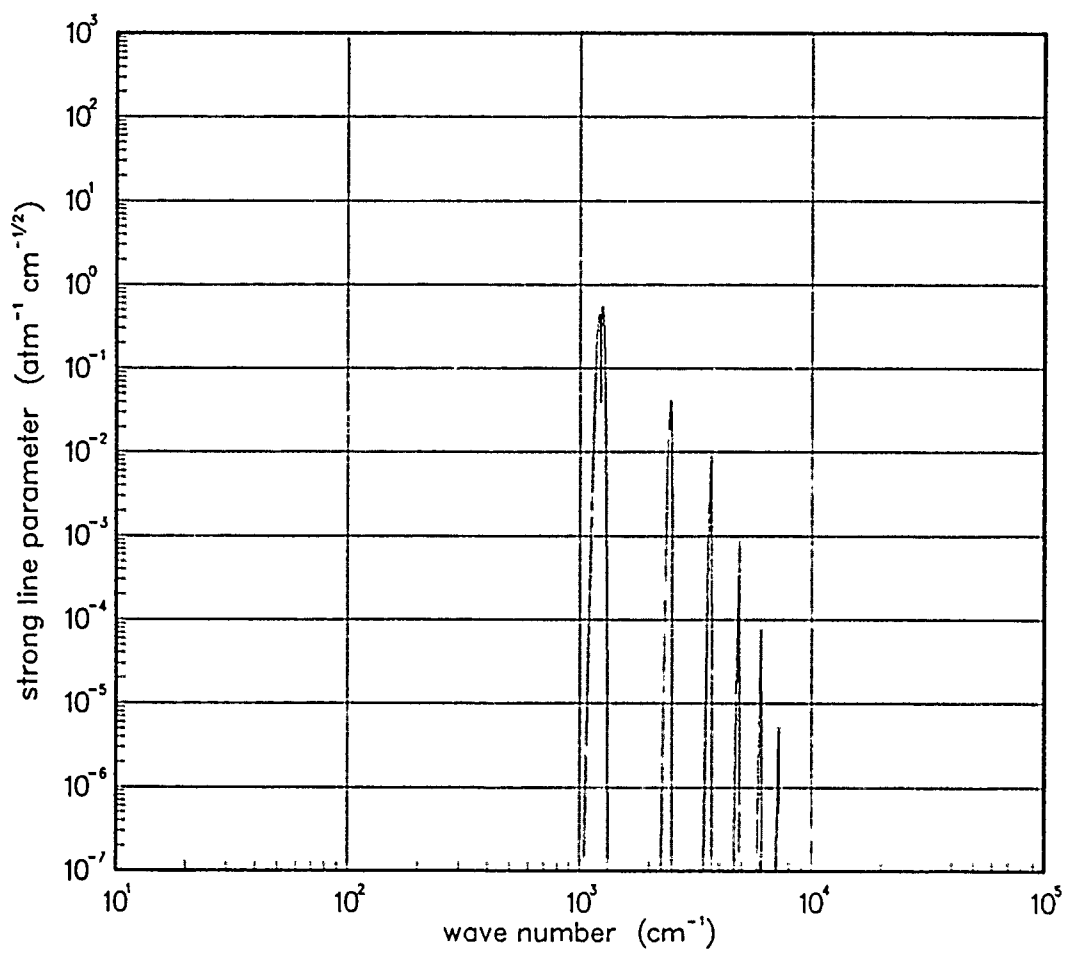


Figure 442. Strong-line parameter for SiO at 300°K.

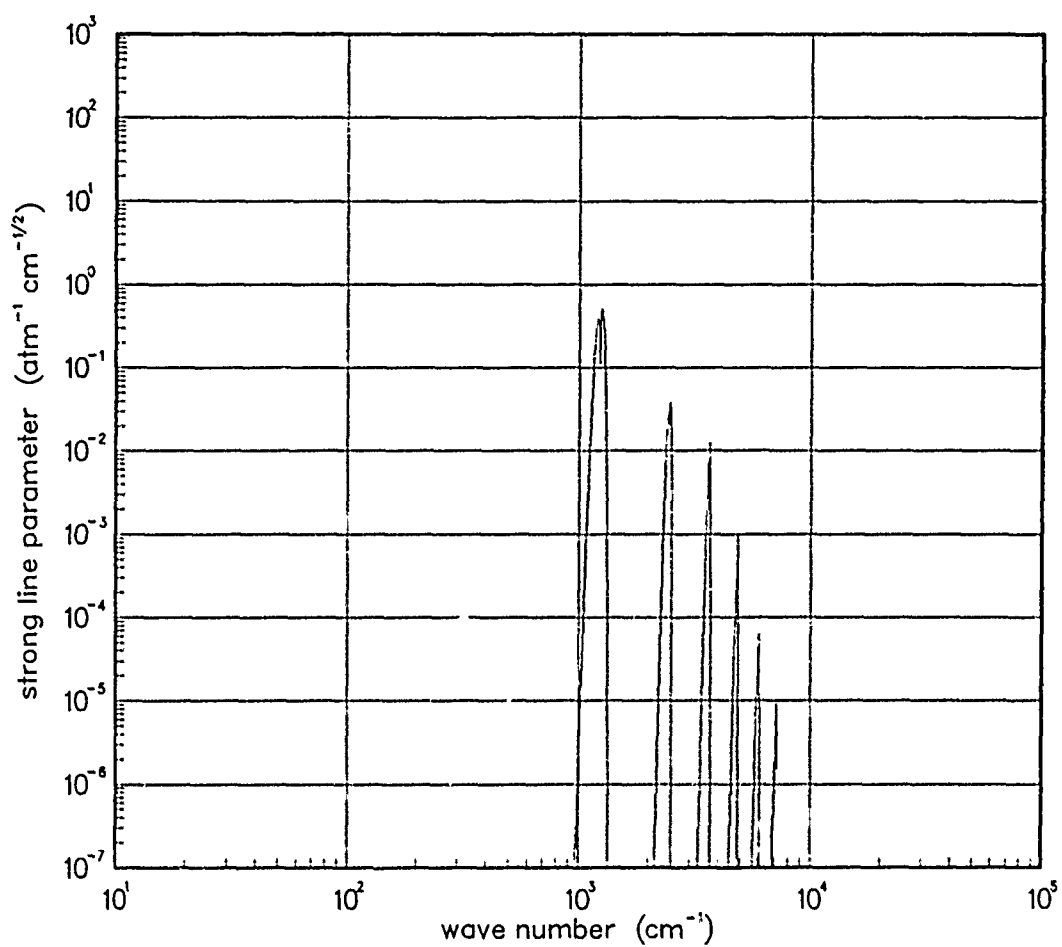


Figure 443. Strong-line parameter for SiO at 500°K.

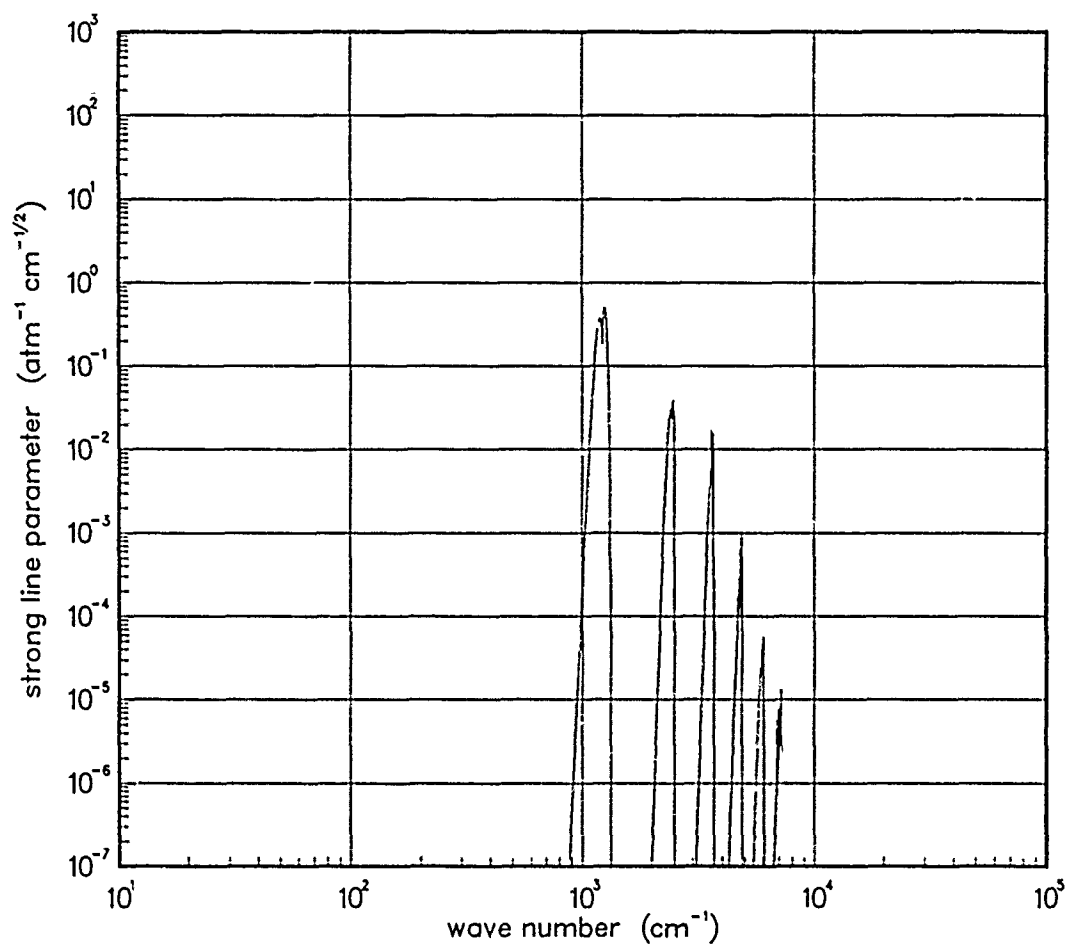


Figure 444. Strong-line parameter for SiO at 750°K.

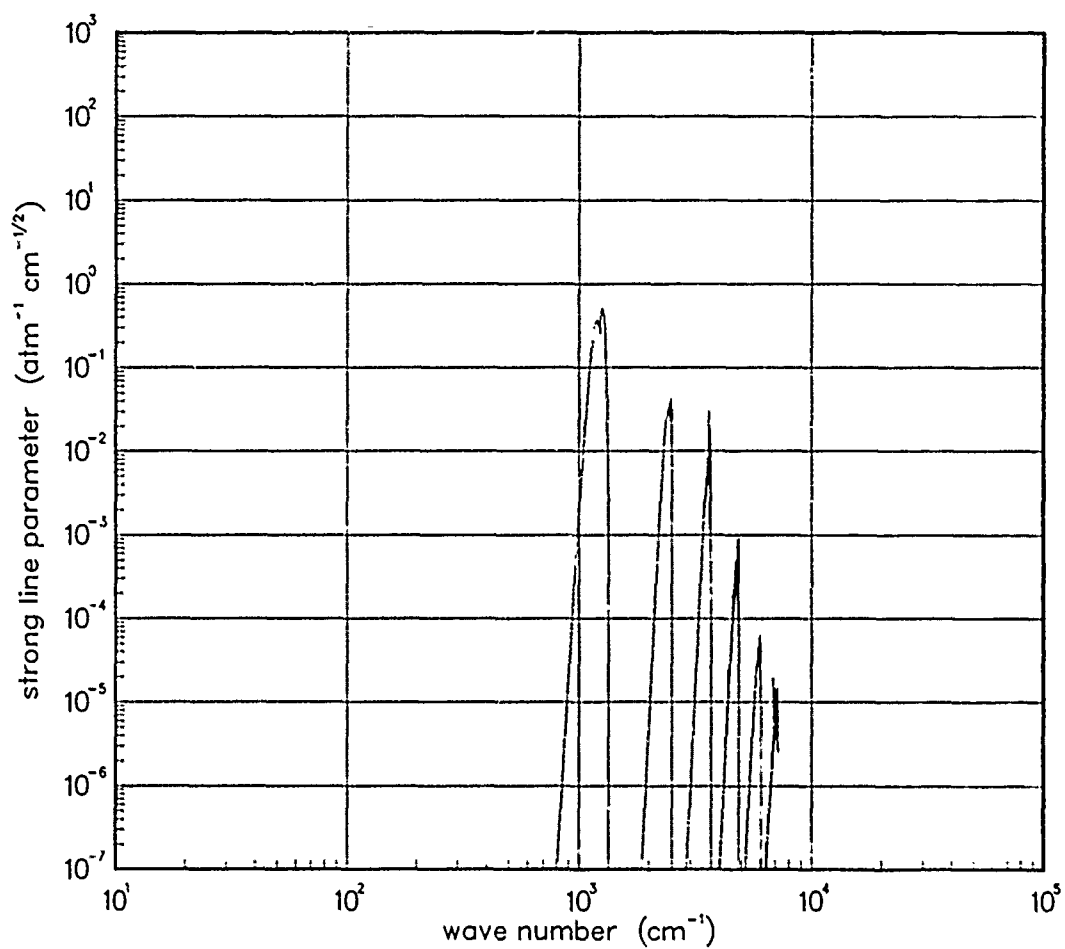


Figure 445. Strong-line parameter for SiO at 1000°K.

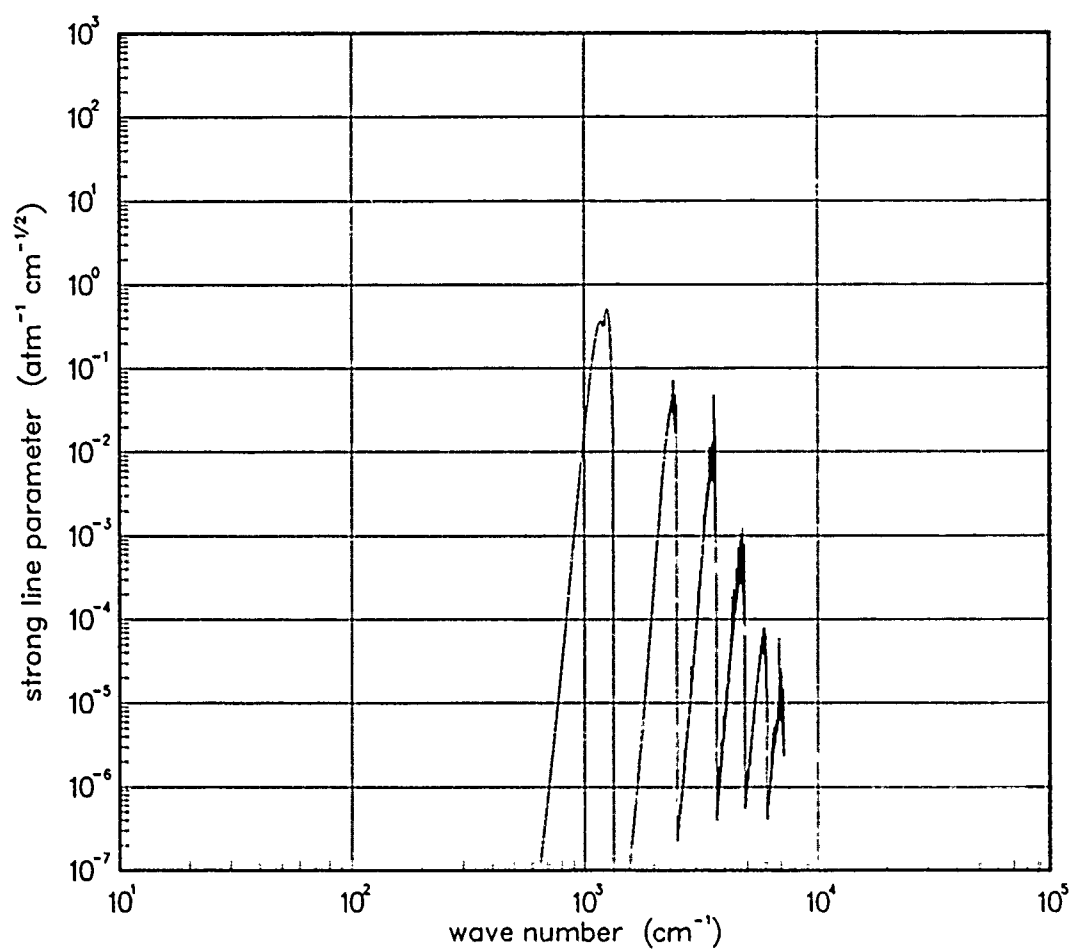


Figure 446. Strong-line parameter for SiO at 1500°K.

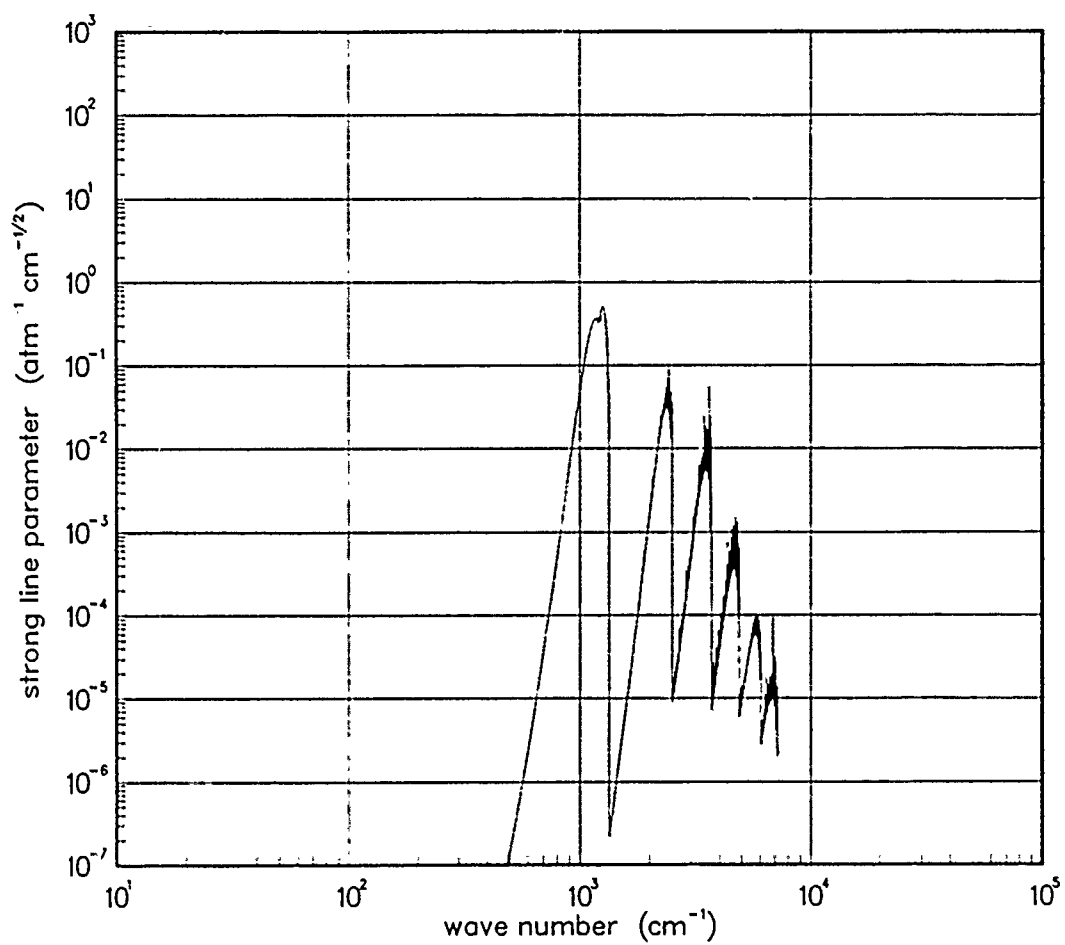


Figure 447. Strong-line parameter for SiO at 2000°K.

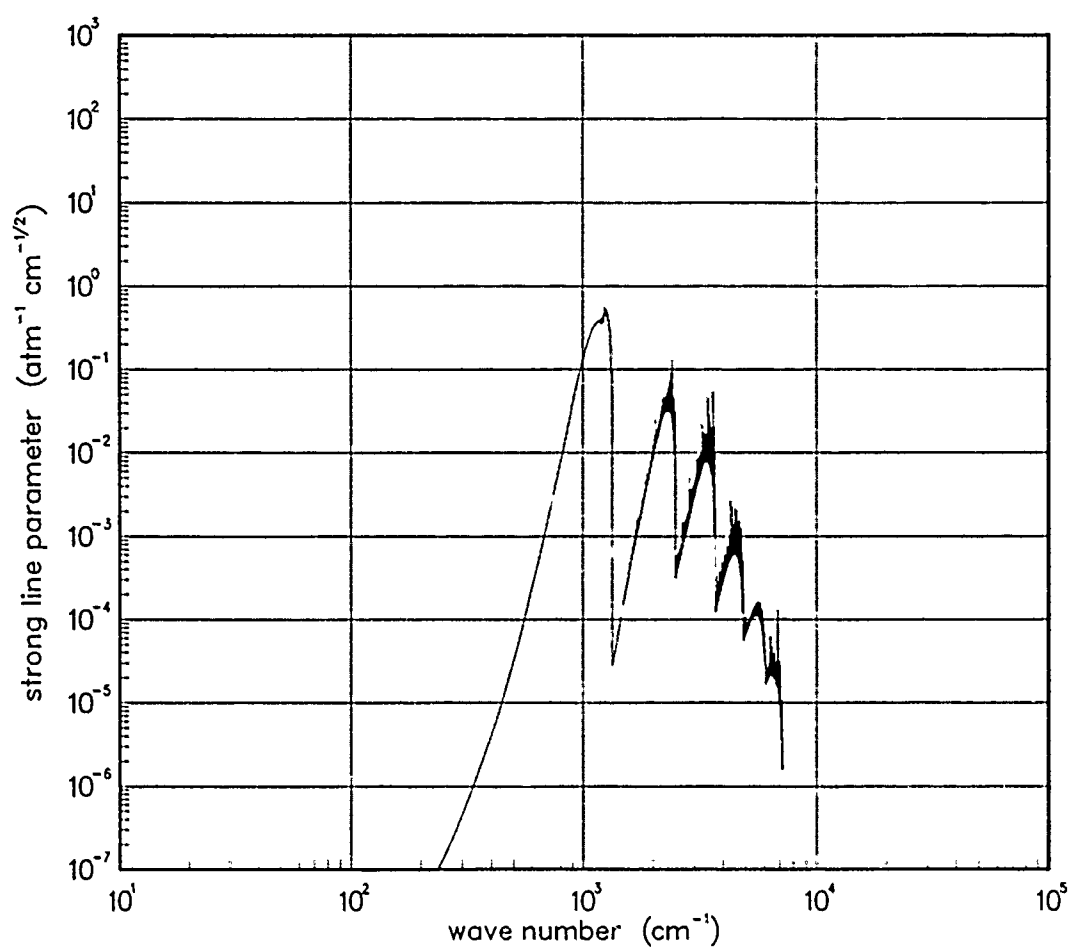


Figure 448. Strong-line parameter for SiO at 3000°K.

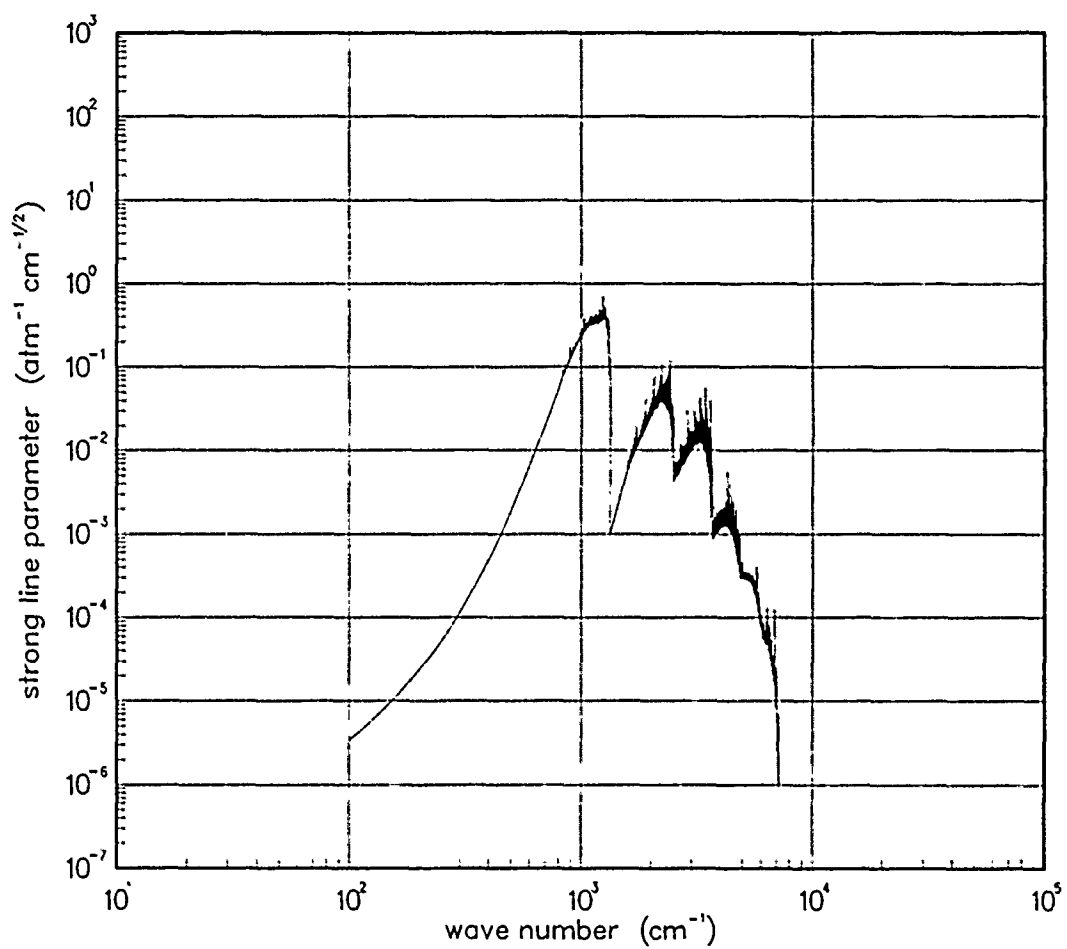


Figure 449. Strong-line parameter for SiO at 5000°K.

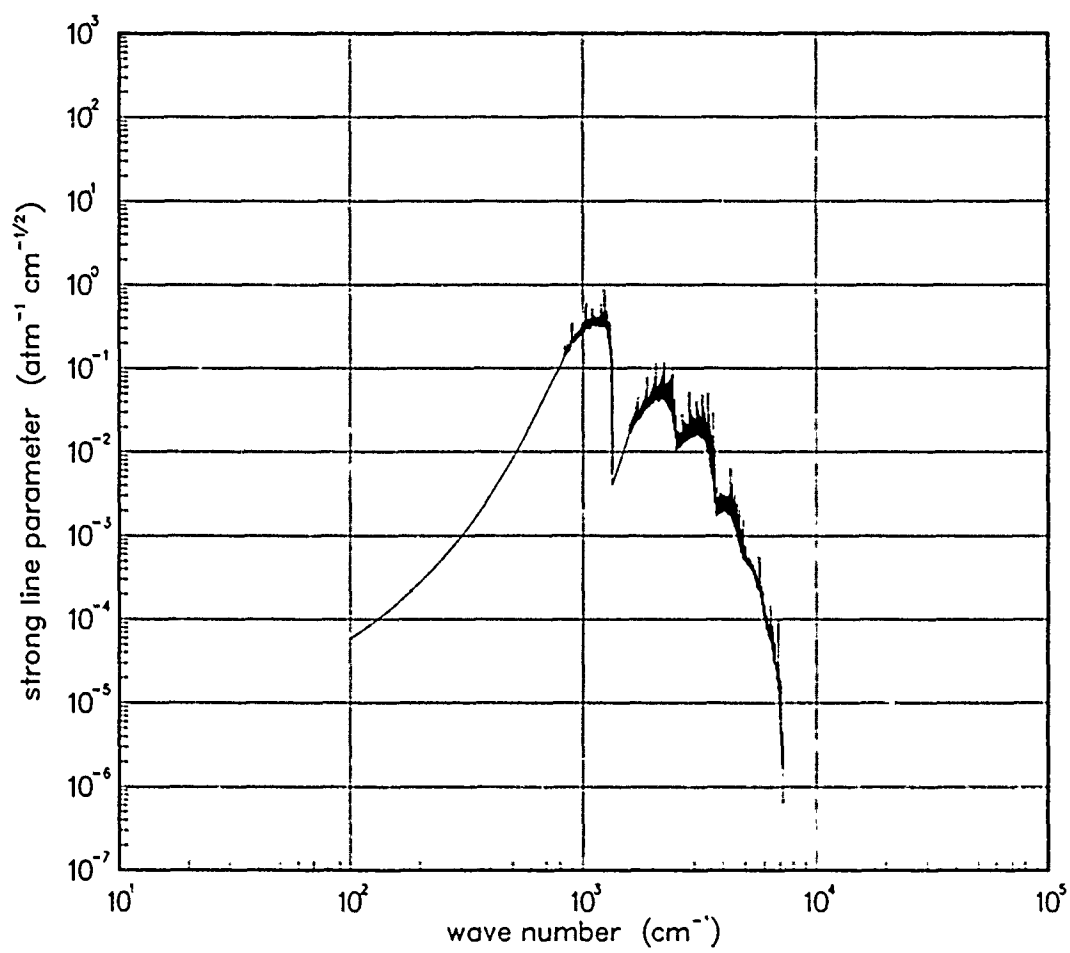


Figure 450. Strong-line parameter for SiO at 7000°K.

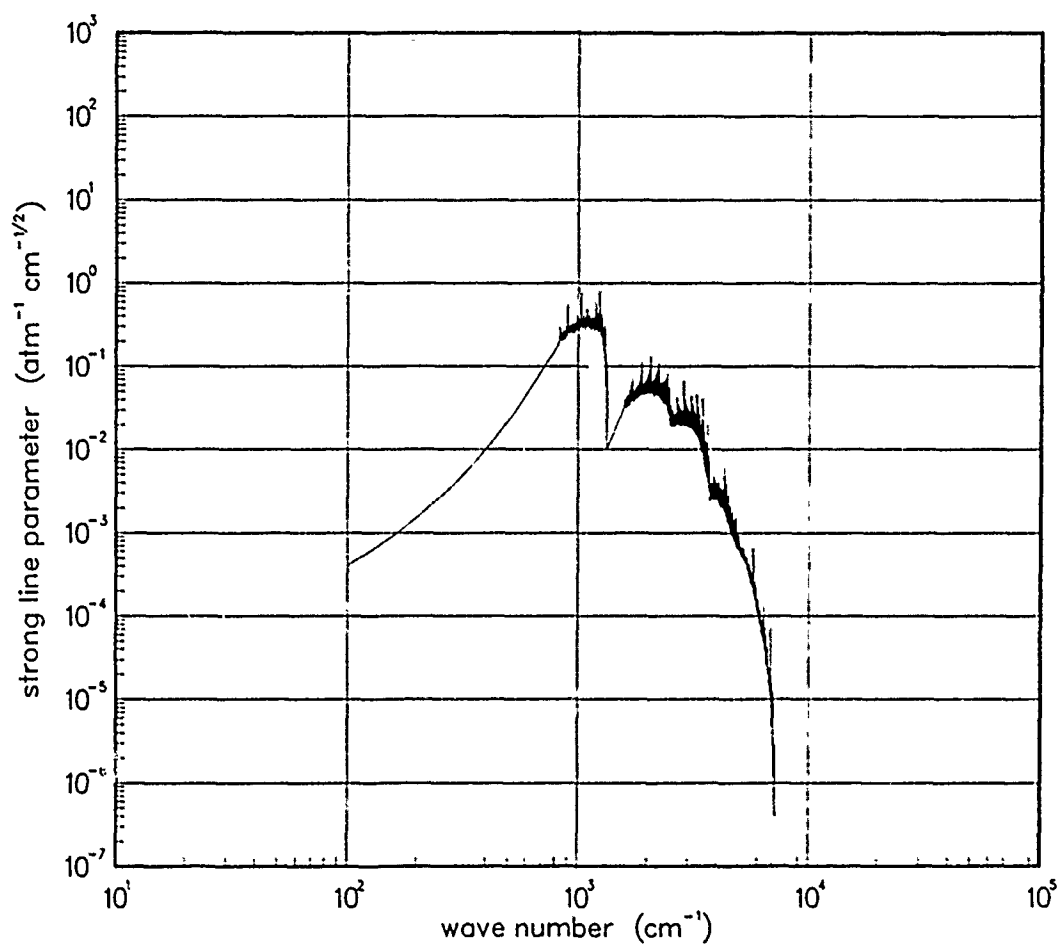


Figure 451. Strong-line parameter for SiO at 10000°K.

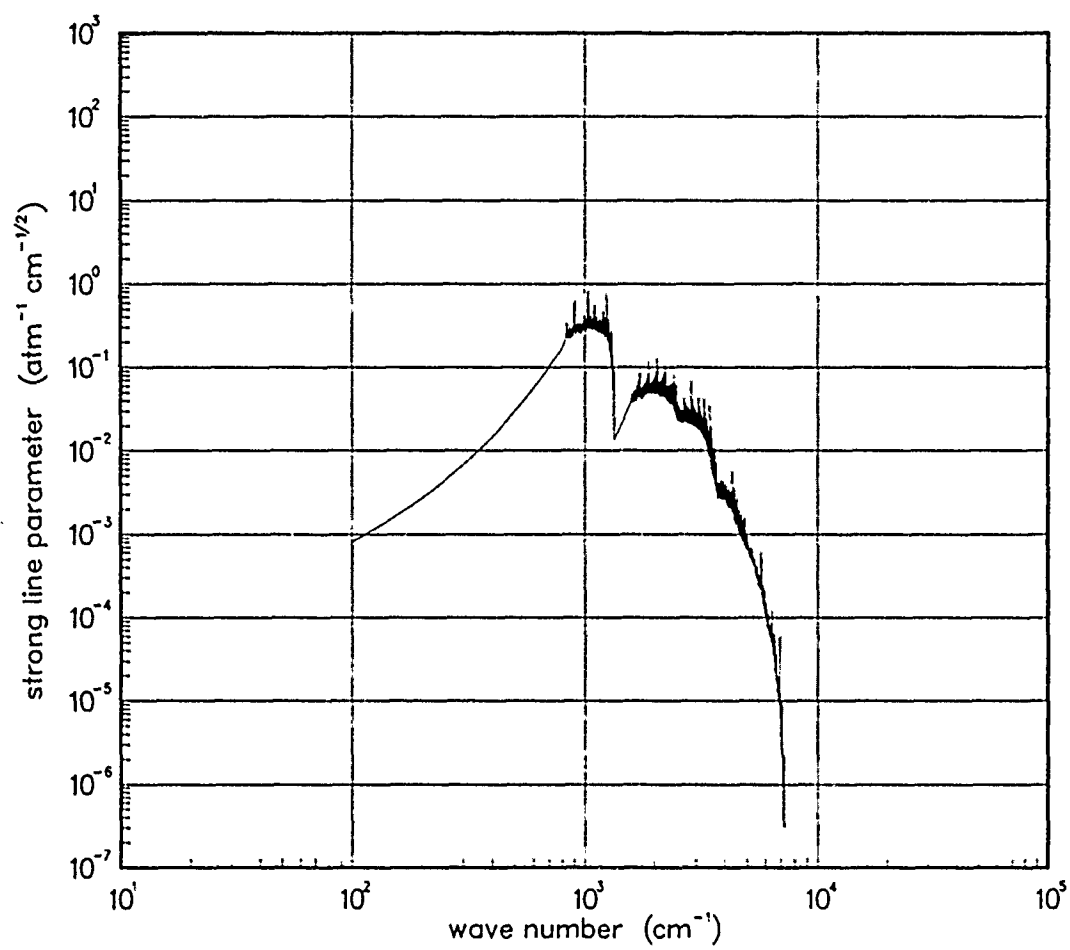


Figure 452. Strong-line parameter for SiO at 12000°K.

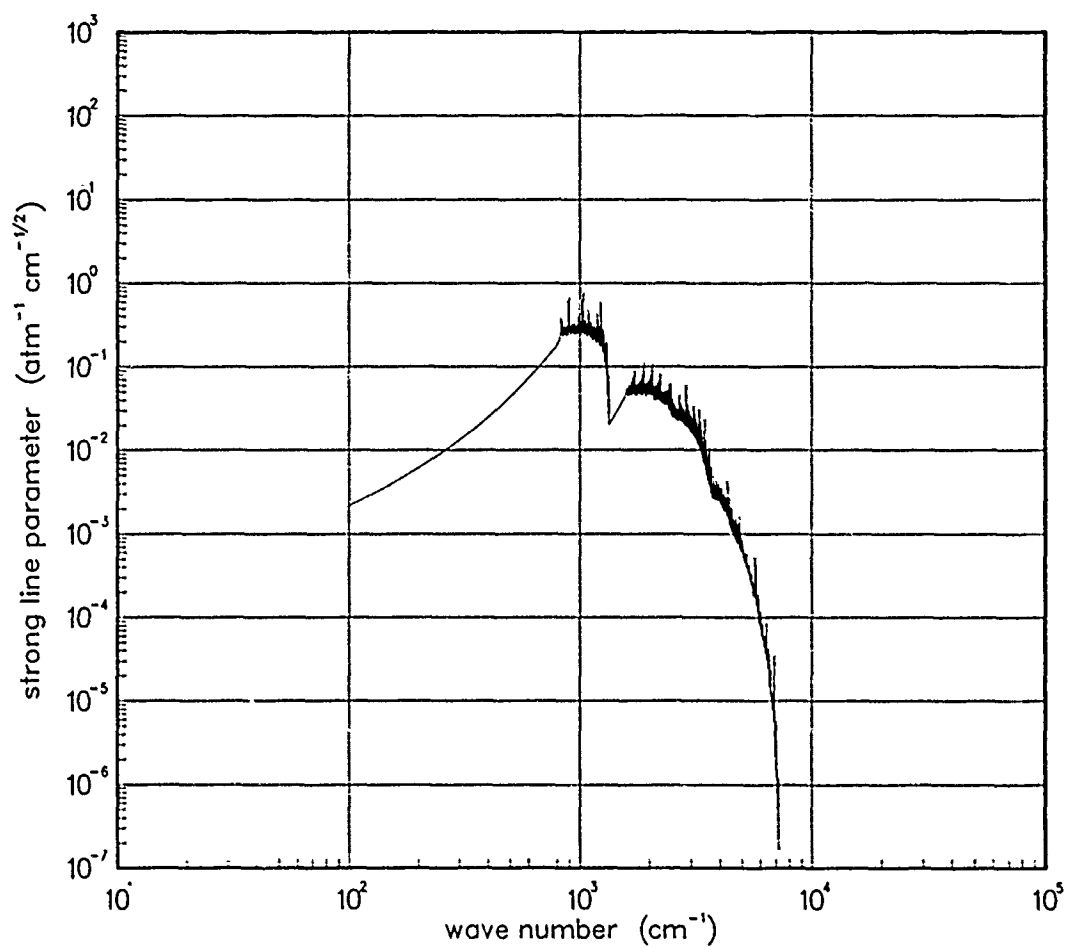


Figure 453. Strong-line parameter for SiO at 18000°K.

6.7 TITANIUM OXIDE (TiO).

Table 13. Spectroscopic data for TiO.

$X^3\Delta$			
$\omega_e = 1008.26^\dagger$	$\omega_e x_e = 4.13^\dagger$		
$\alpha_e = .0031^\dagger$	$A_e = 48.3^*$	$B_e = .5354^\dagger$	$E_e = 0.0$
$S_{10} = 149.0^\ddagger$	$S_{20} = .549^\ddagger$	$S_{30} = 0.076^\ddagger$	

Data Source:

*J.D. Phillips, *Astrophys. J.* 169, 185 (1971).

†B. Rosen, ed., Spectroscopic Data Relative to Diatomic Molecules, Pergamon Press, New York (1970).

‡H.H. Michels, *Diatomic Oxide Vibrational Band Intensities*, United Aircraft Research Laboratories, K921094-4 (May 1971).

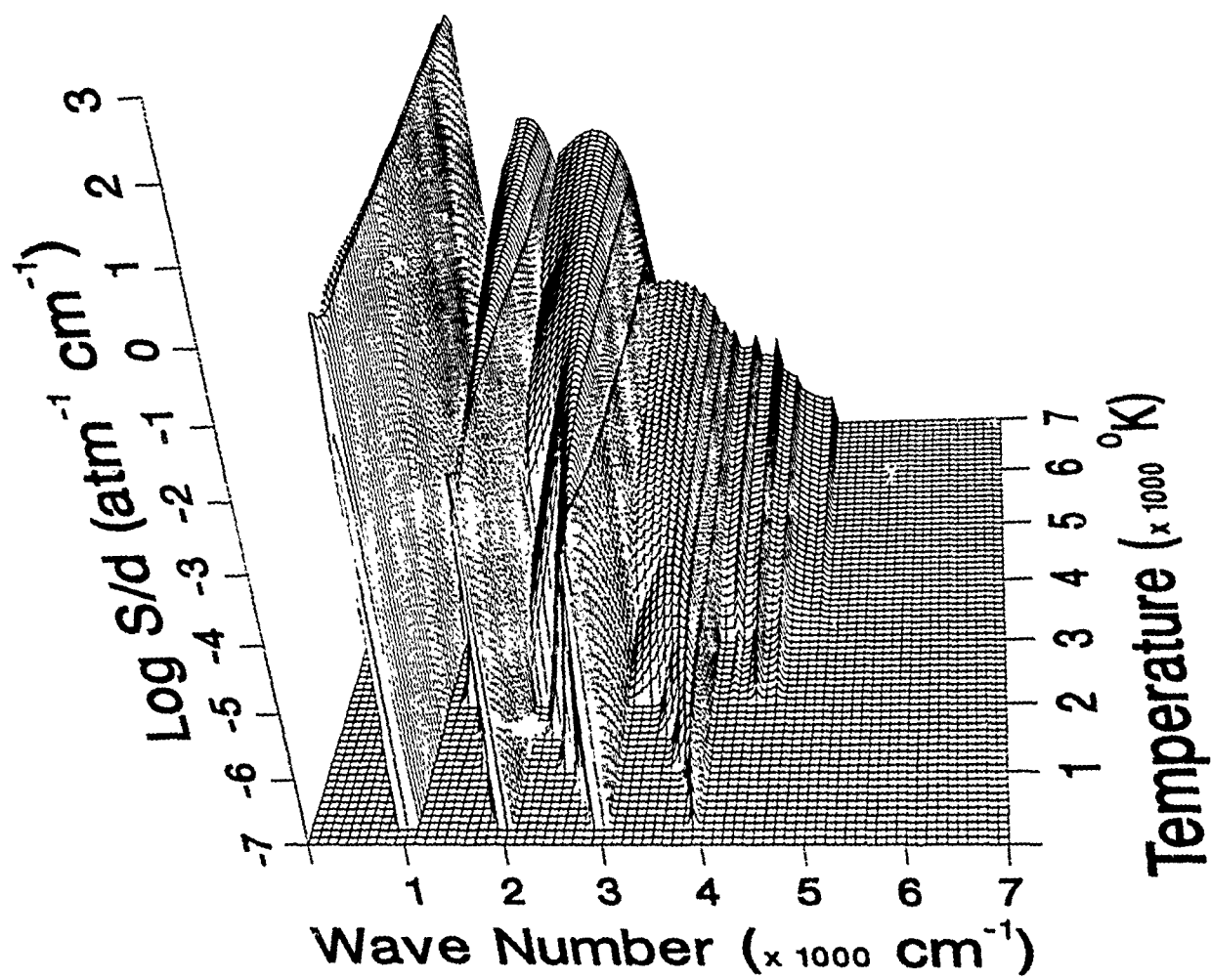


Figure 454. Weak-line parameter for TiO.

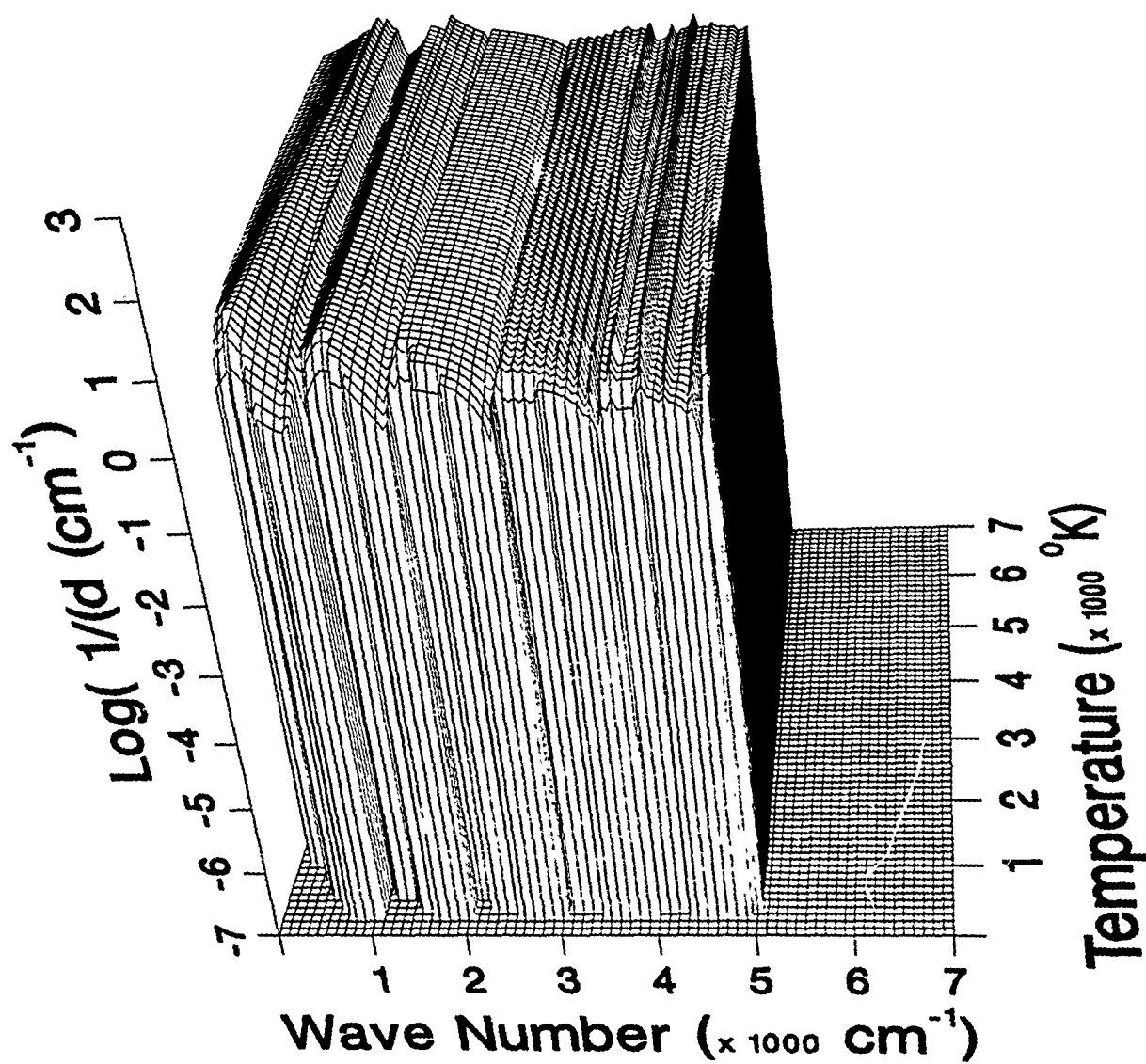


Figure 455. Inverse line spacing for TiO.

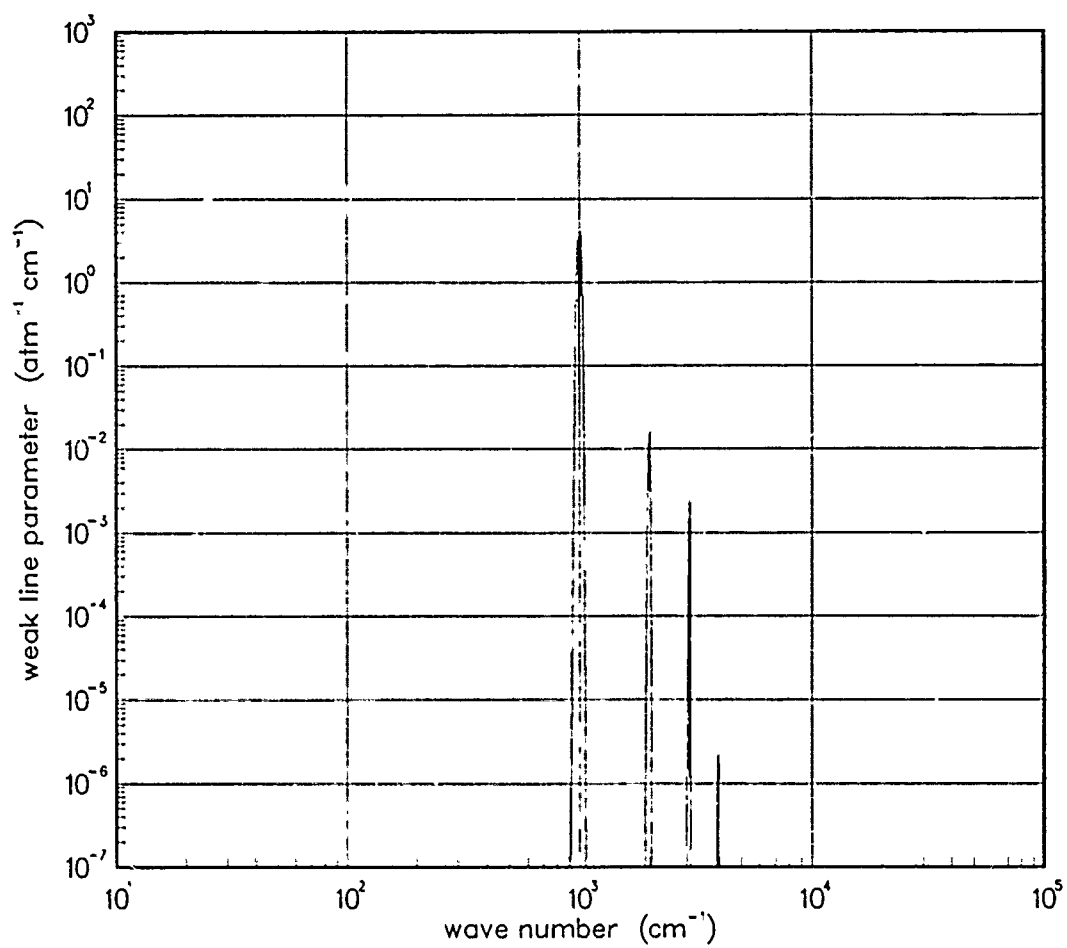


Figure 456. Weak-line parameter for TiO at 200°K.

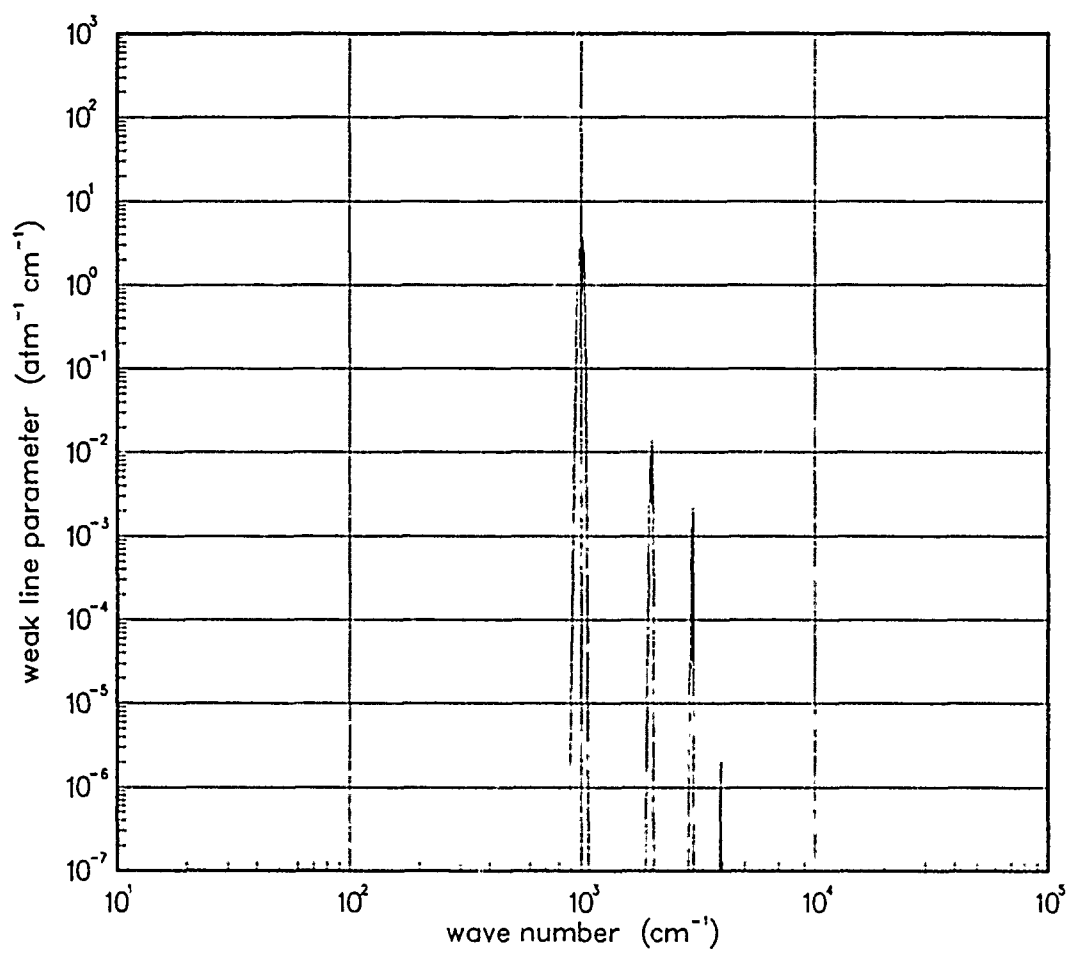


Figure 457. Weak-line parameter for TiO at 300°K.

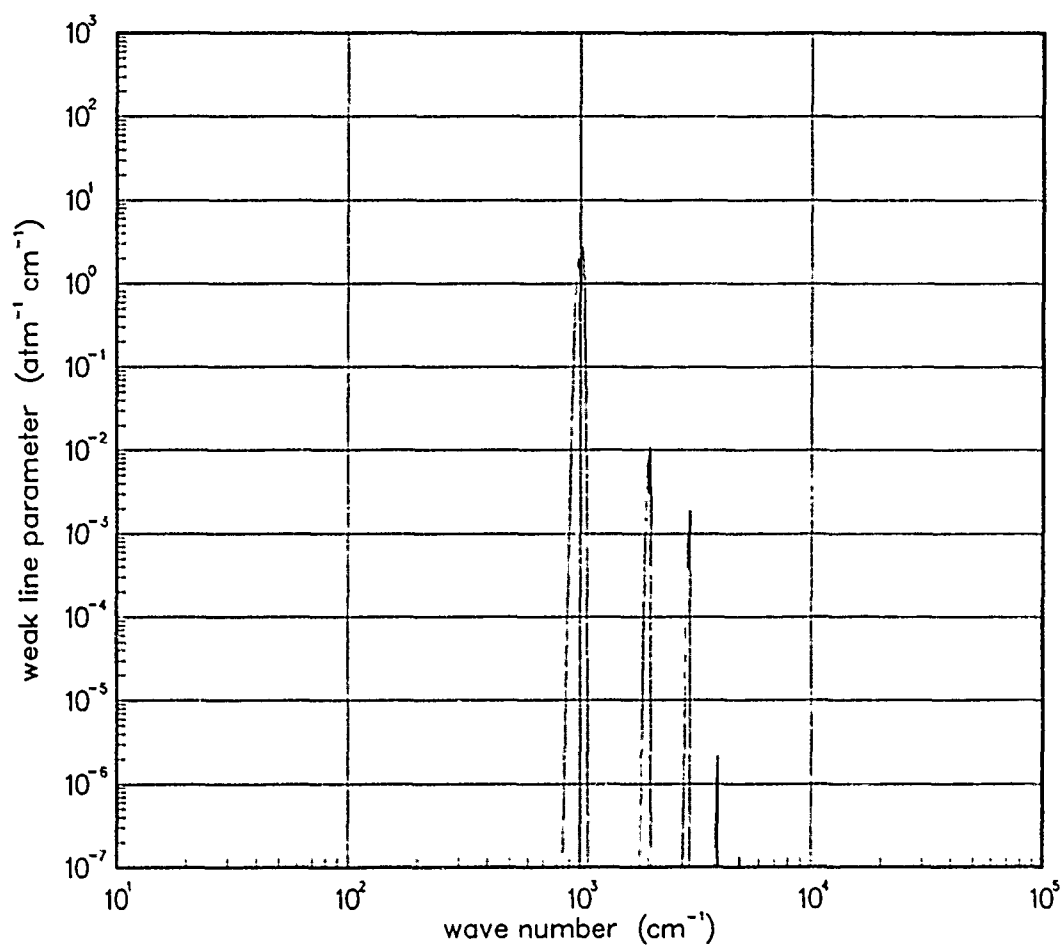


Figure 458. Weak-line parameter for TiO at 500°K.

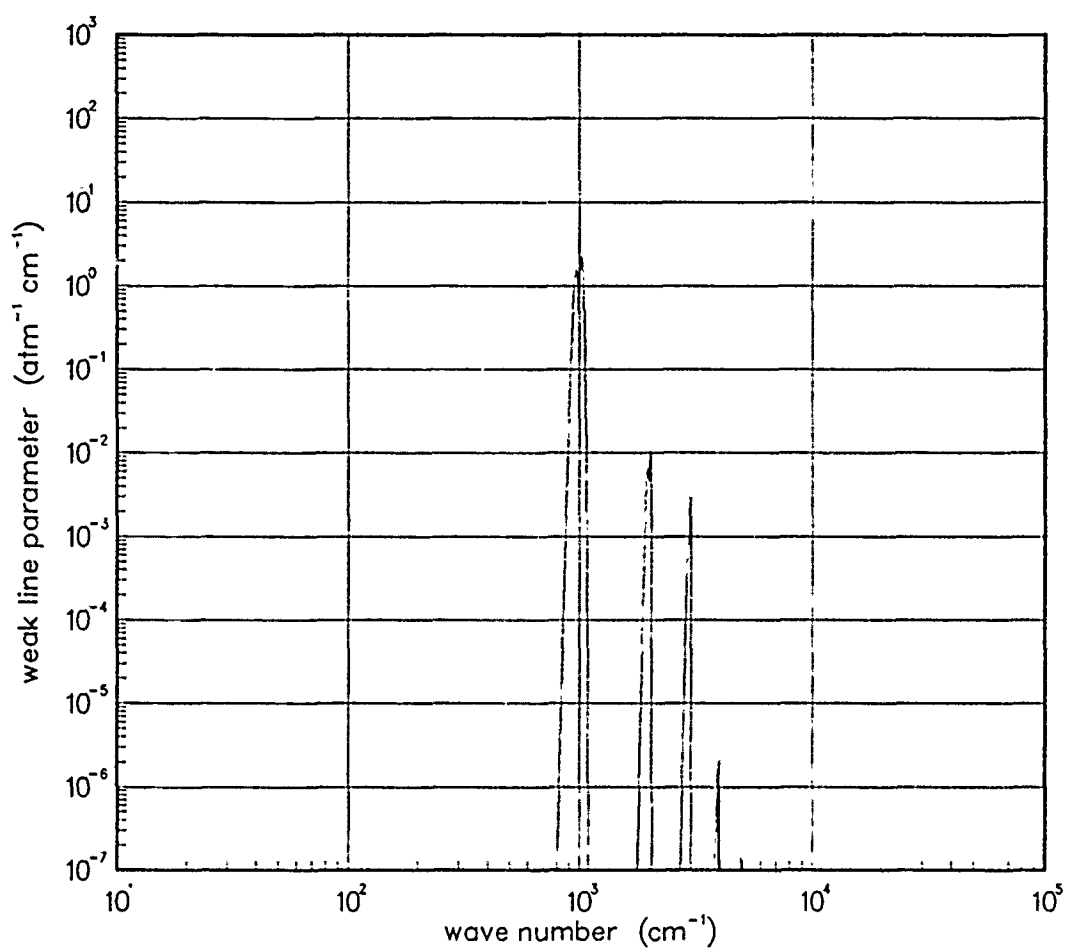


Figure 459. Weak-line parameter for TiO at 750°K.

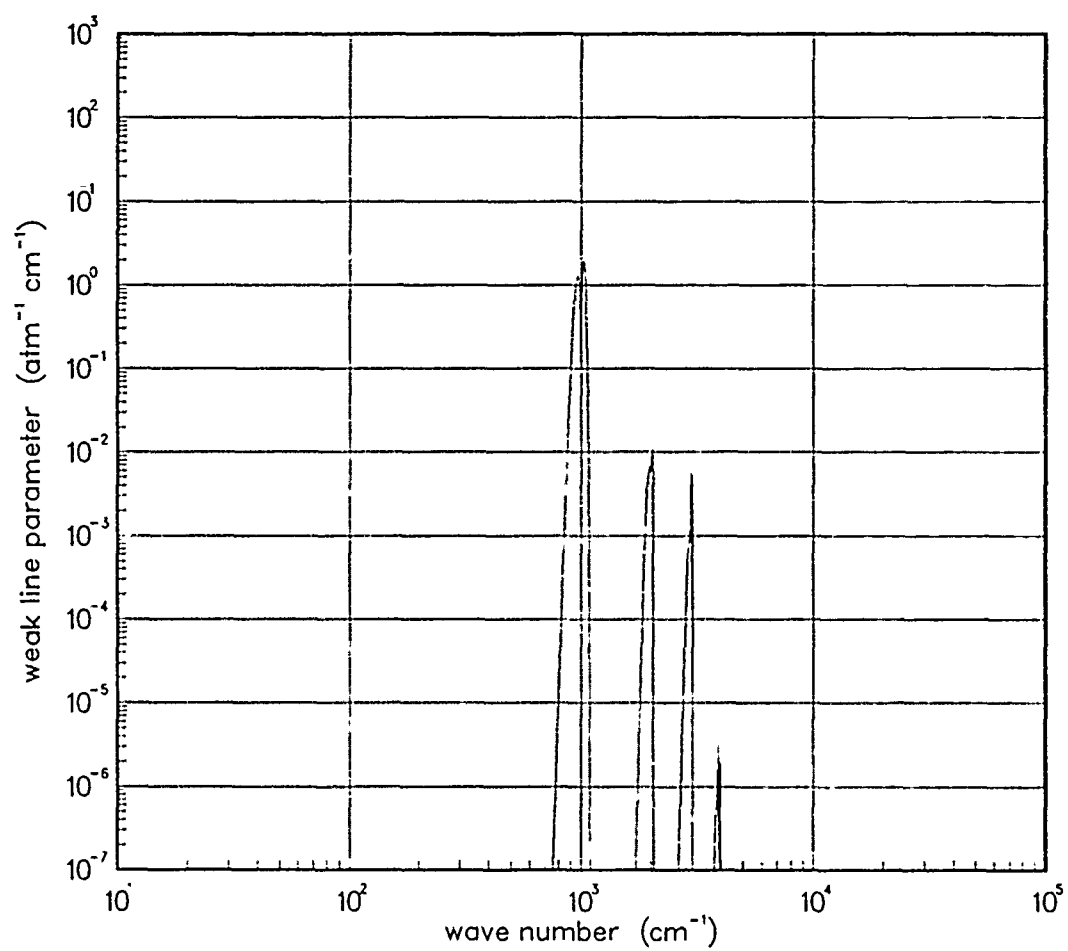


Figure 460. Weak-line parameter for TiO at 1000°K.

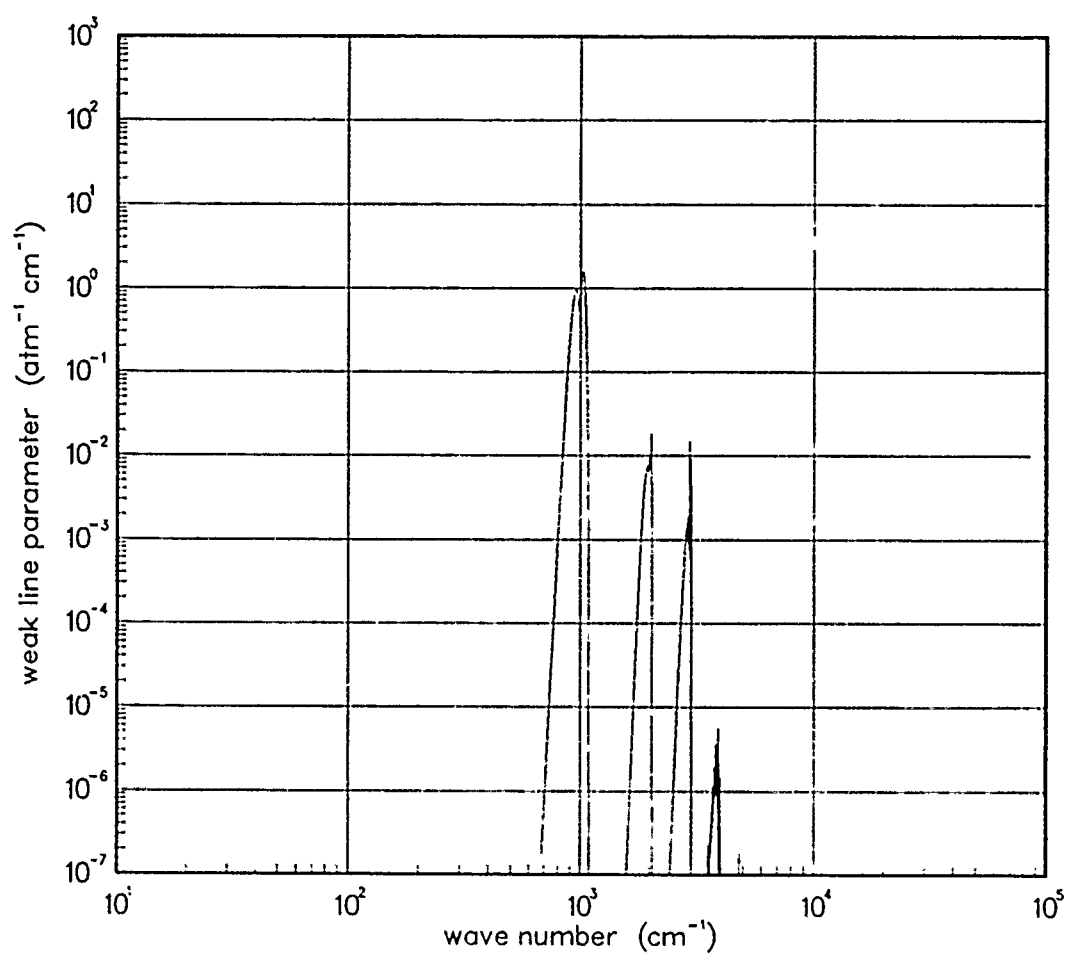


Figure 461. Weak-line parameter for TiO at 1500°K.

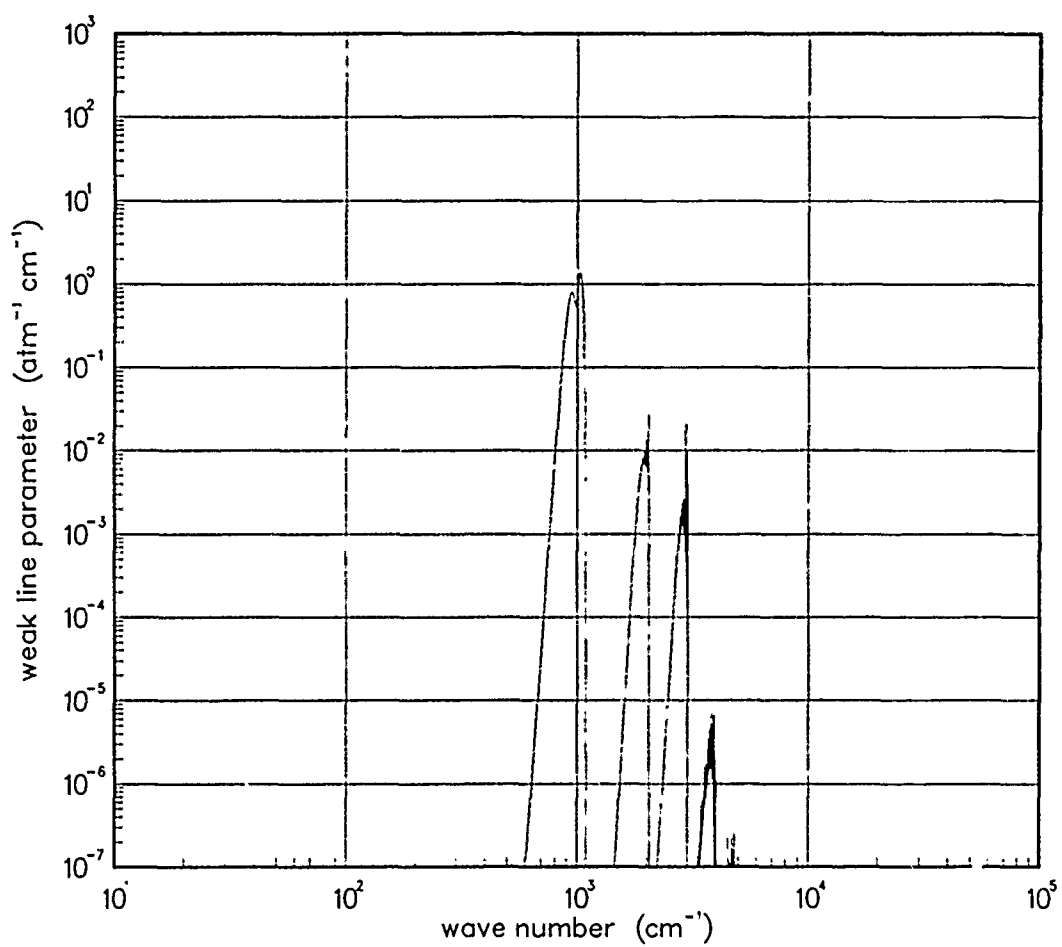


Figure 462. Weak-line parameter for TiO at 2000°K.

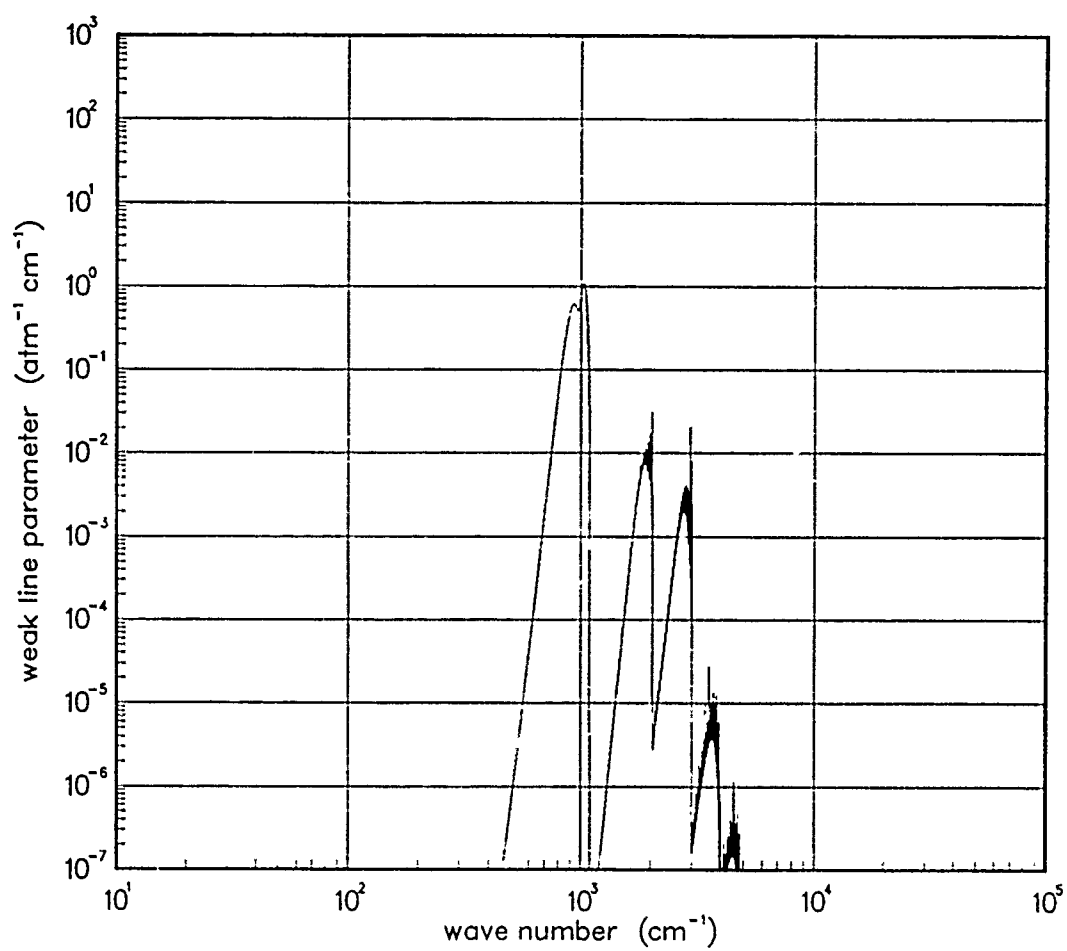


Figure 463. Weak-line parameter for TiO at 3000°K.

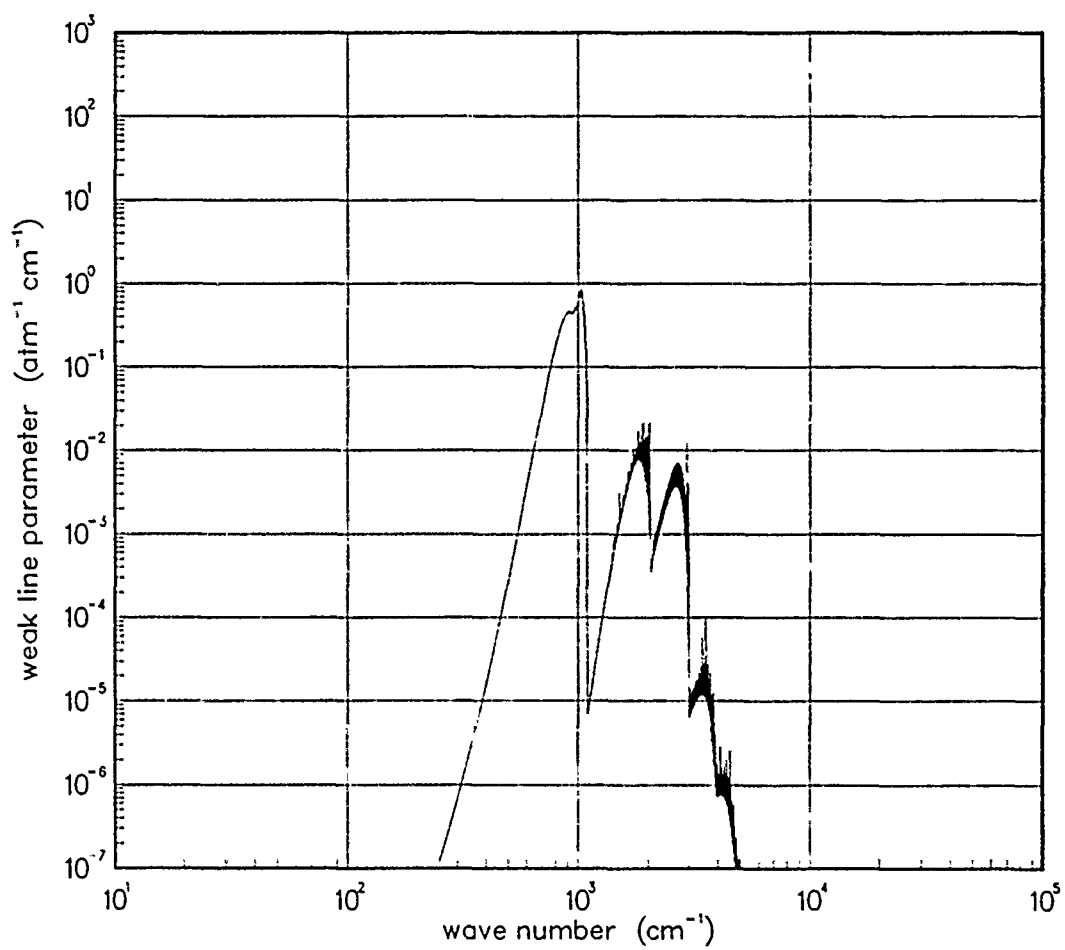


Figure 464. Weak-line parameter for TiO at 5000°K.

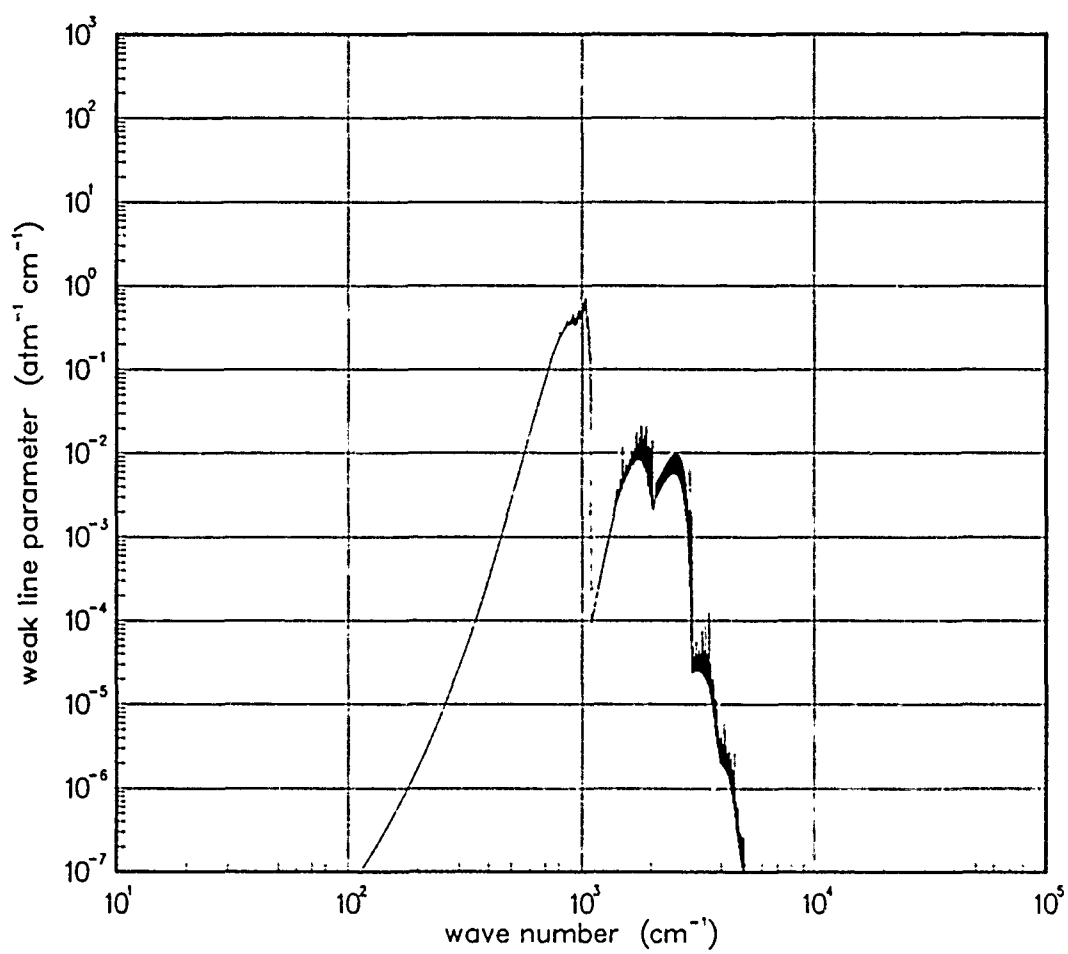


Figure 465. Weak-line parameter for TiO at 7000°K.

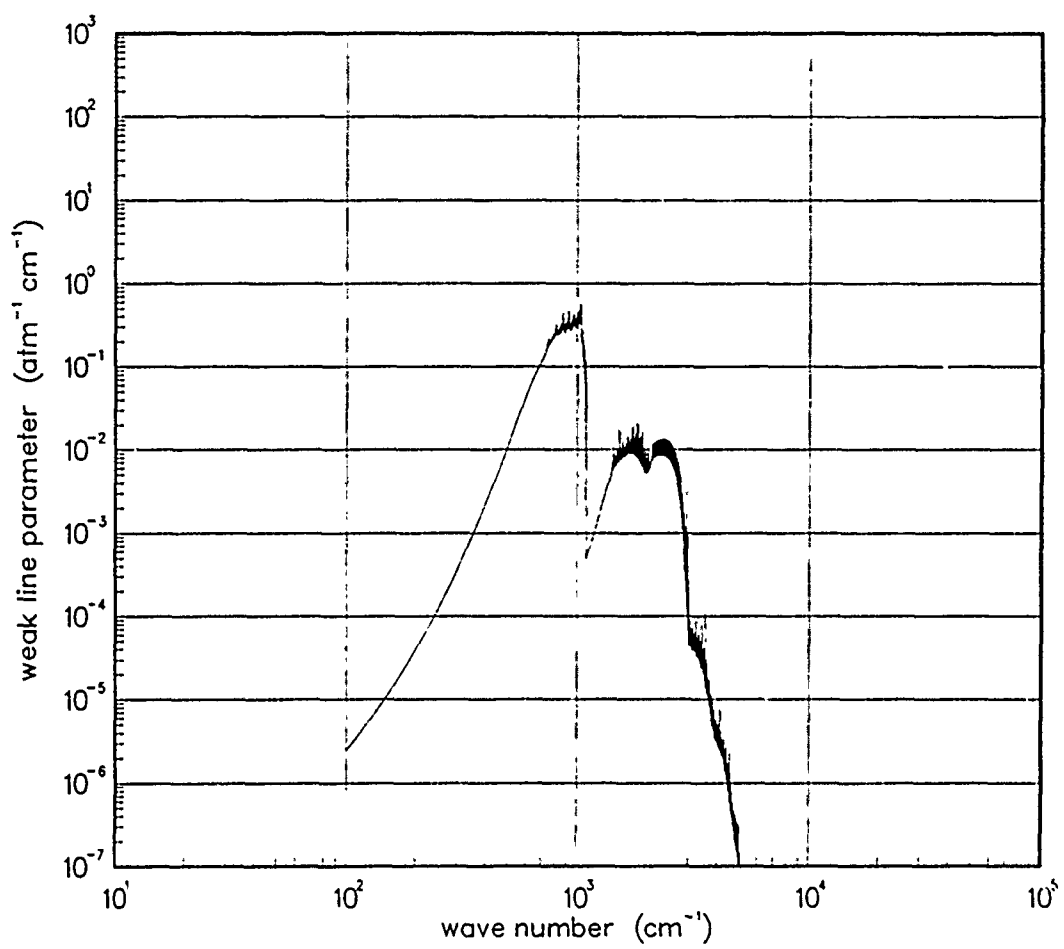


Figure 466. Weak-line parameter for TiO at 10000°K.

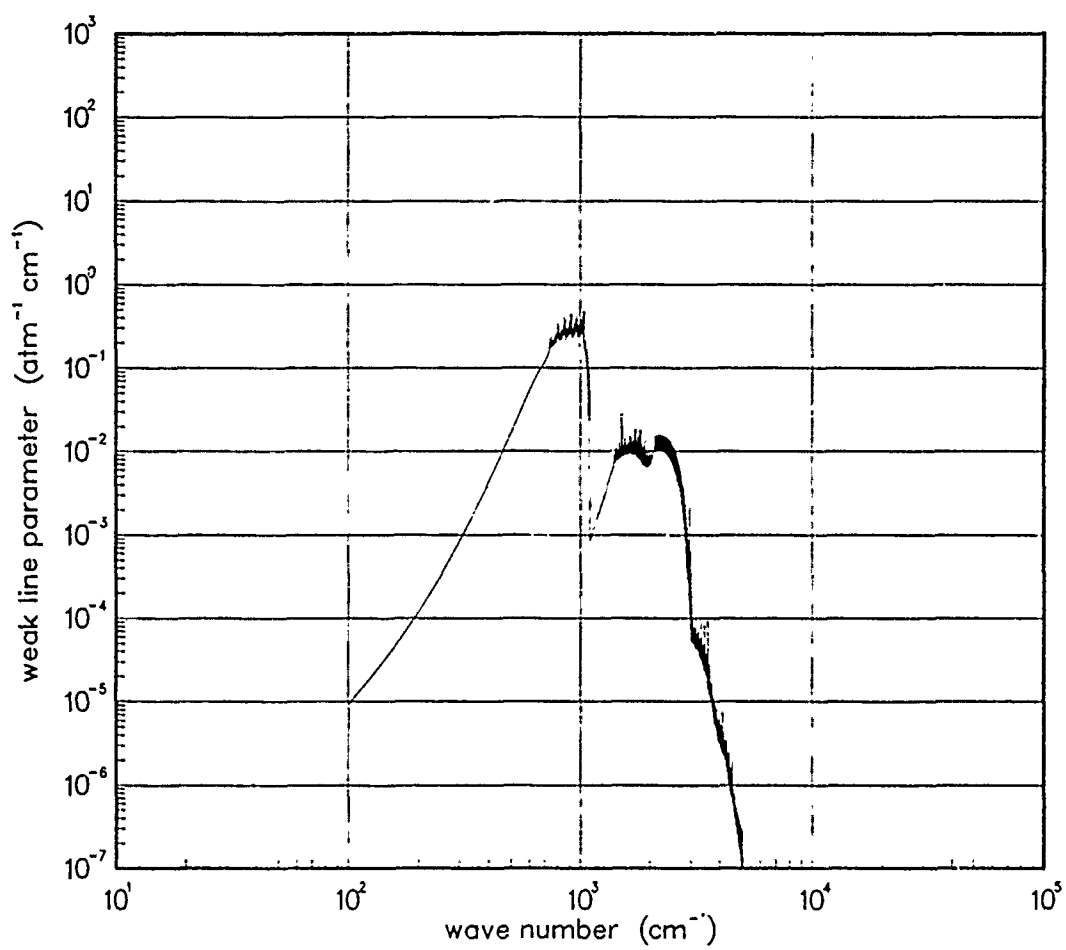


Figure 467. Weak-line parameter for TiO at 12000°K.

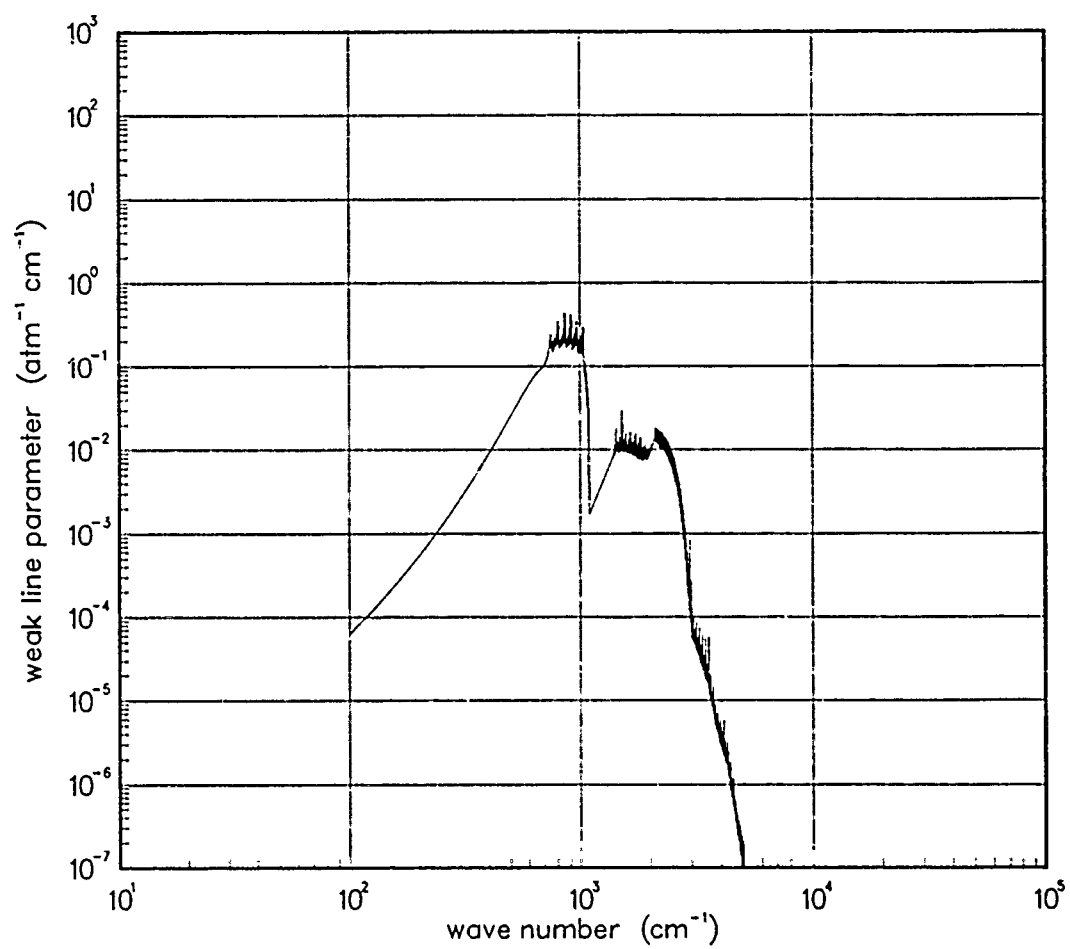


Figure 468. Weak-line parameter for TiO at 18000°K.

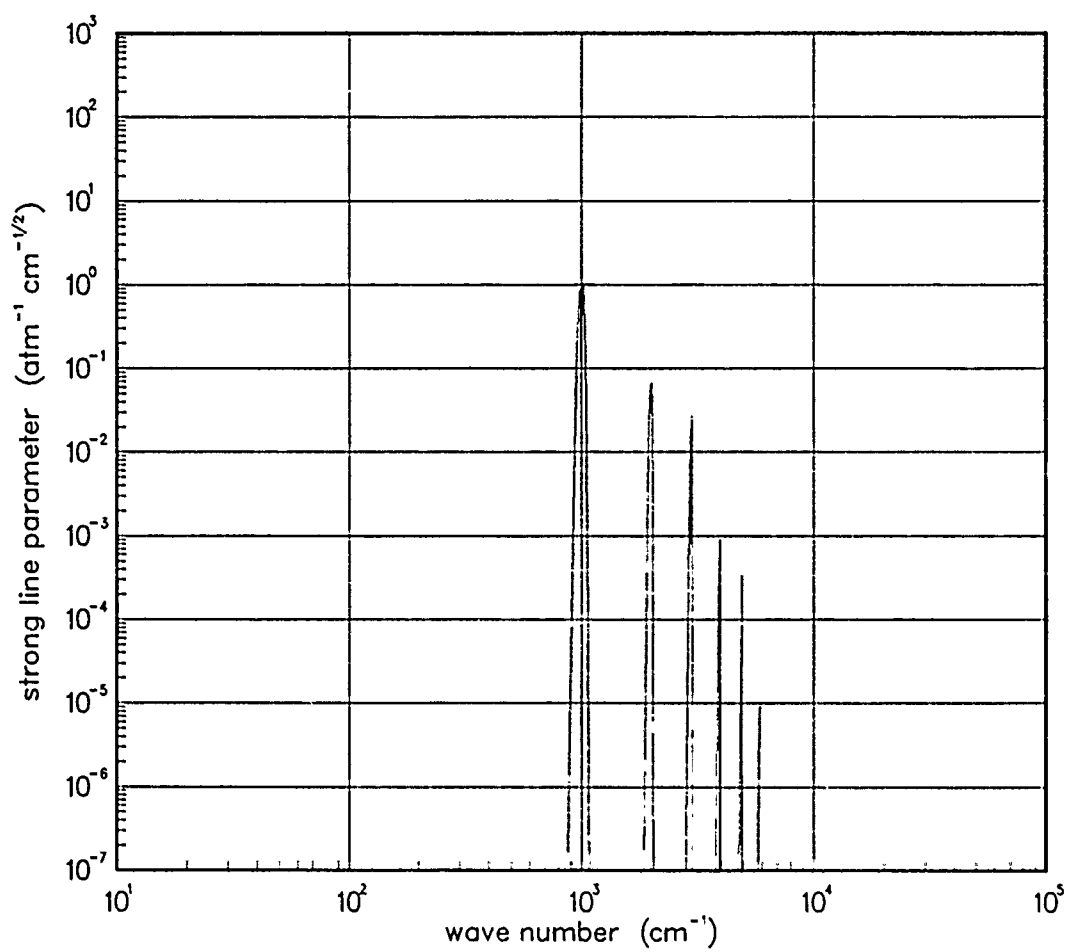


Figure 469. Strong-line parameter for TiO at 200°K.

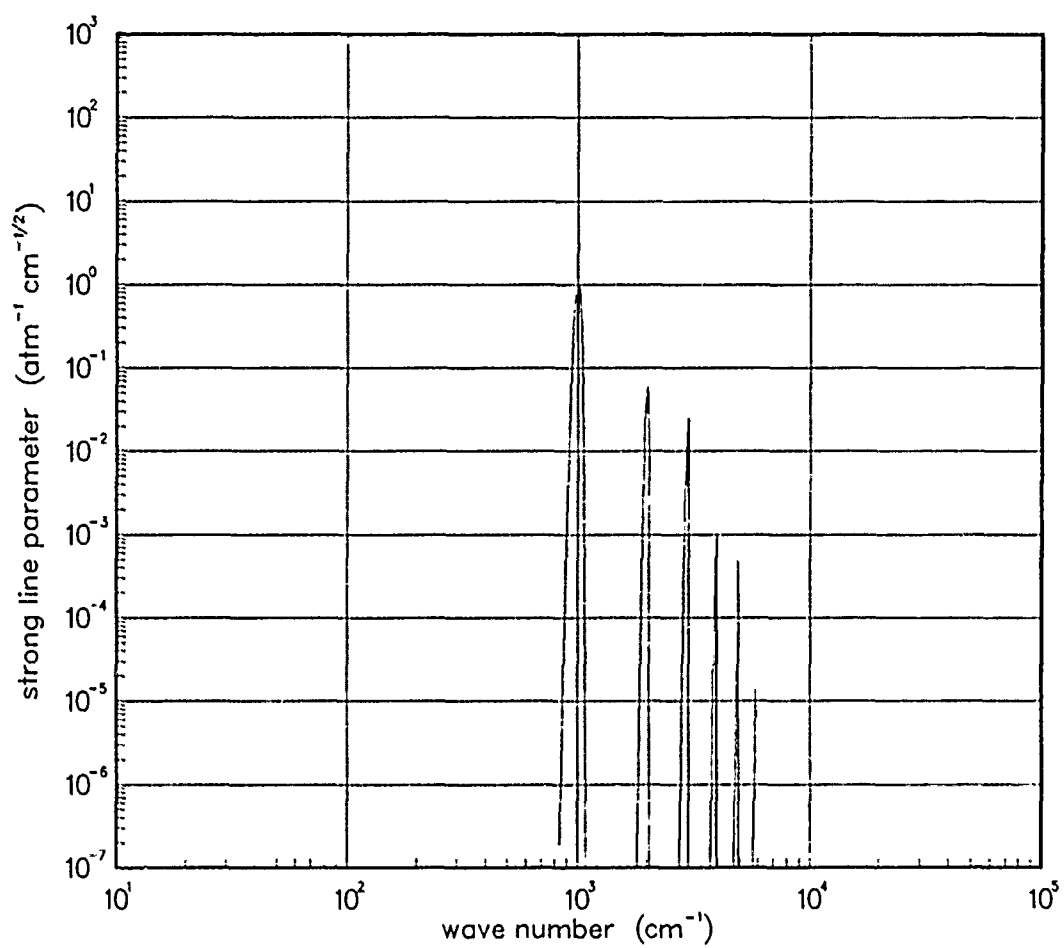


Figure 470. Strong-line parameter for TiO at 300°K.

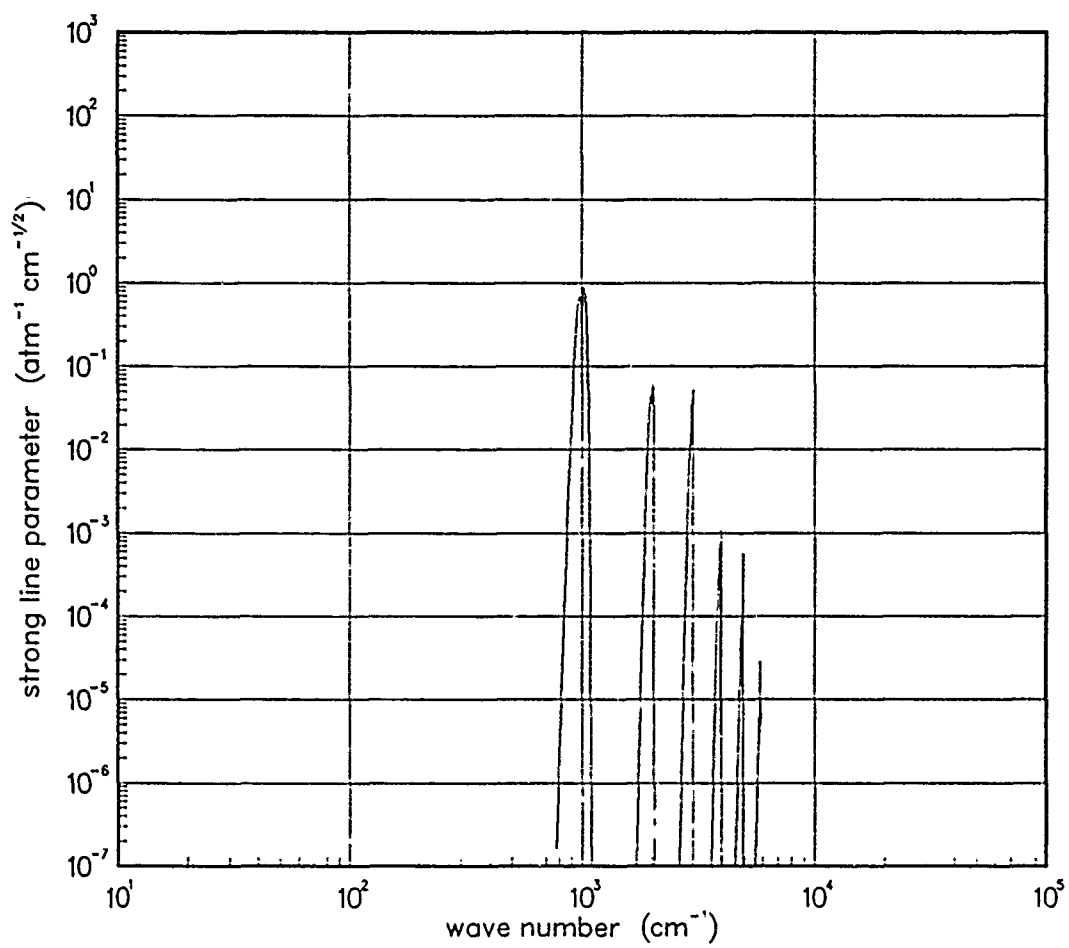


Figure 471. Strong-line parameter for TiO at 500°K.

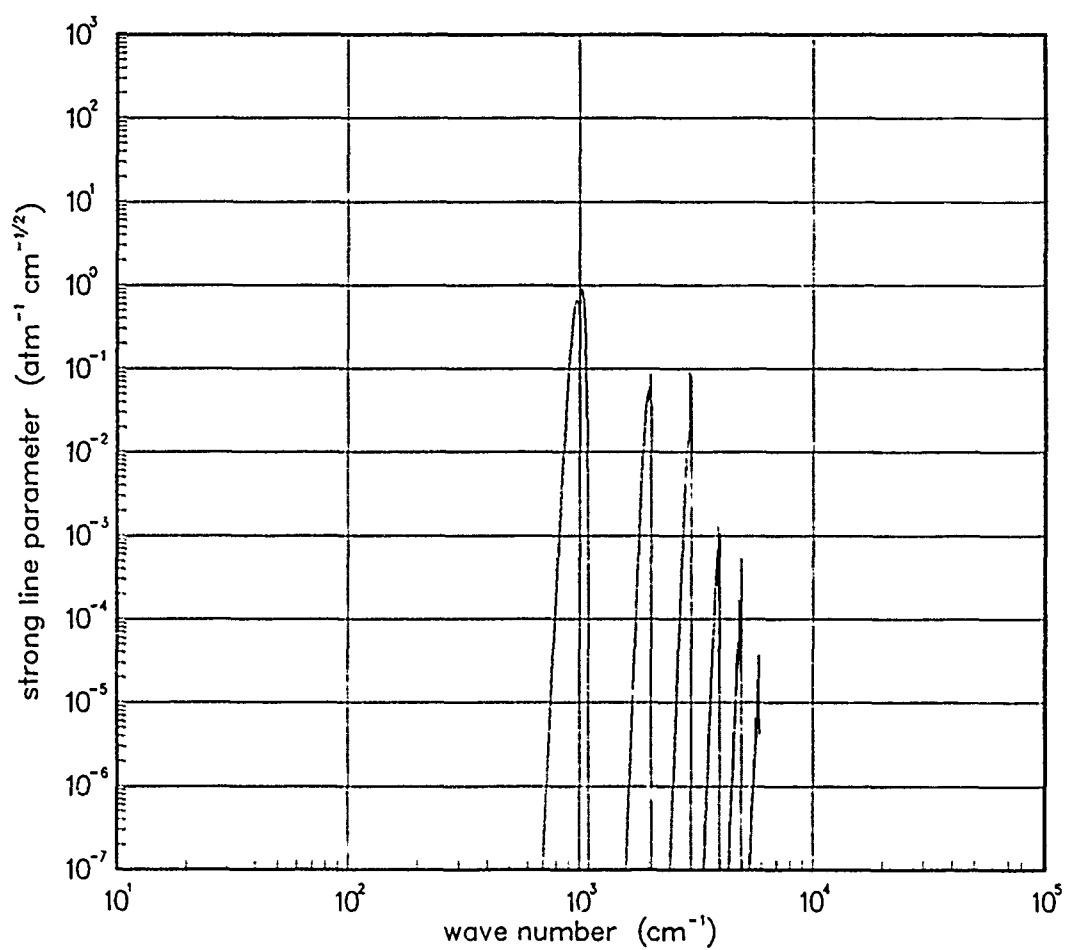


Figure 472. Strong-line parameter for TiO at 750°K.

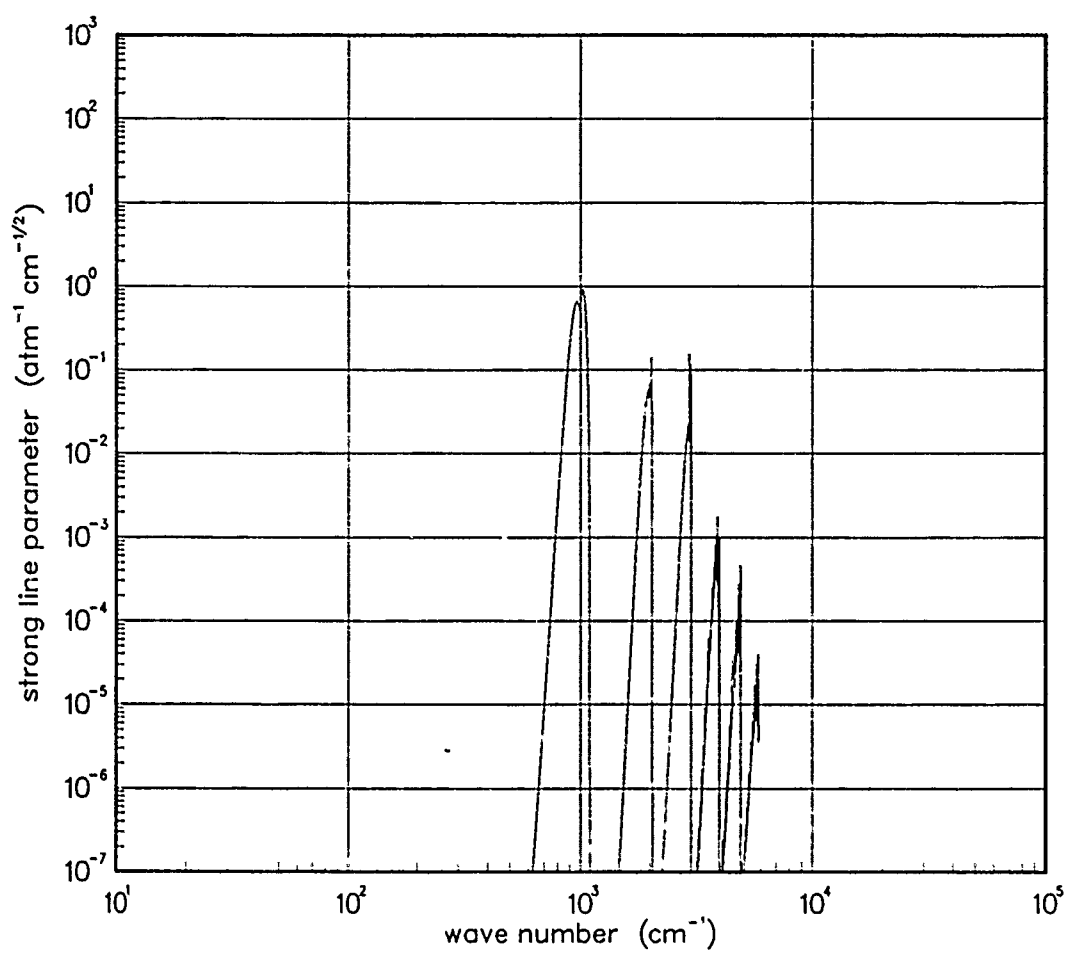


Figure 473. Strong-line parameter for TiO at 1000°K.

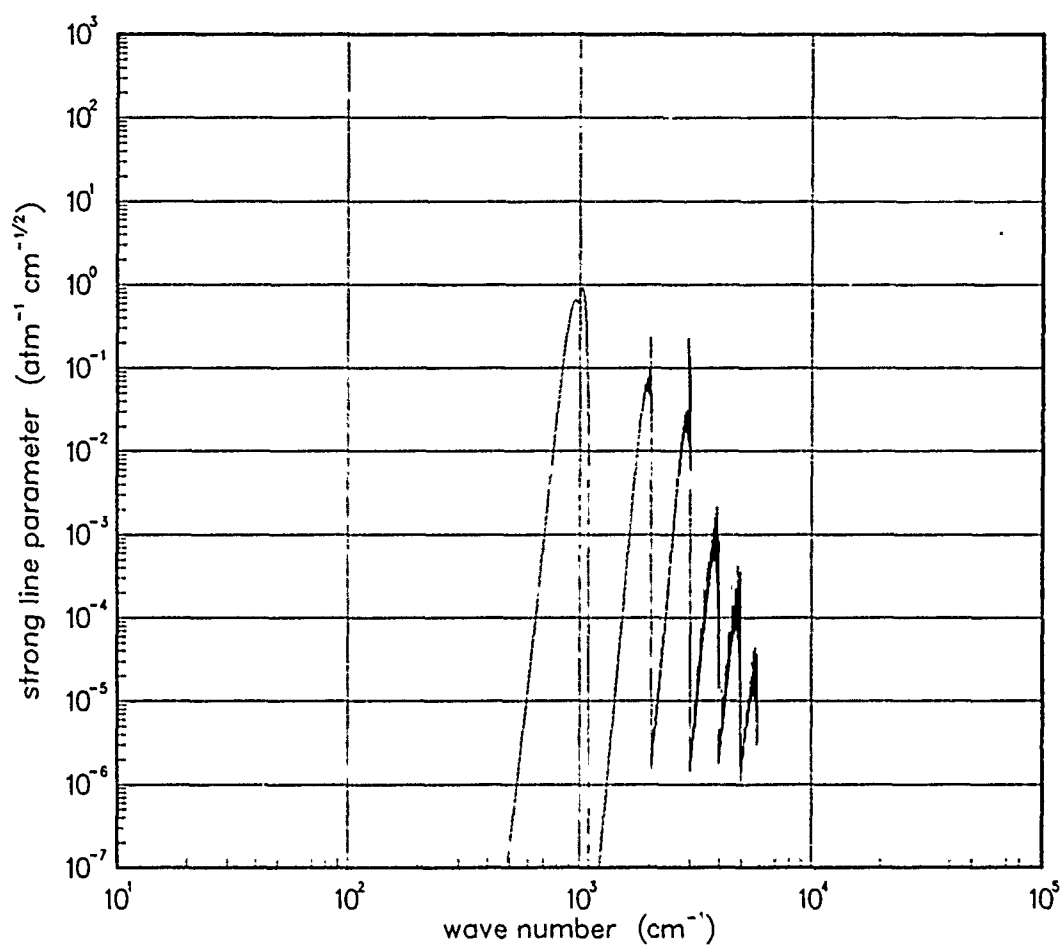


Figure 474. Strong-line parameter for TiO at 1500°K.

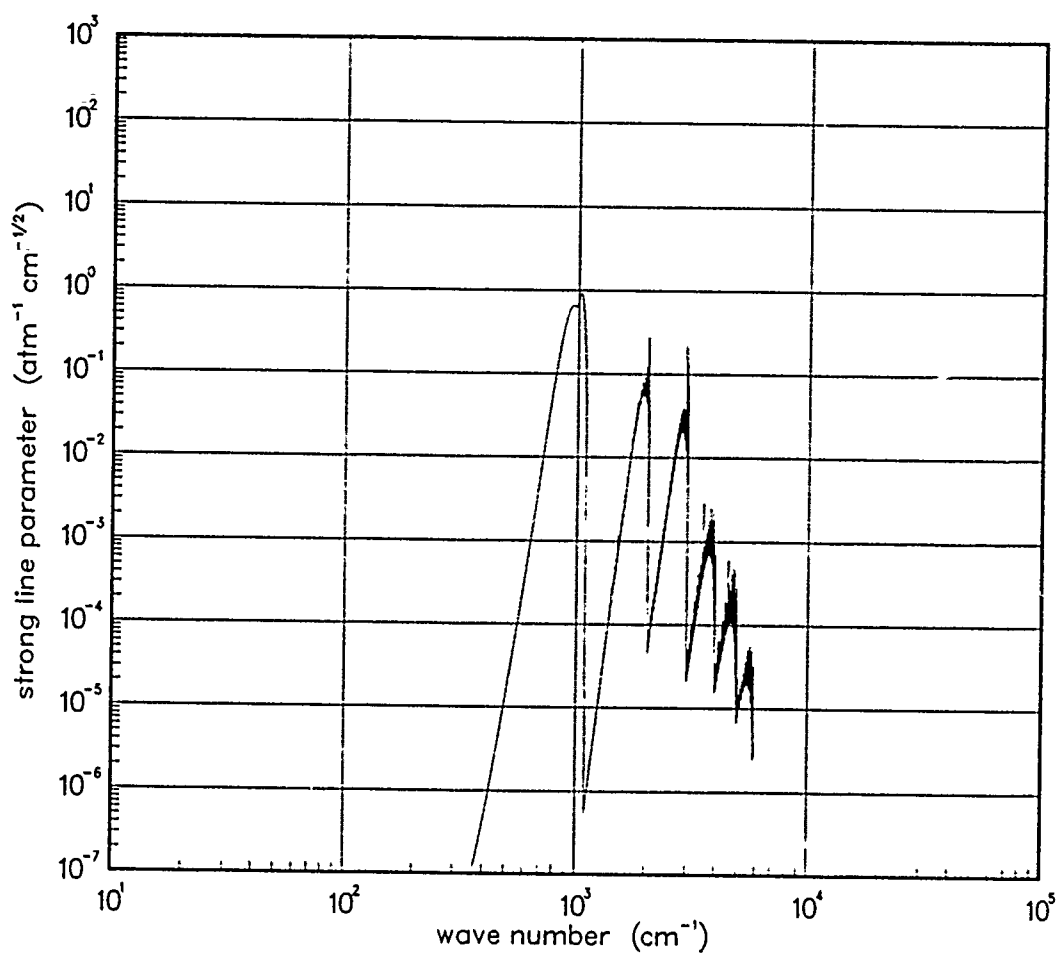


Figure 475. Strong-line parameter for TiO at 2000°K.

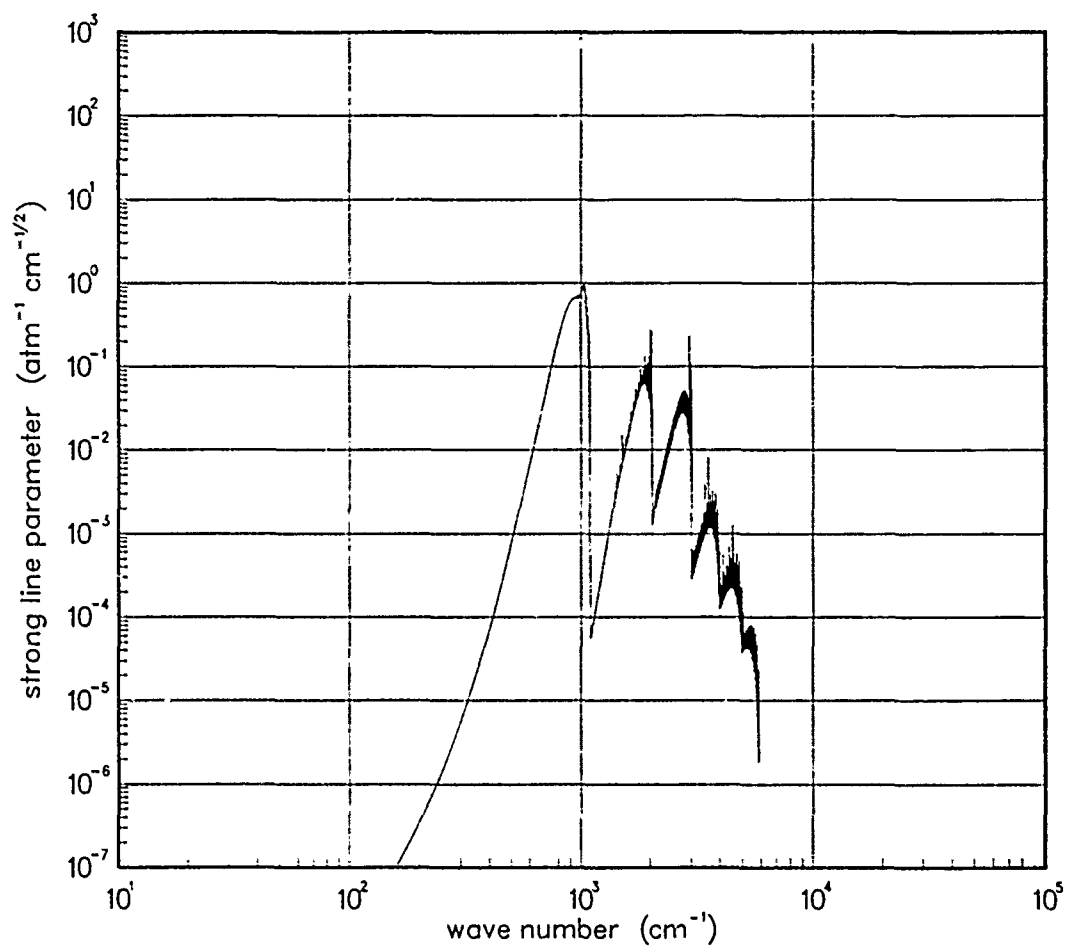


Figure 476. Strong-line parameter for TiO at 3000°K.

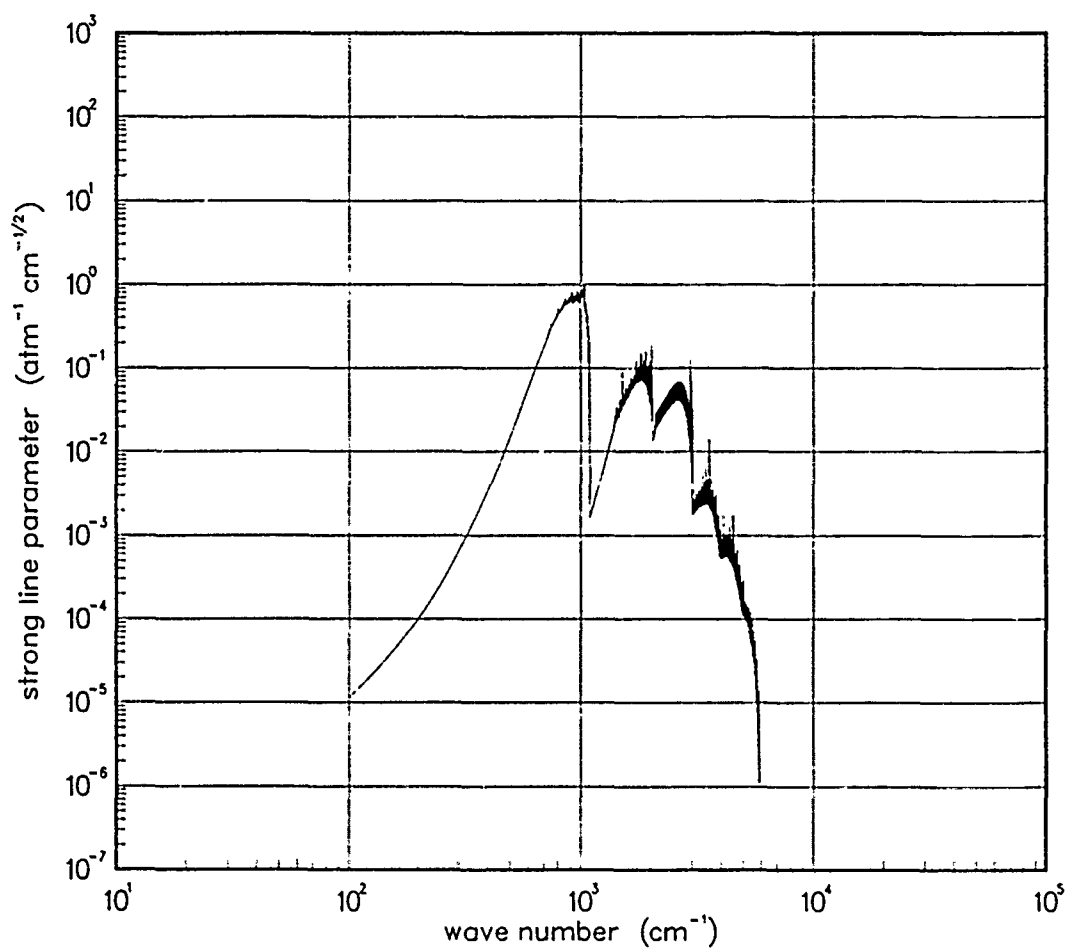


Figure 477. Strong-line parameter for TiO at 5000°K.

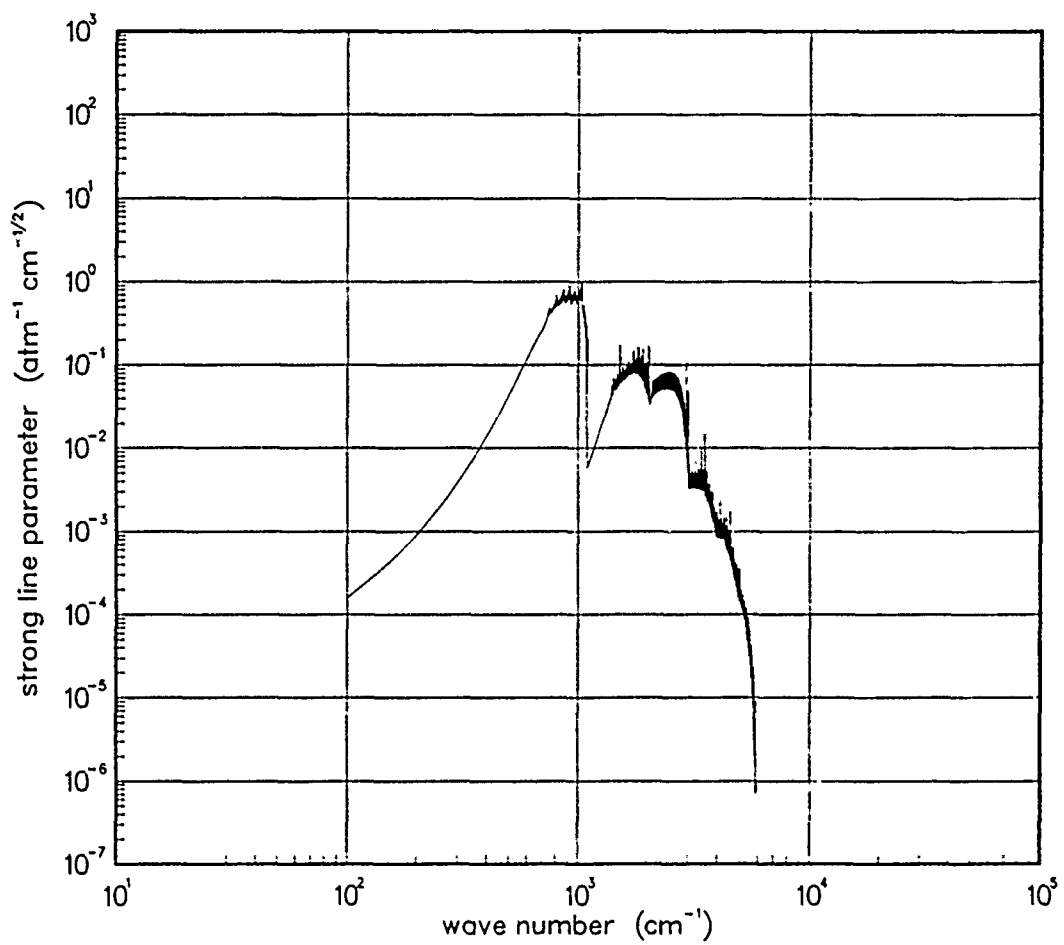


Figure 478. Strong-line parameter for TiO at 7000°K.

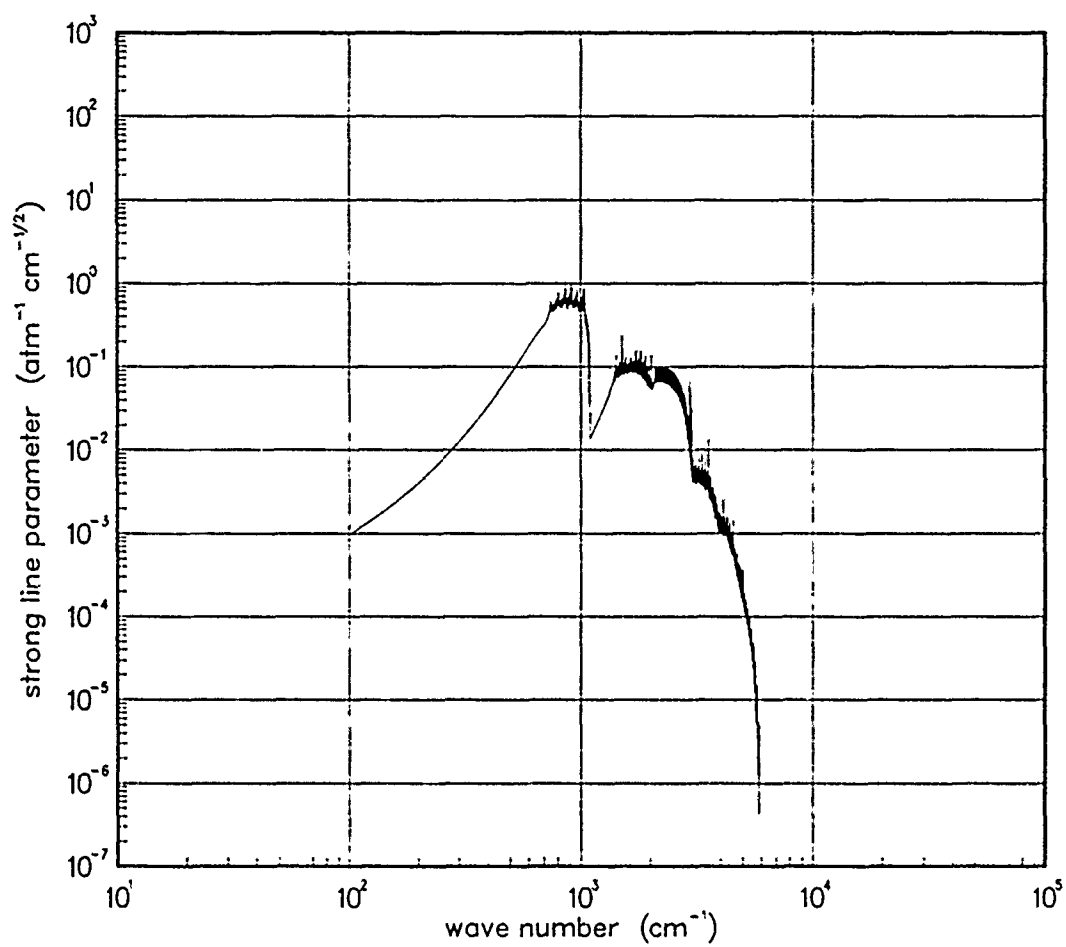


Figure 479. Strong-line parameter for TiO at 10000°K.

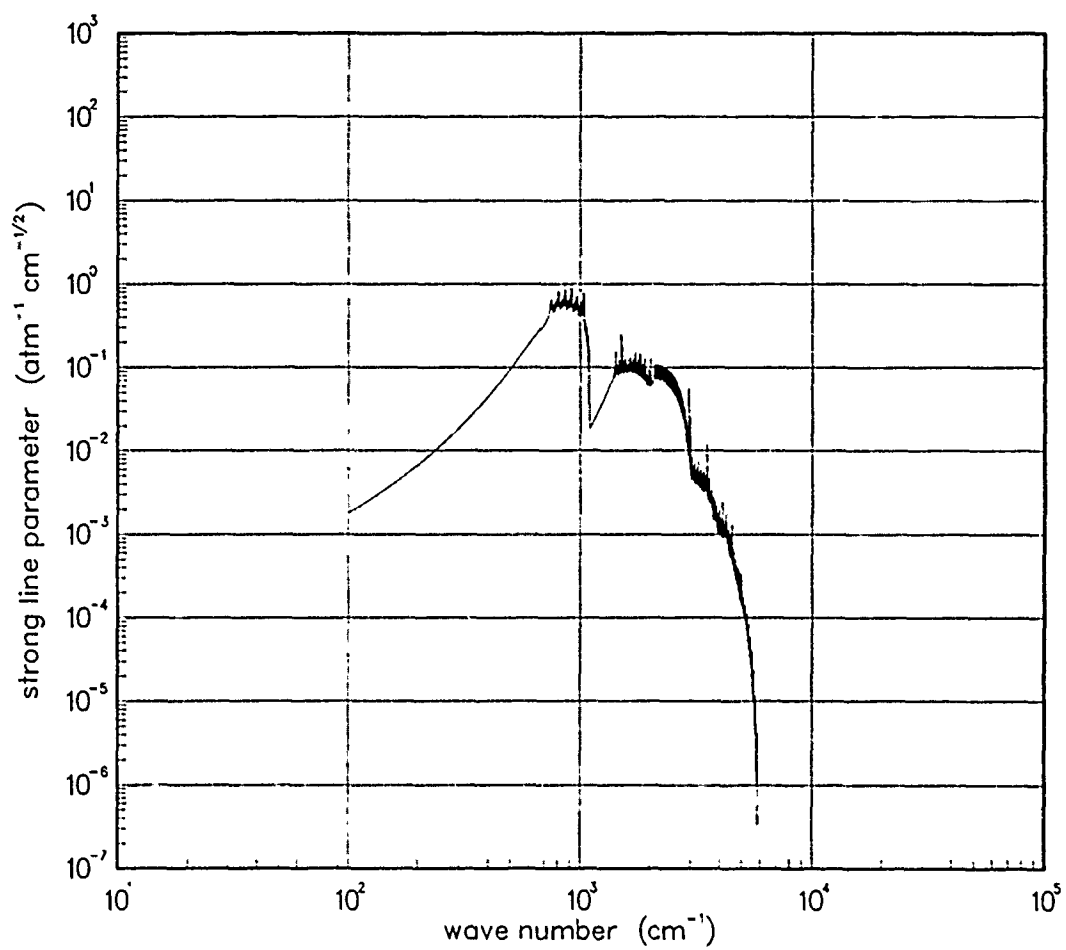


Figure 480. Strong-line parameter for TiO at 12000°K.

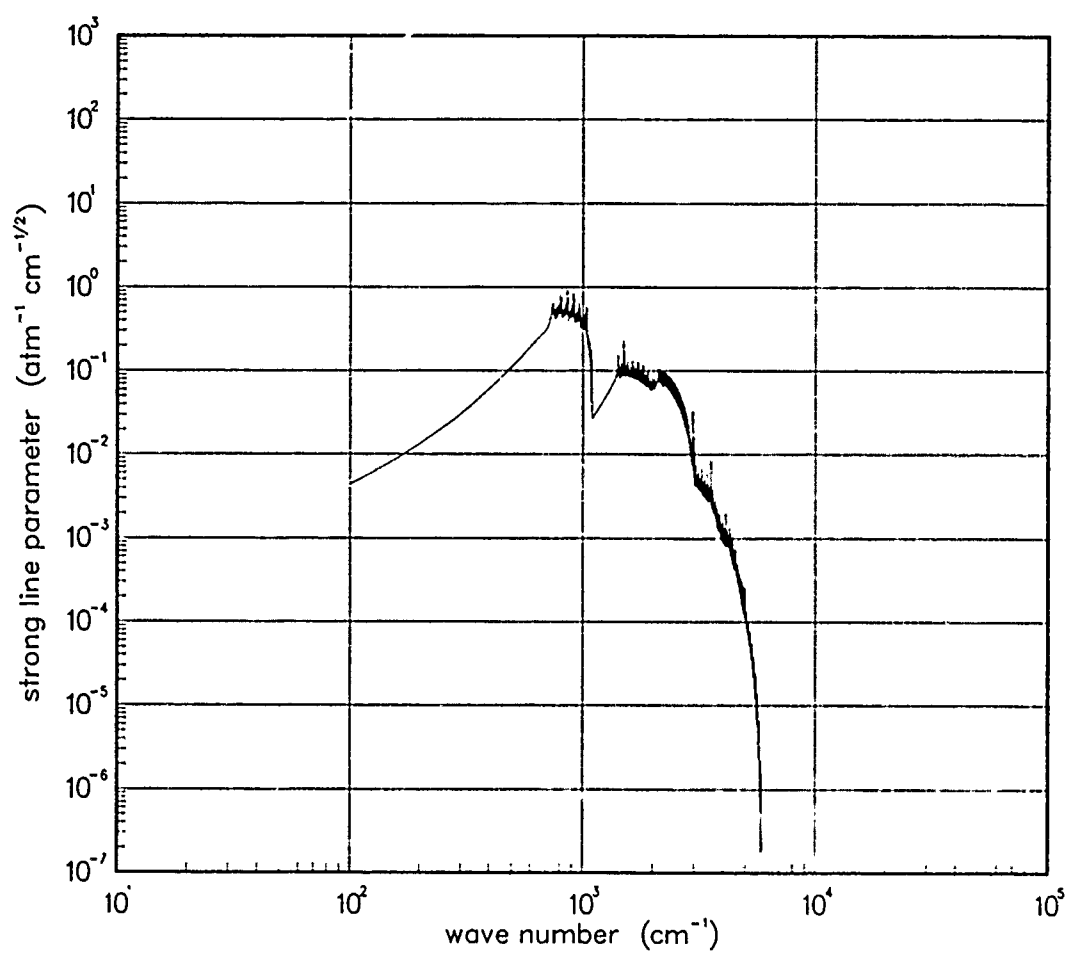


Figure 481. Strong-line parameter for TiO at 18000°K.

6.8 URANIUM OXIDE (UO).

The emissions from the Uranium Oxide molecule and Uranium Oxide Ion were calculated with the DATE program.

Table 14. Spectroscopic data for UO.

$X \ ^1\Sigma^+$	
$\omega_e = 783.2^\dagger$	$\omega_e x_e = 5.09^\dagger$
$\alpha_e = .0028^\dagger$	$B_e = 0.368^\dagger$
$S_{10} = 450.^\ddagger$	
$\gamma_e(300^\circ\text{K}) = 0.04^\S$	

Data Source:

*The symmetry of the ground state is not known. However, the nature of the state will affect only the strong-line parameter to any significant degree.

$^\dagger\omega_e$ is calculated using the band center (773 cm^{-1}) given in Note $\parallel$ along with an estimate of 0.0065 for x_e . See Note ‡ .

‡ T.L. Stephens, and J.G. DeVore, Band Models for Calculating Fireball Thermal Emission (U) , 71TMP-35, General Electric-TEMPO, Santa Barbara, California, (May 1971).

§ Estimate.

$\parallel$ H.J. Leary, et al., High Temp. Sci. 3, 433 (1971).

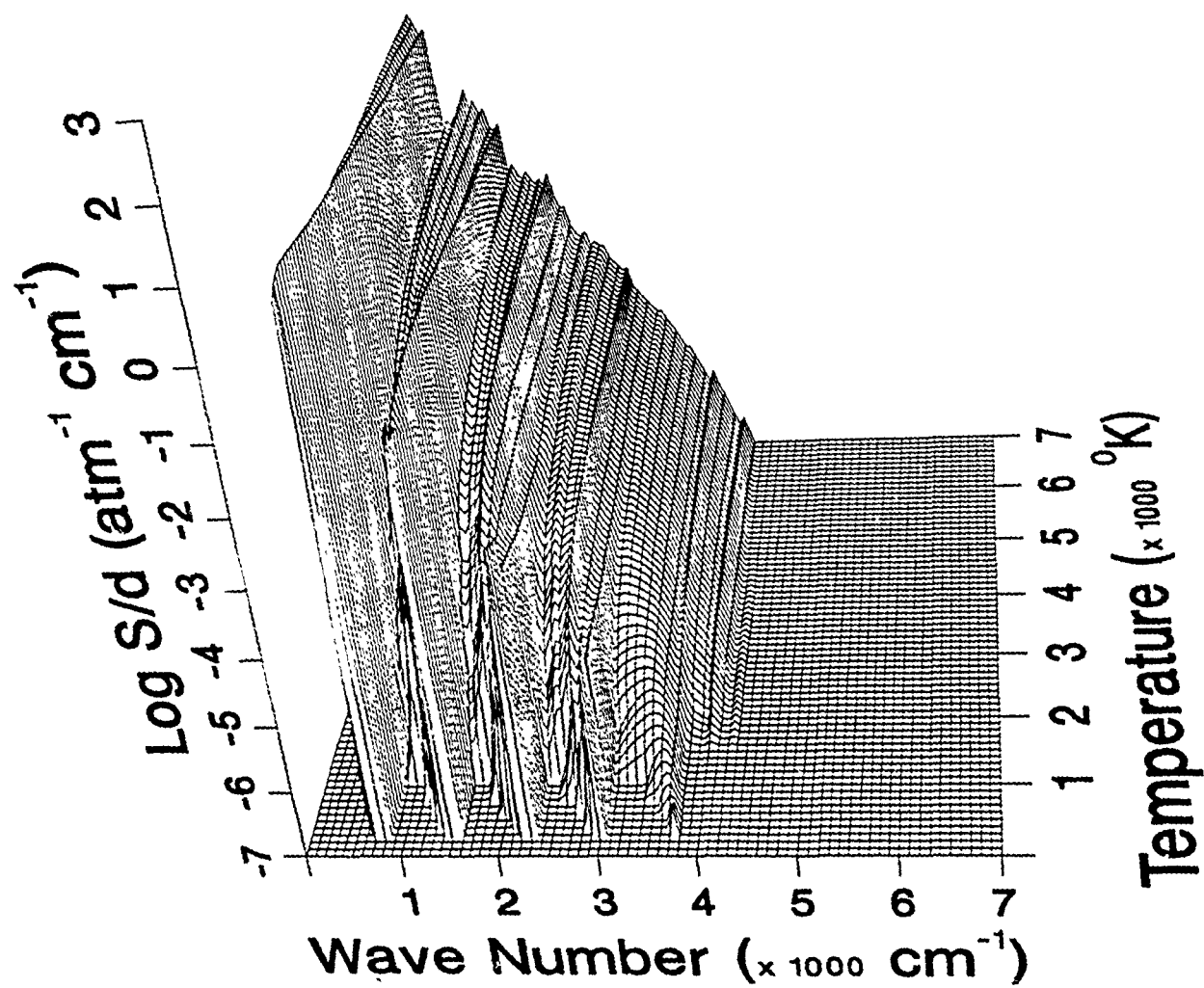


Figure 482. Weak-line parameter for UO.

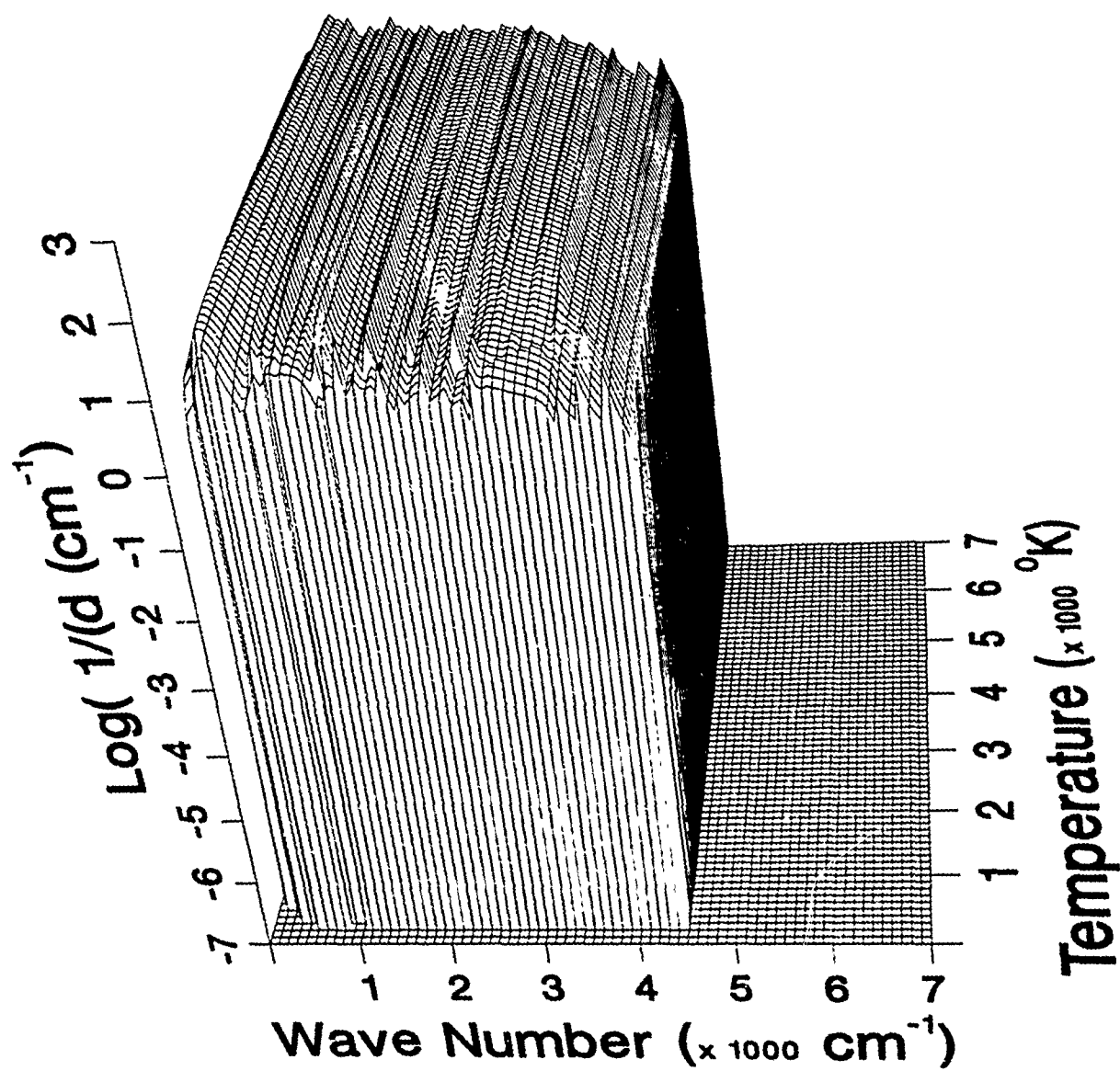


Figure 483. Inverse line spacing for UO.

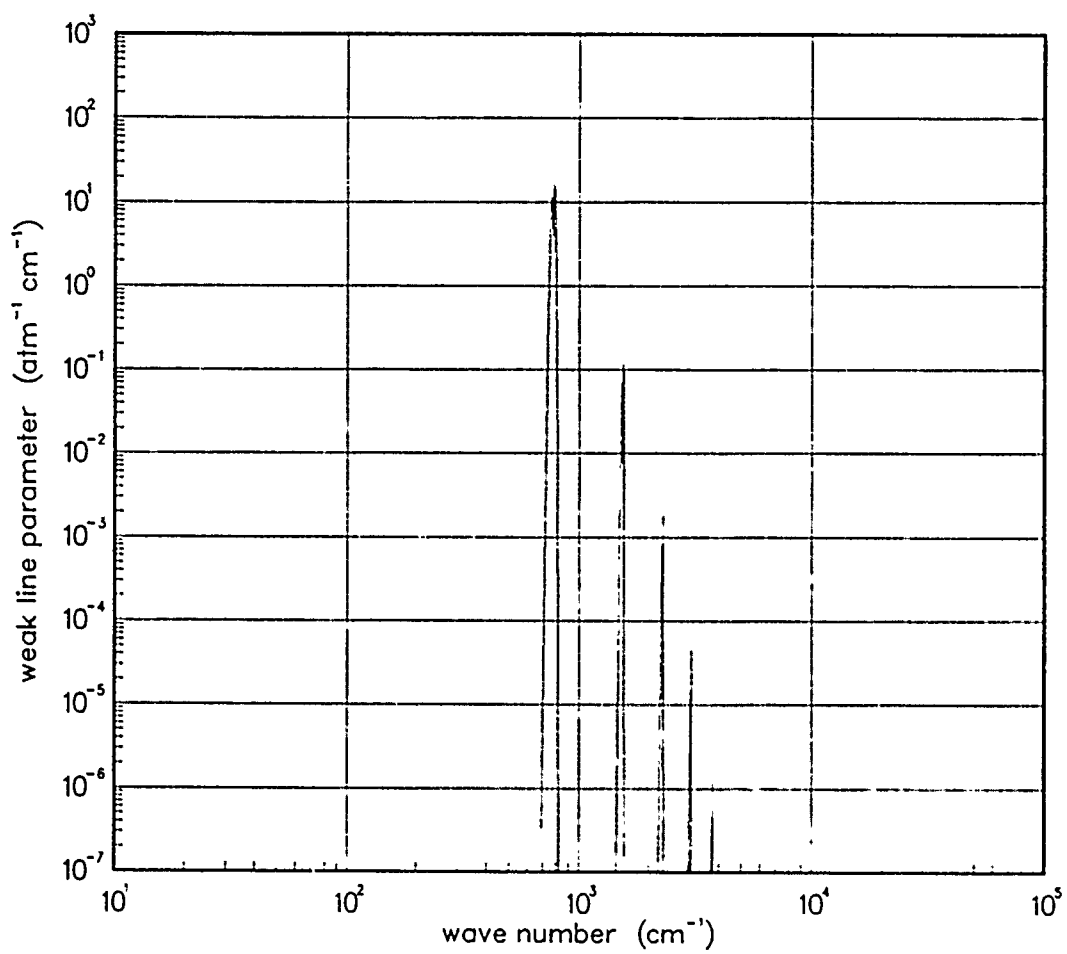


Figure 484. Weak-line parameter for UO at 200°K.

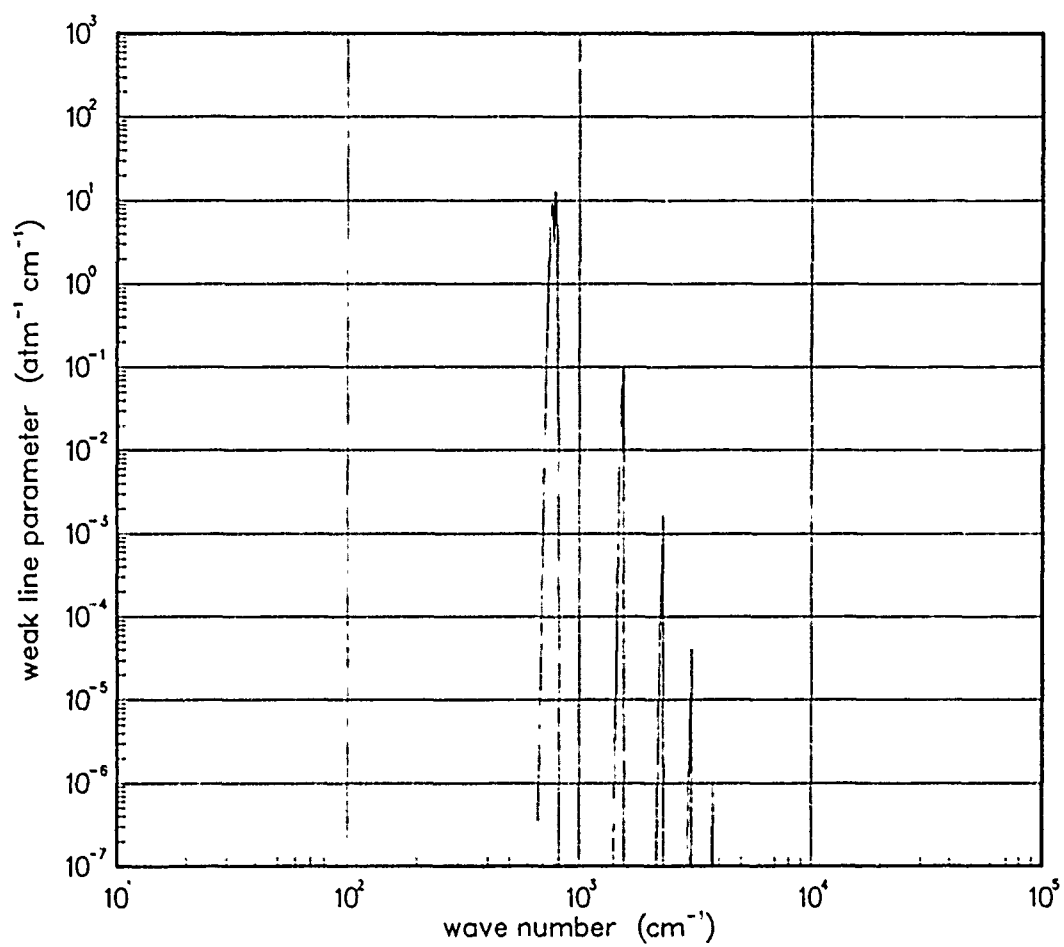


Figure 485. Weak-line parameter for UO at 300°K.

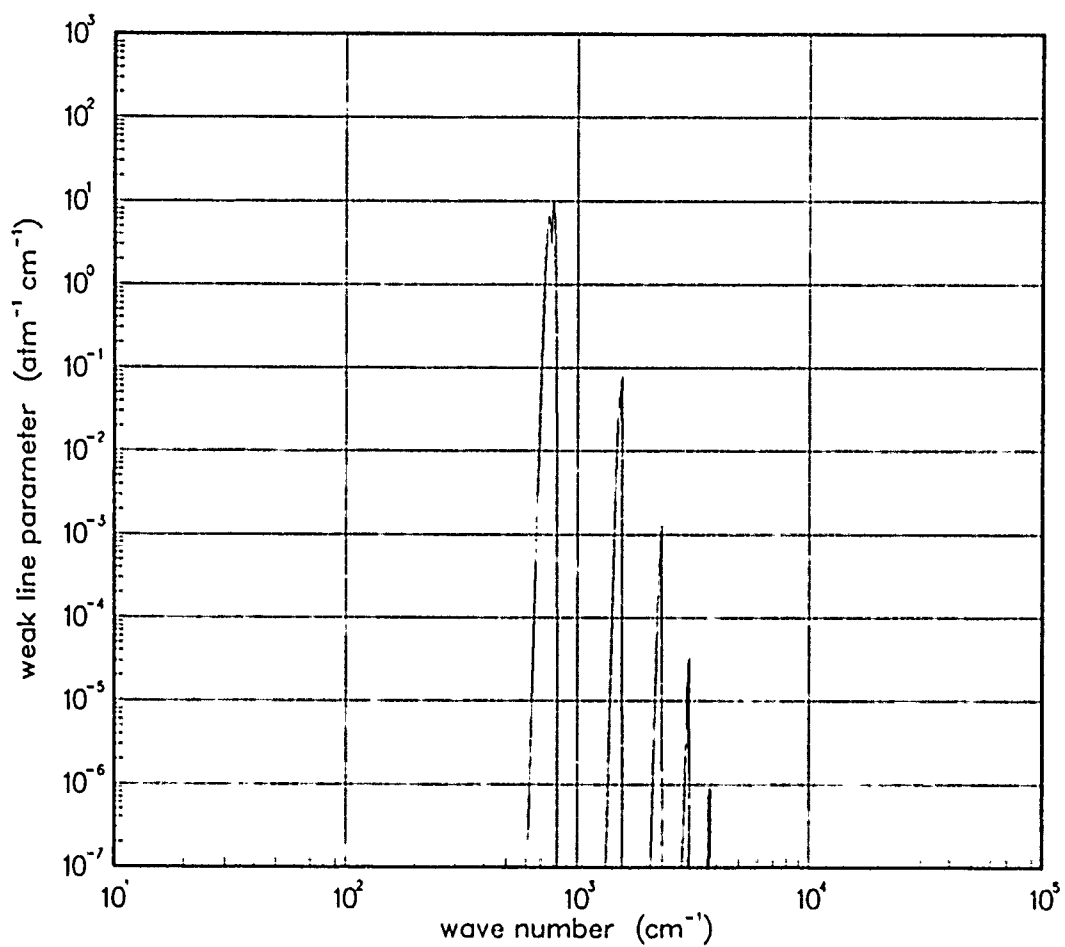


Figure 486. Weak-line parameter for UO at 500°K.

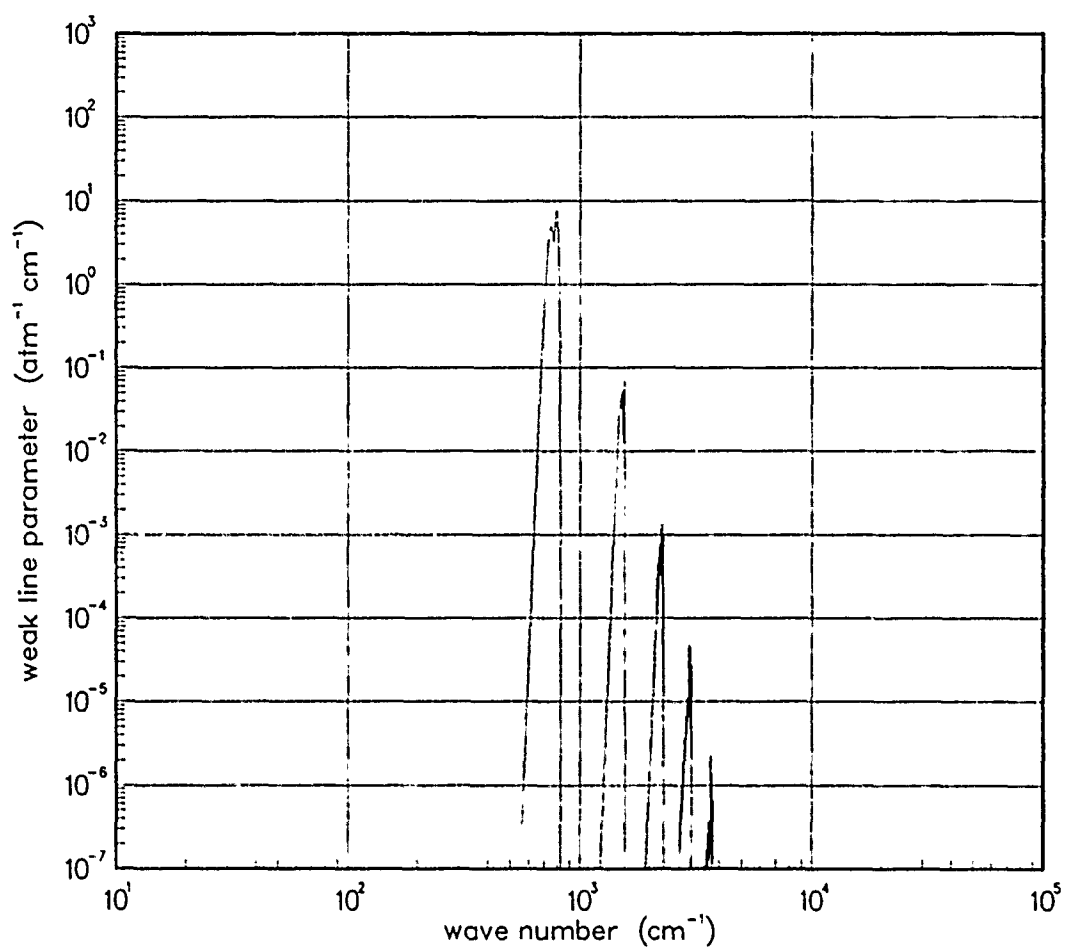


Figure 487. Weak-line parameter for UO at 750°K.

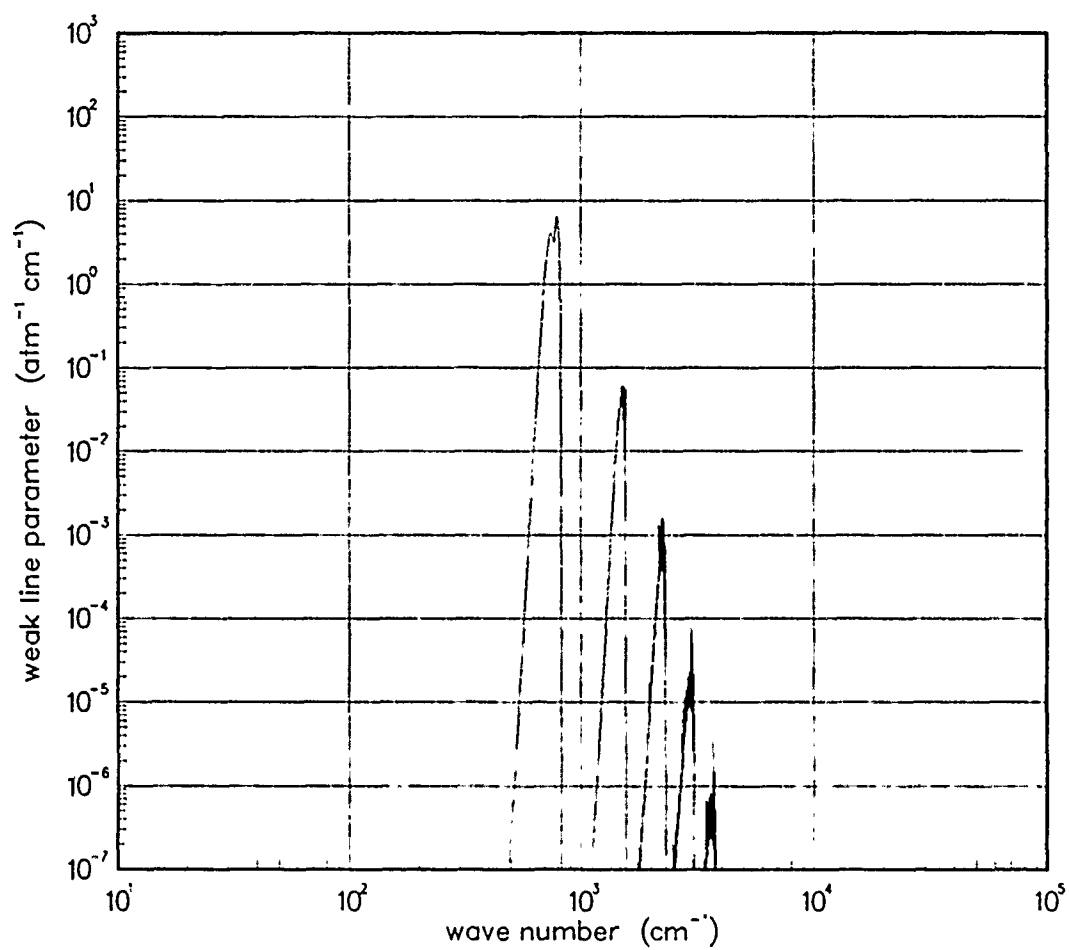


Figure 488. Weak-line parameter for UO at 1000°K.

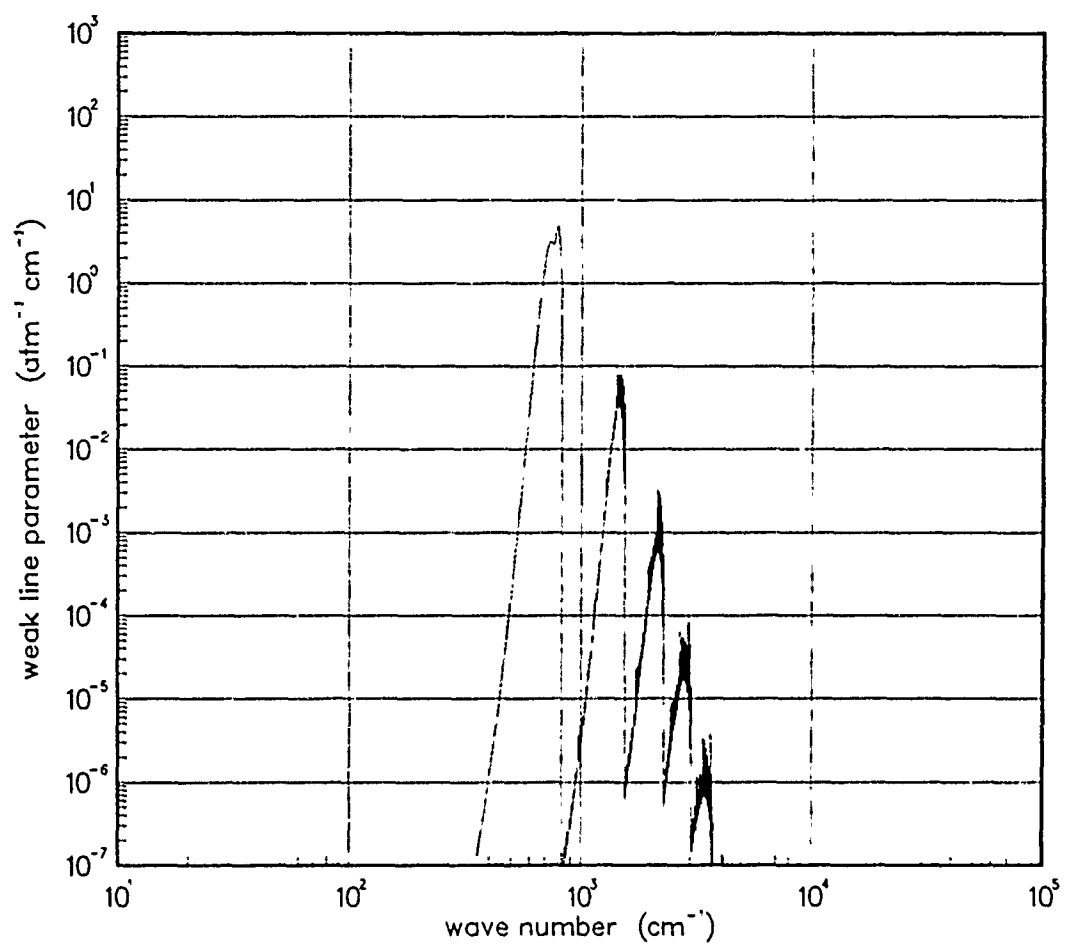


Figure 489. Weak-line parameter for UO at 1500°K.

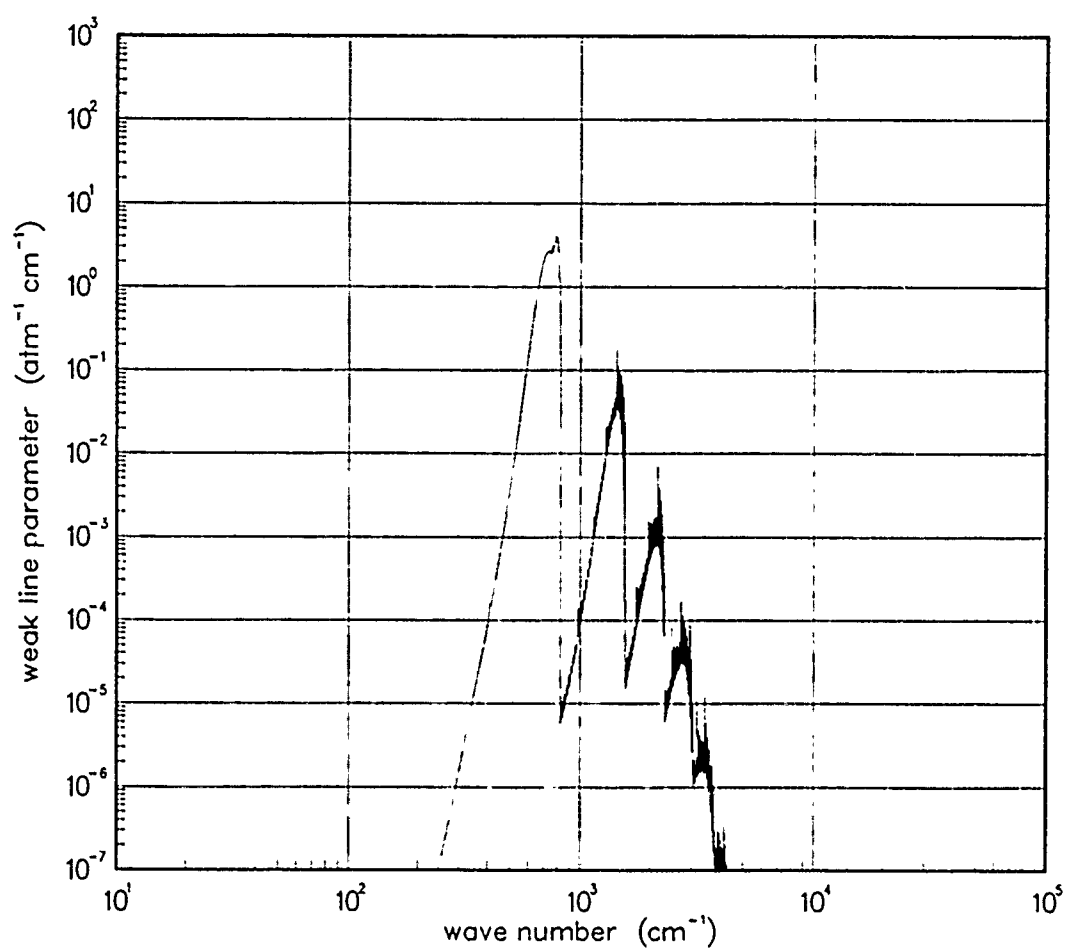


Figure 490. Weak-line parameter for UO at 2000°K.

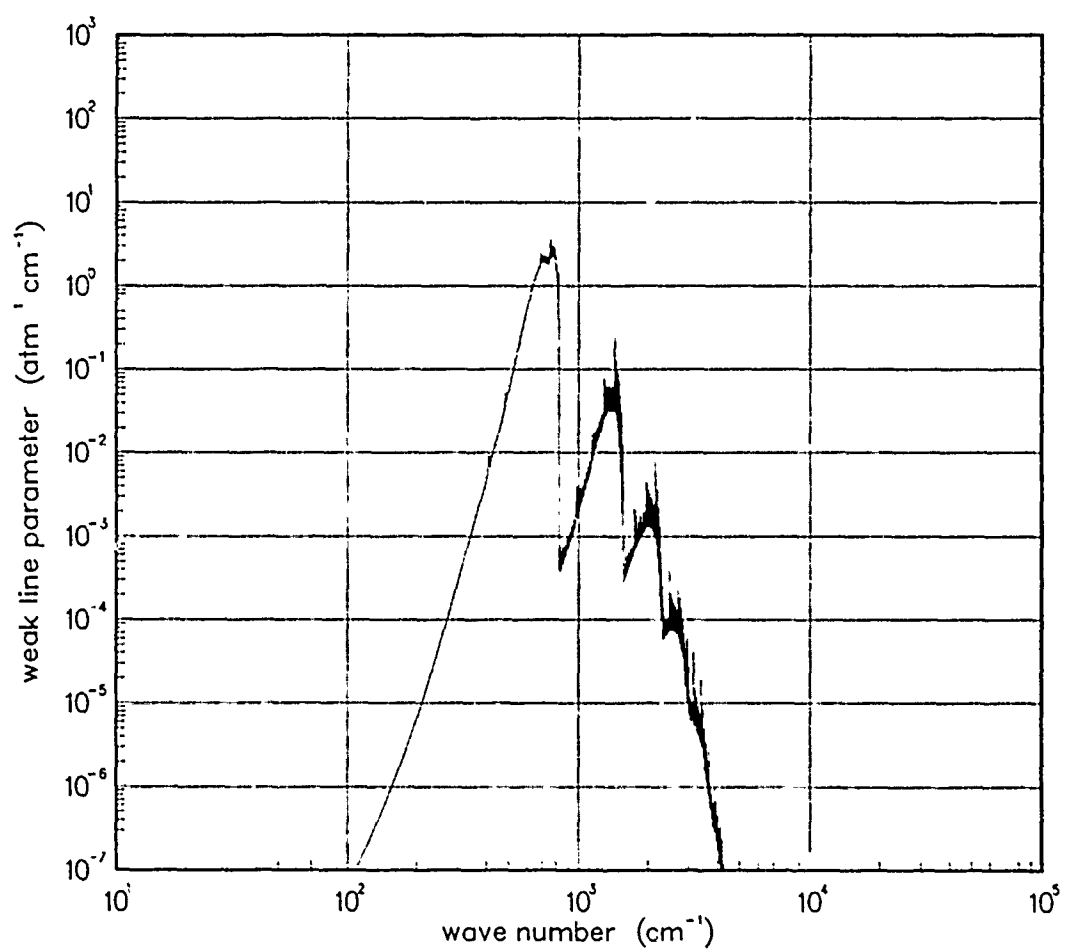


Figure 491. Weak-line parameter for UO at 3000°K.

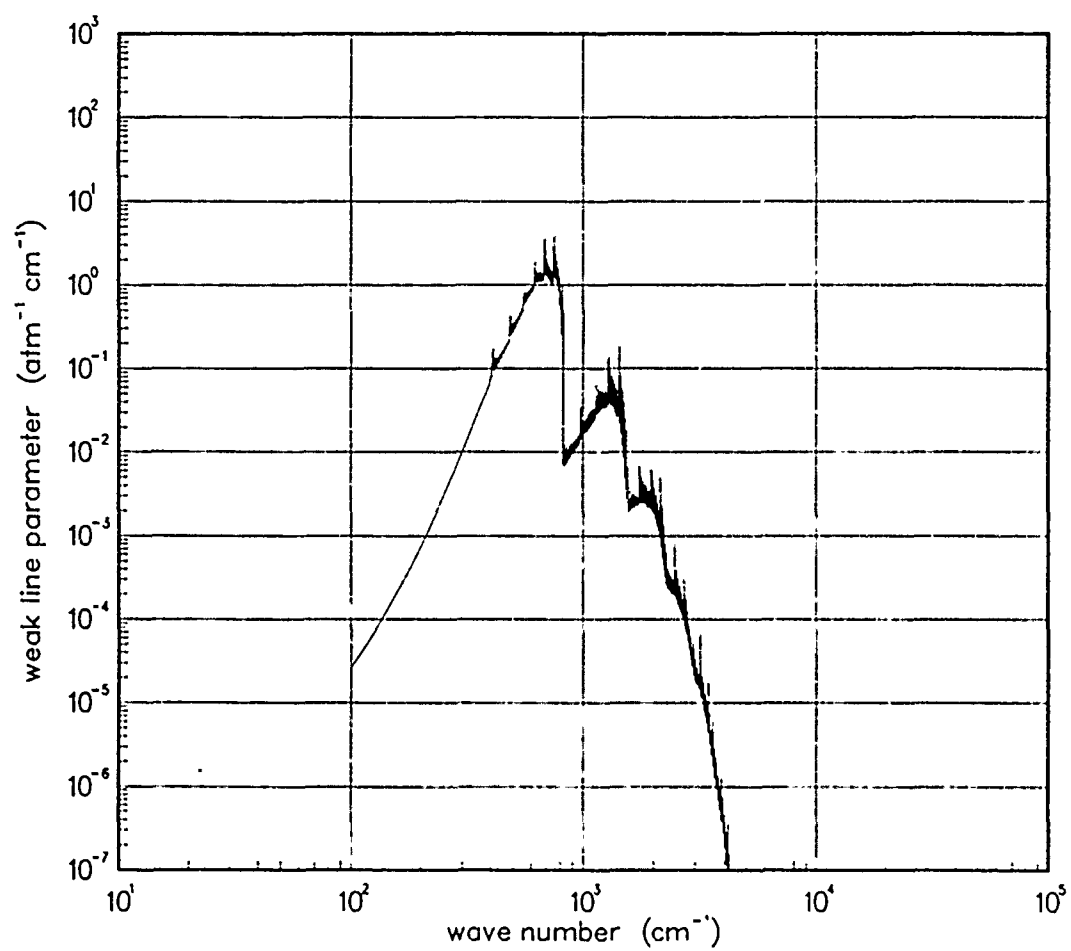


Figure 492. Weak-line parameter for UO at 5000°K.

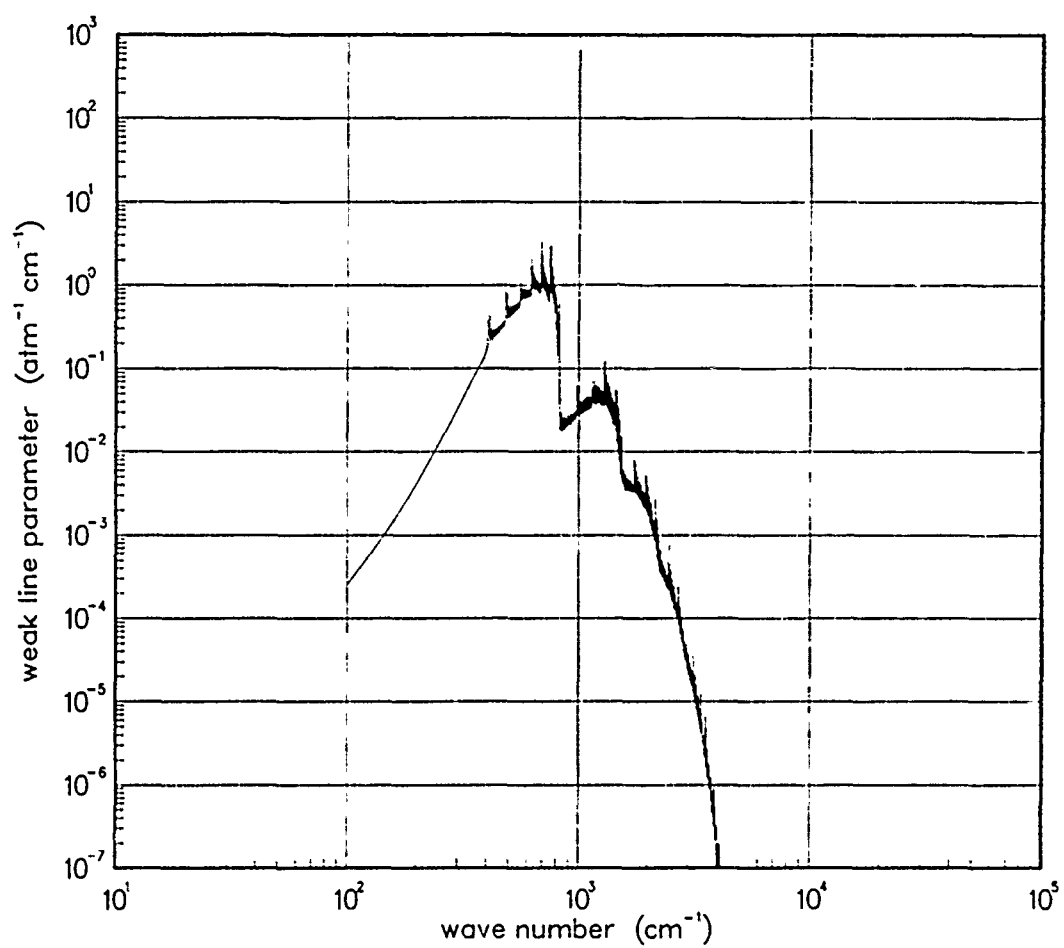


Figure 493. Weak-line parameter for UO at 7000°K.

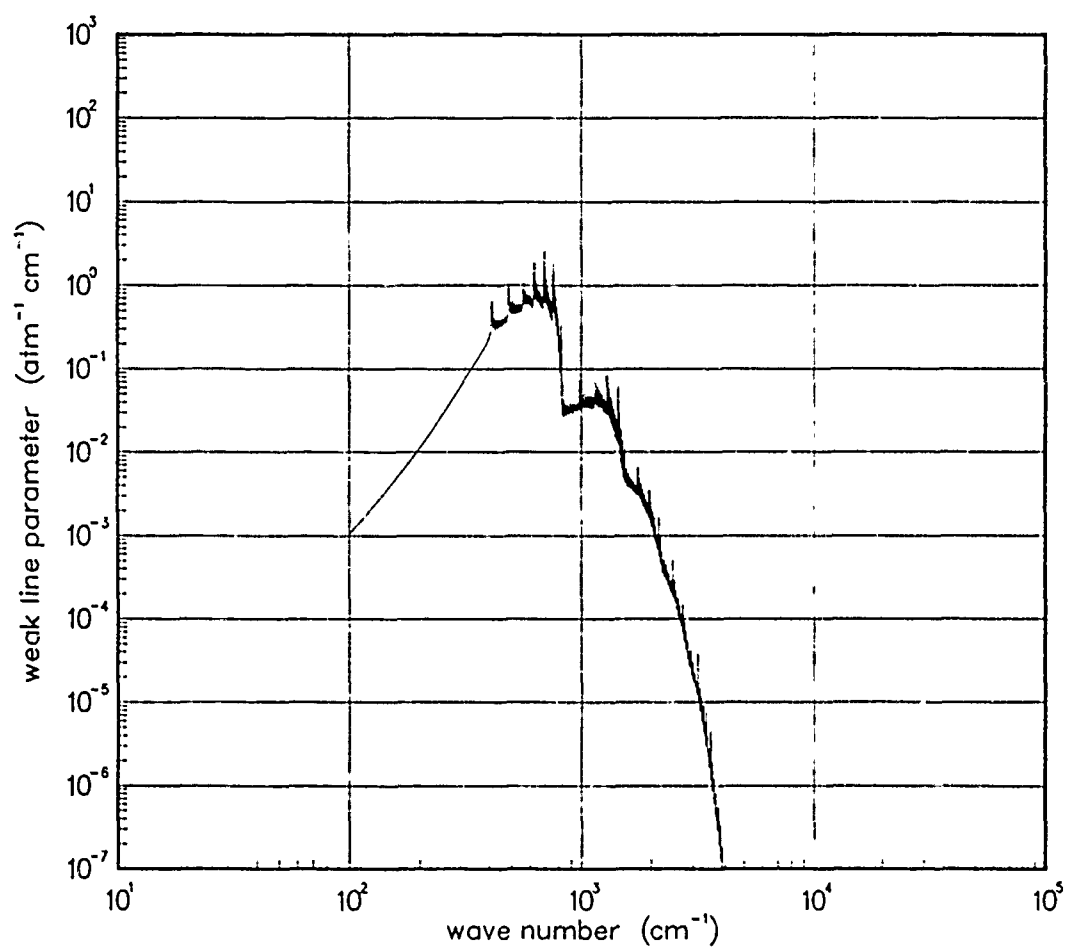


Figure 494. Weak-line parameter for UO at 10000°K.

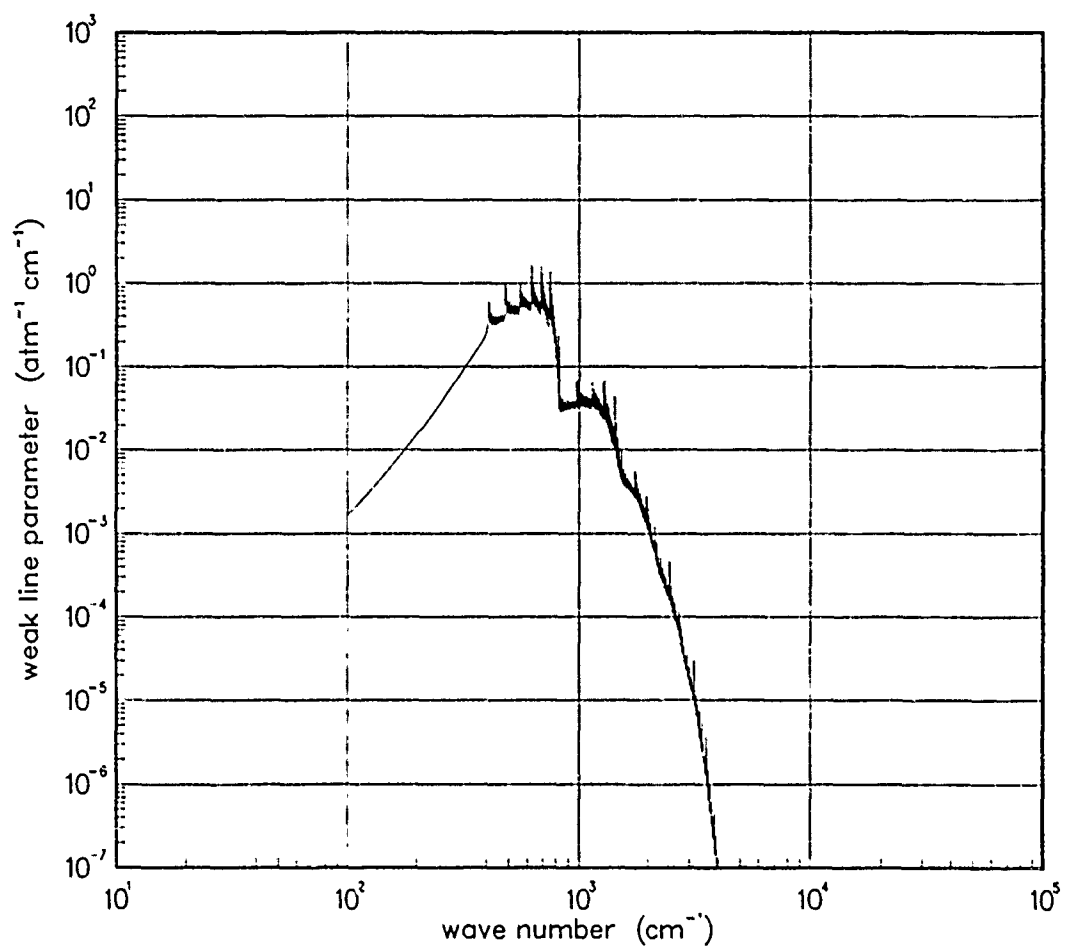


Figure 495. Weak-line parameter for UO at 12000°K.

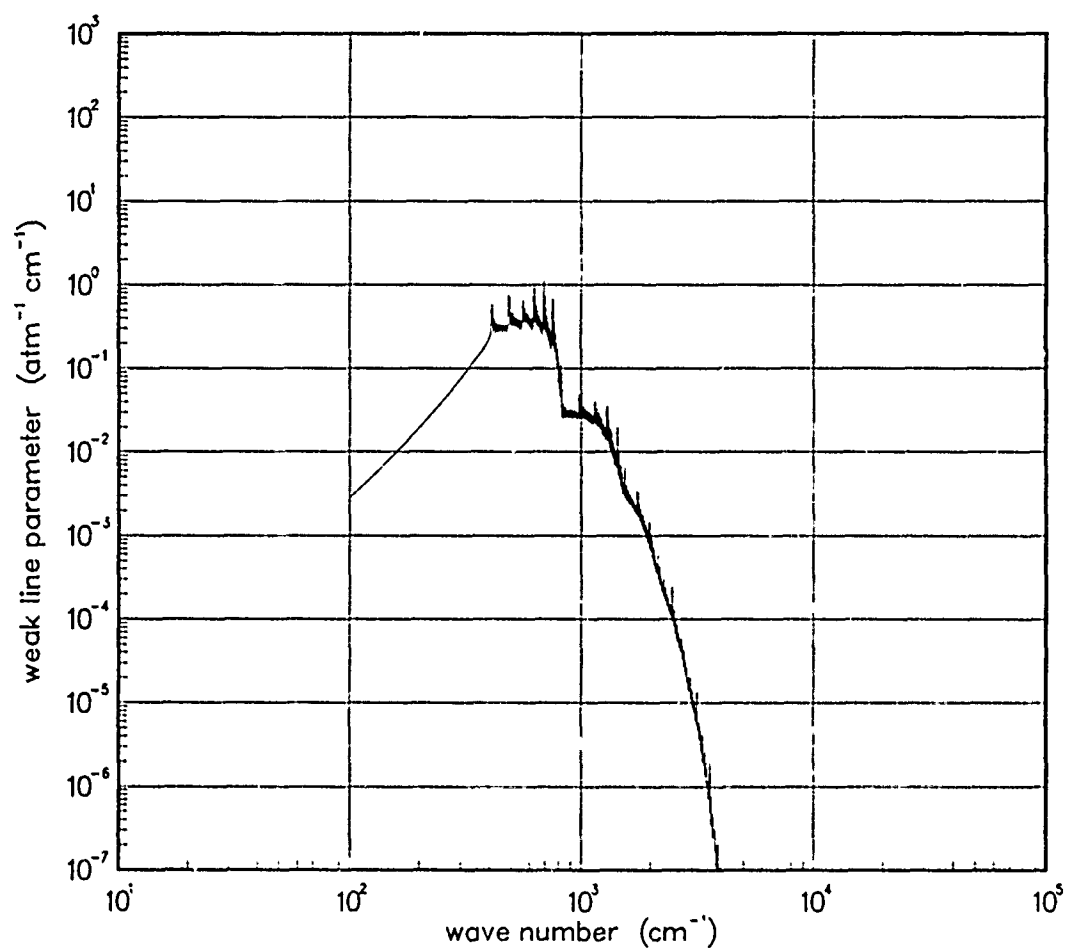


Figure 496. Weak-line parameter for UO at 1800°K .

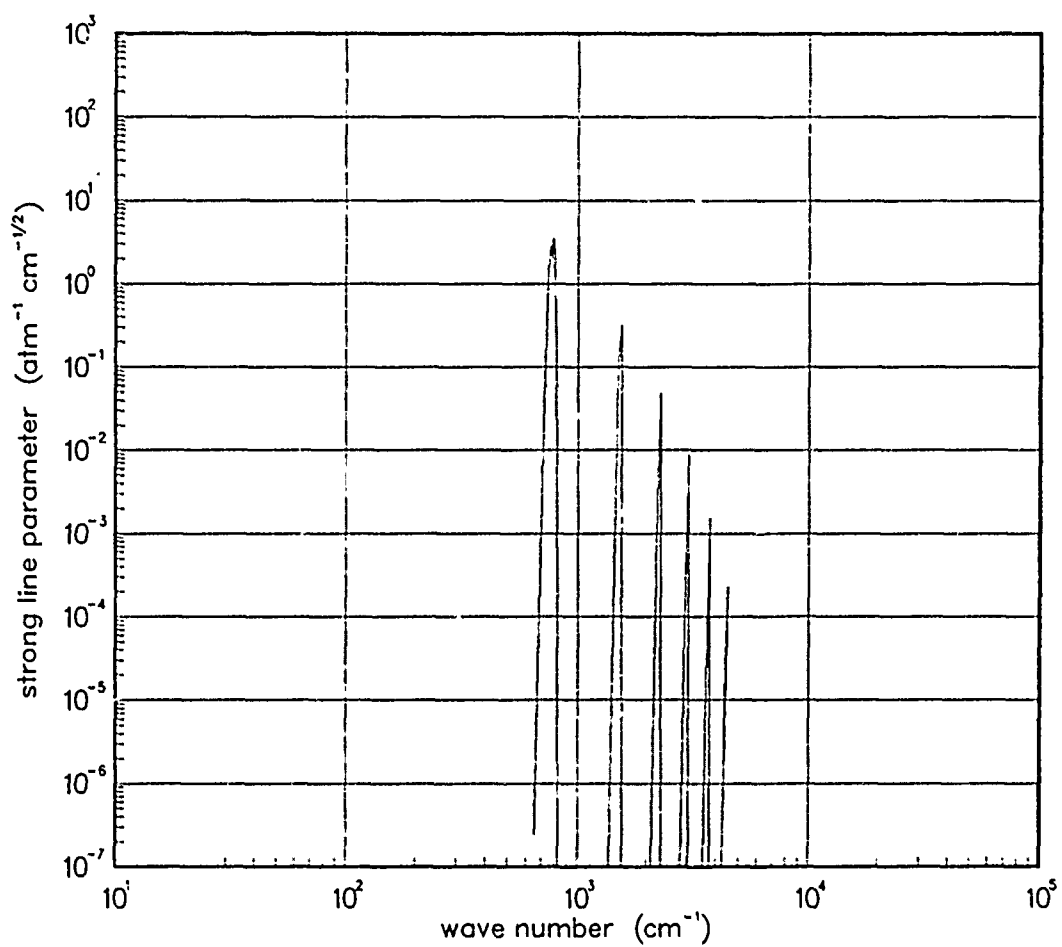


Figure 497. Strong-line parameter for UO at 200°K.

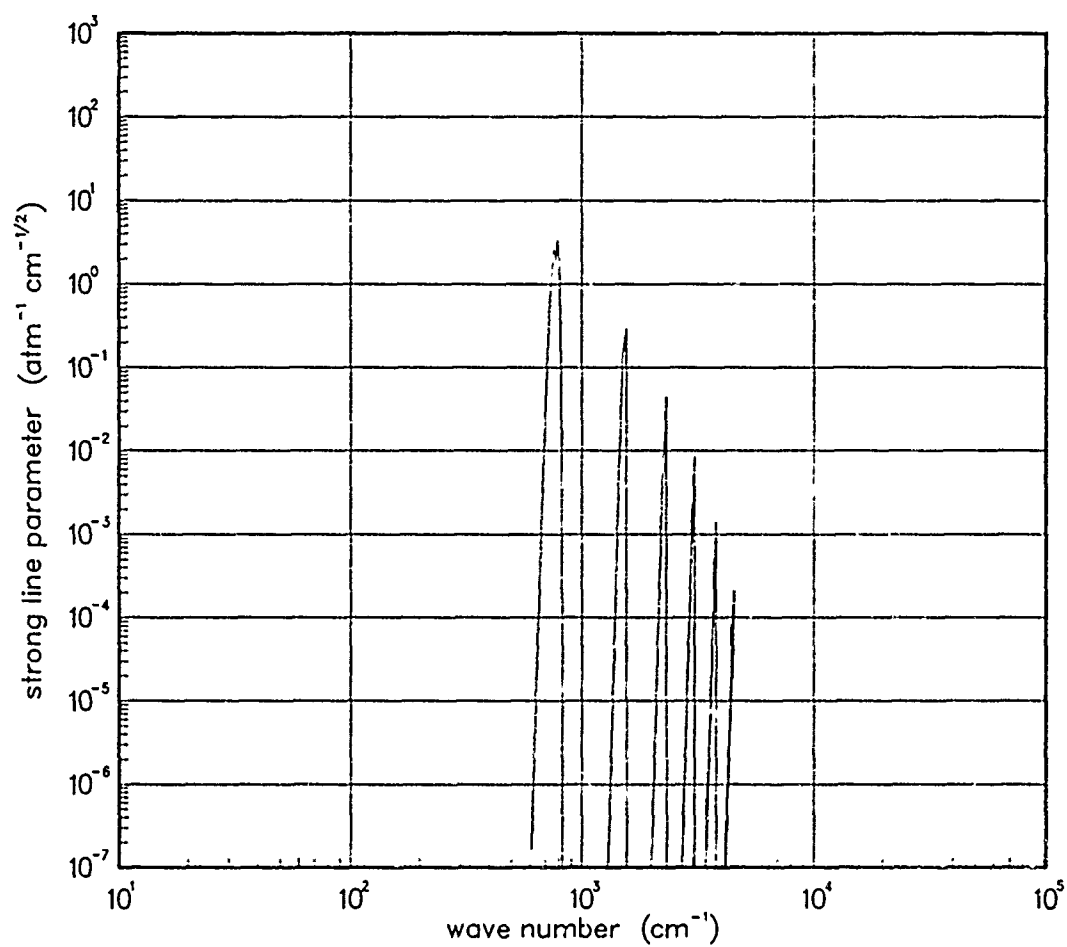


Figure 498. Strong-line parameter for UO at 300°K.

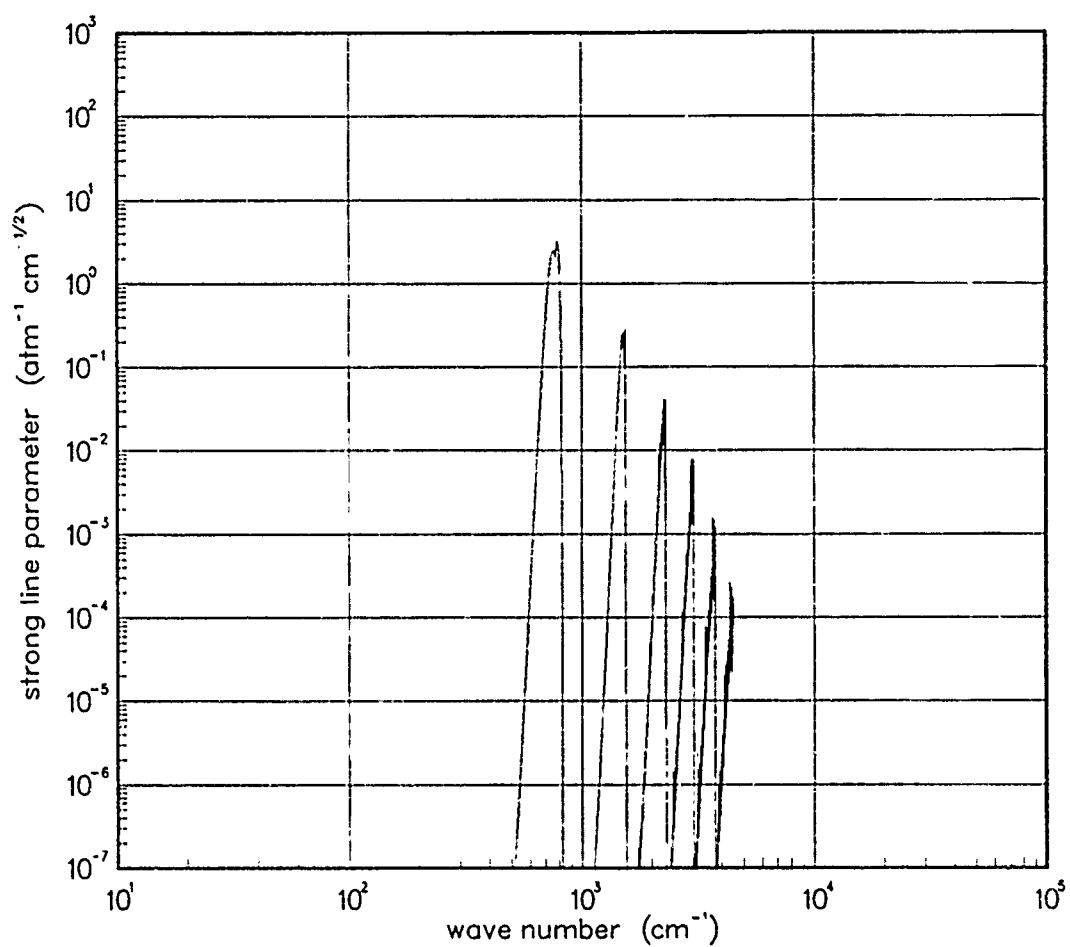


Figure 499. Strong-line parameter for UO at 500°K.

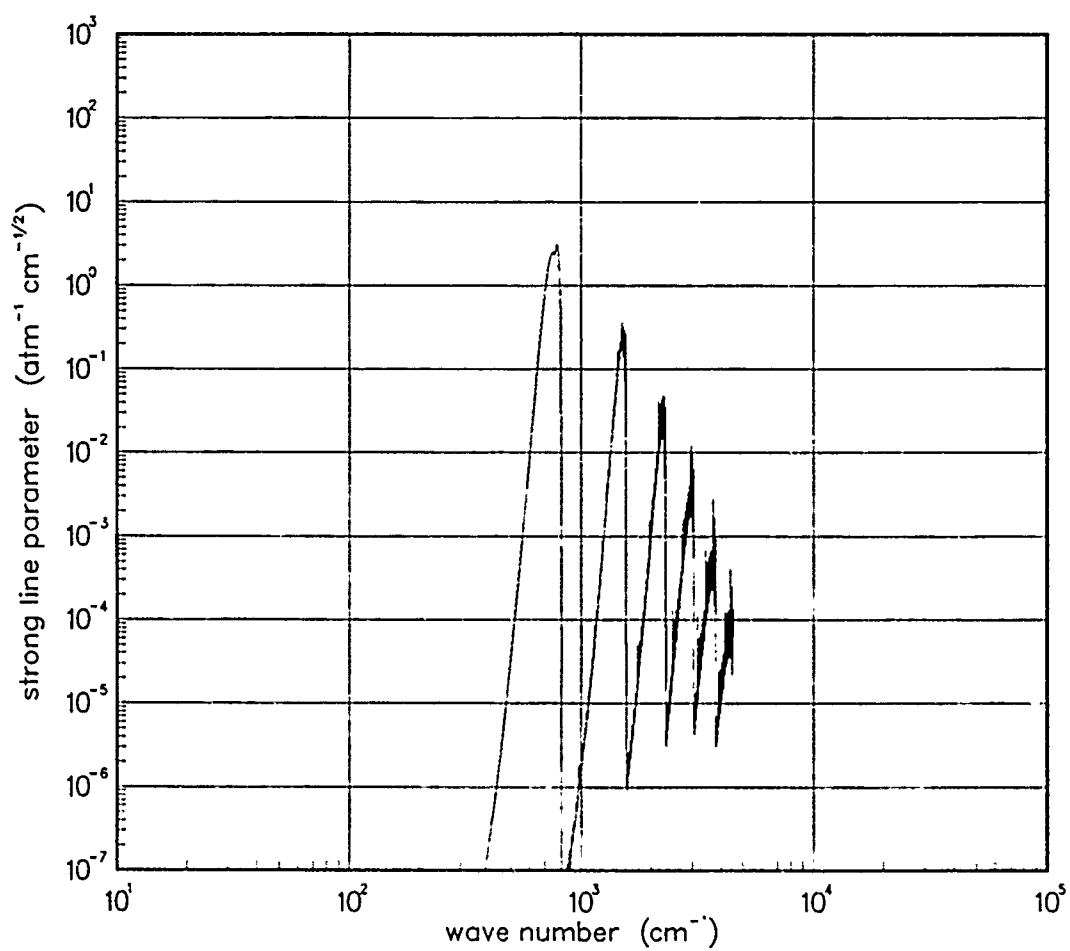


Figure 500. Strong-line parameter for UO at 750°K.

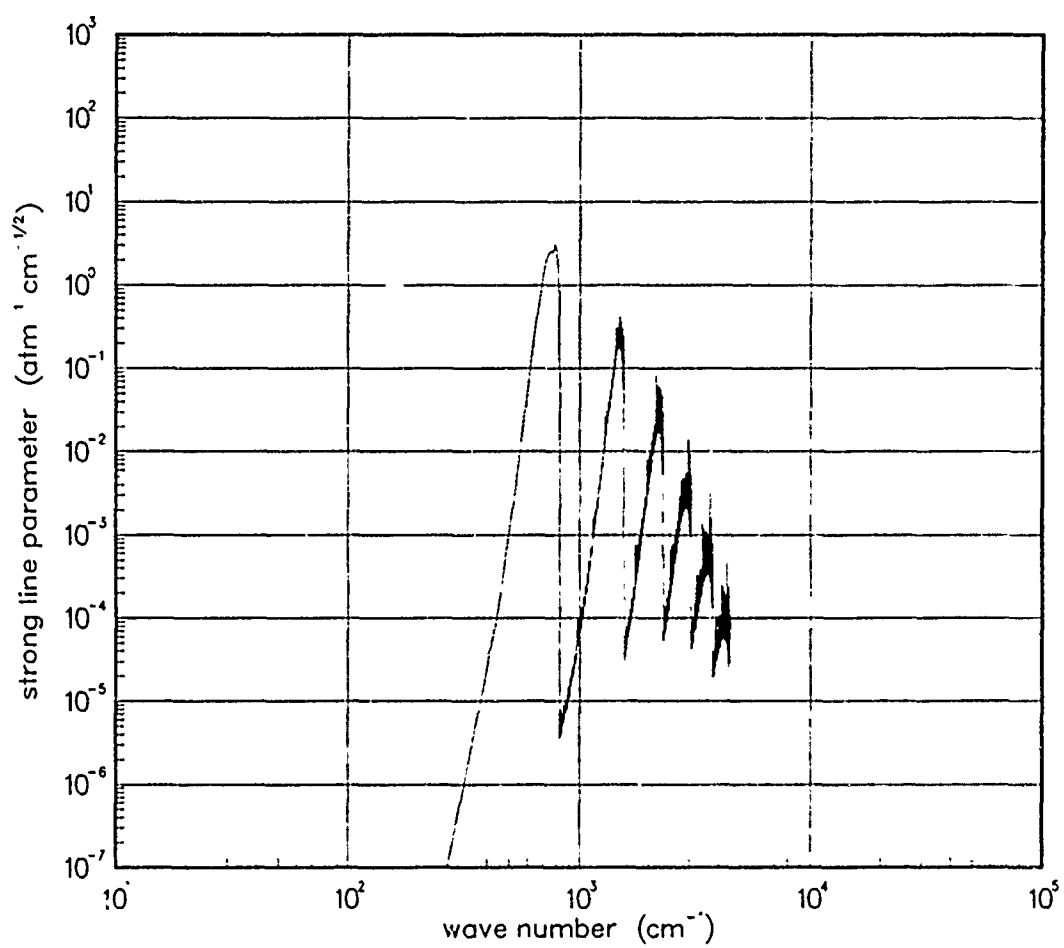


Figure 501. Strong-line parameter for UO at 1000°K.

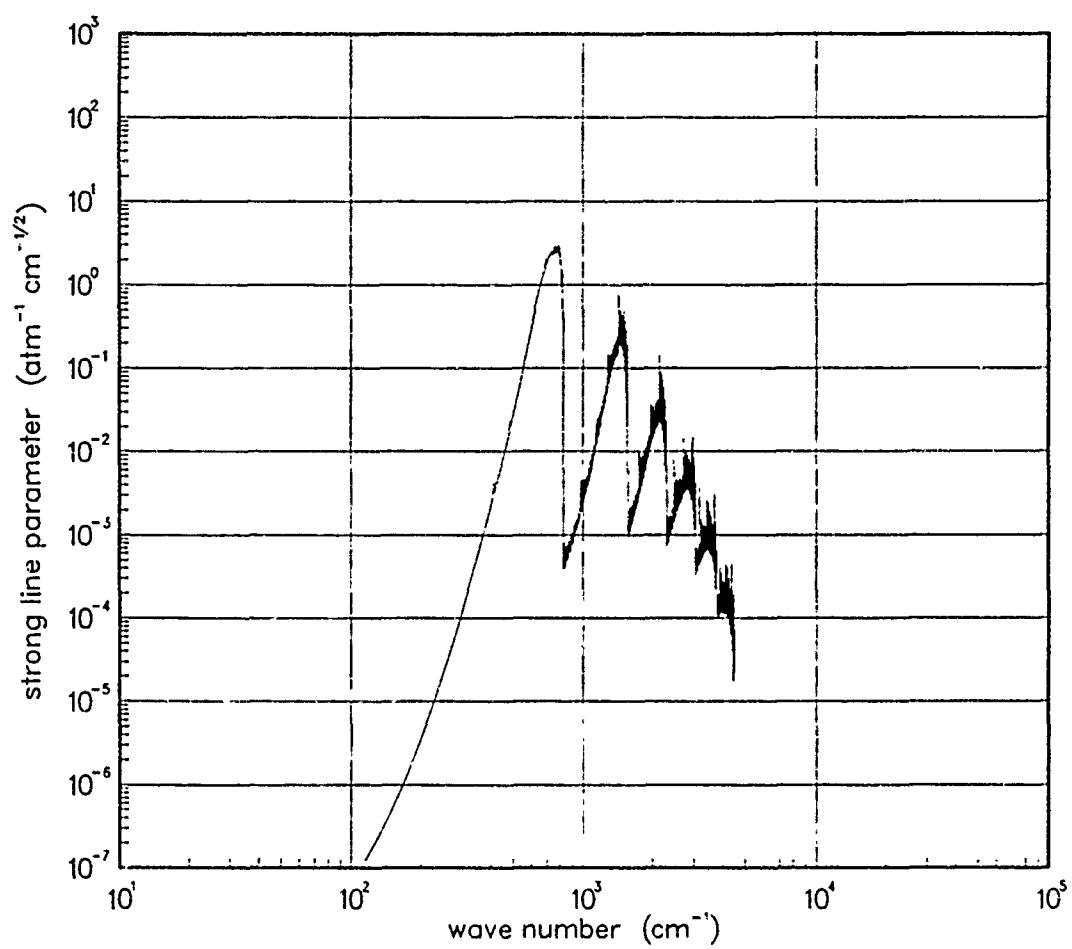


Figure 502. Strong-line parameter for UO at 1500°K.

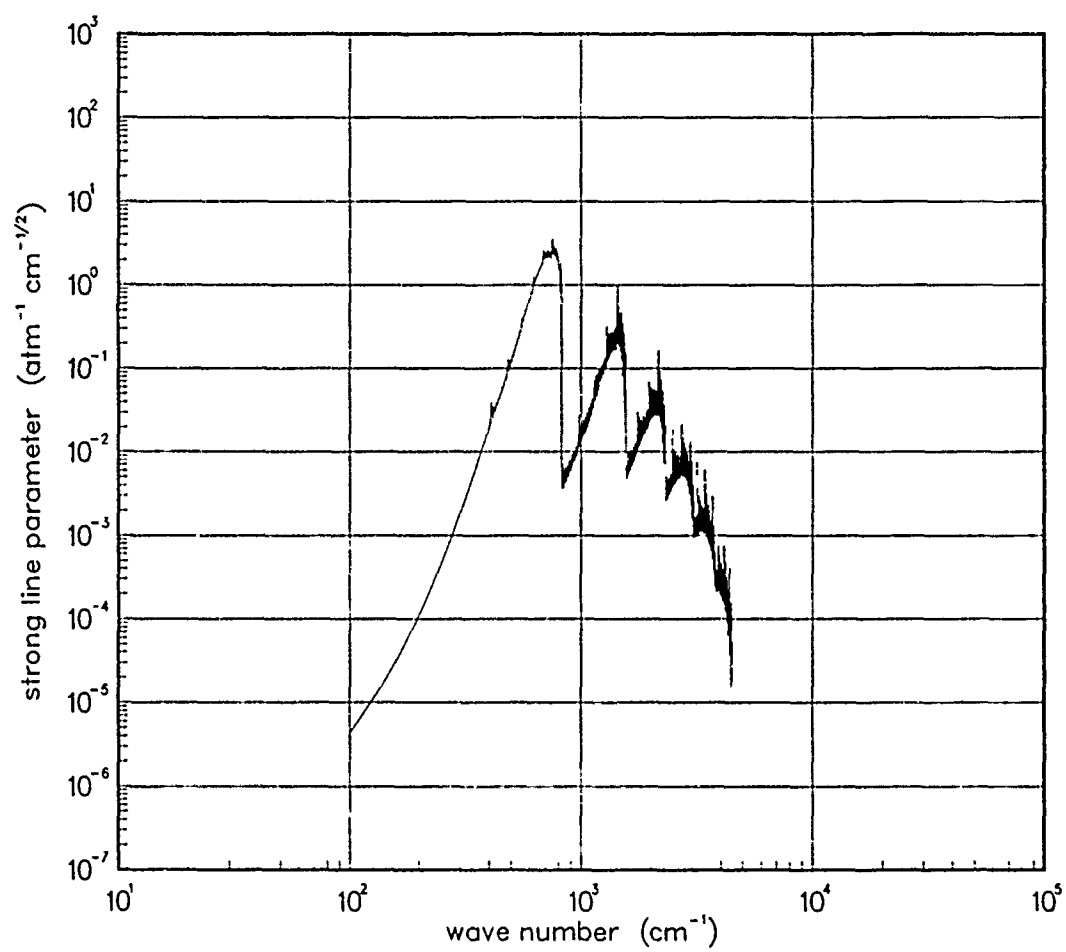


Figure 503. Strong-line parameter for UO at 2000°K.

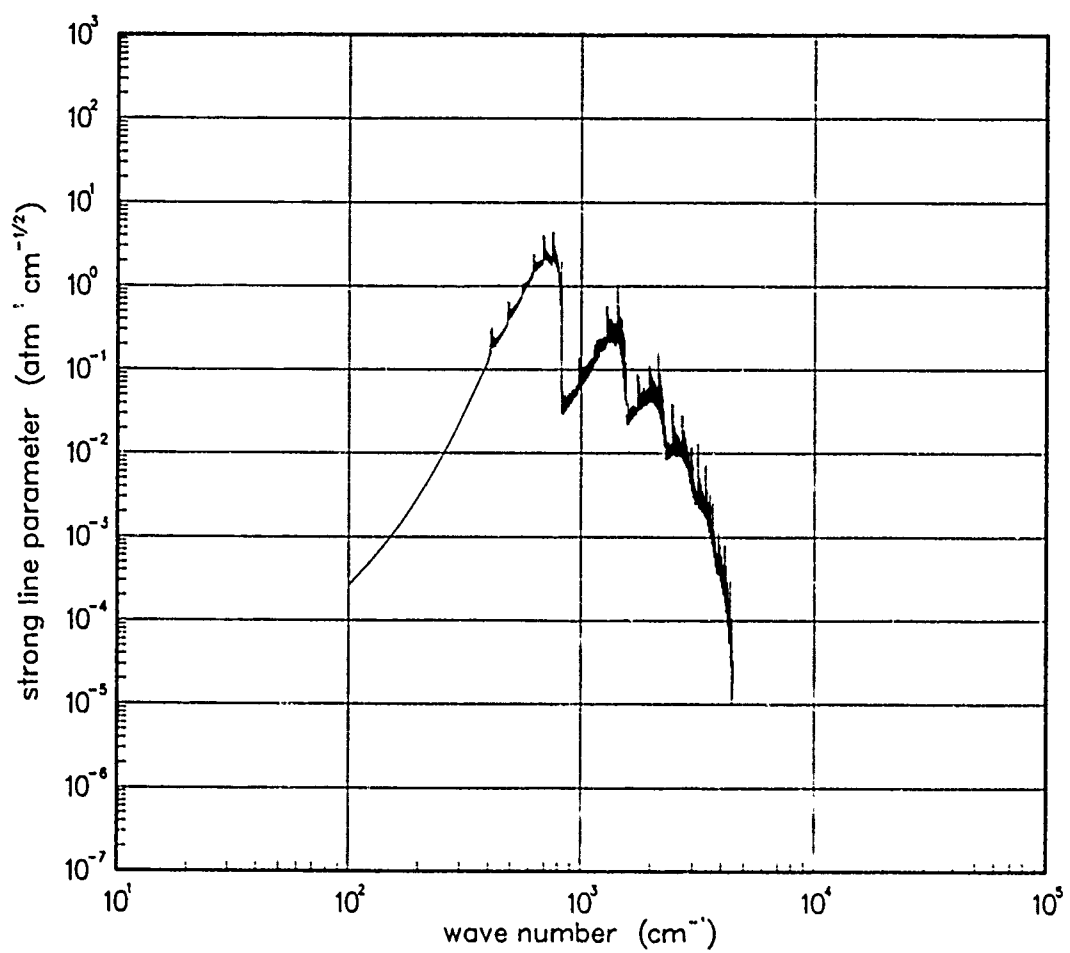


Figure 504. Strong-line parameter for UO at 3000°K.

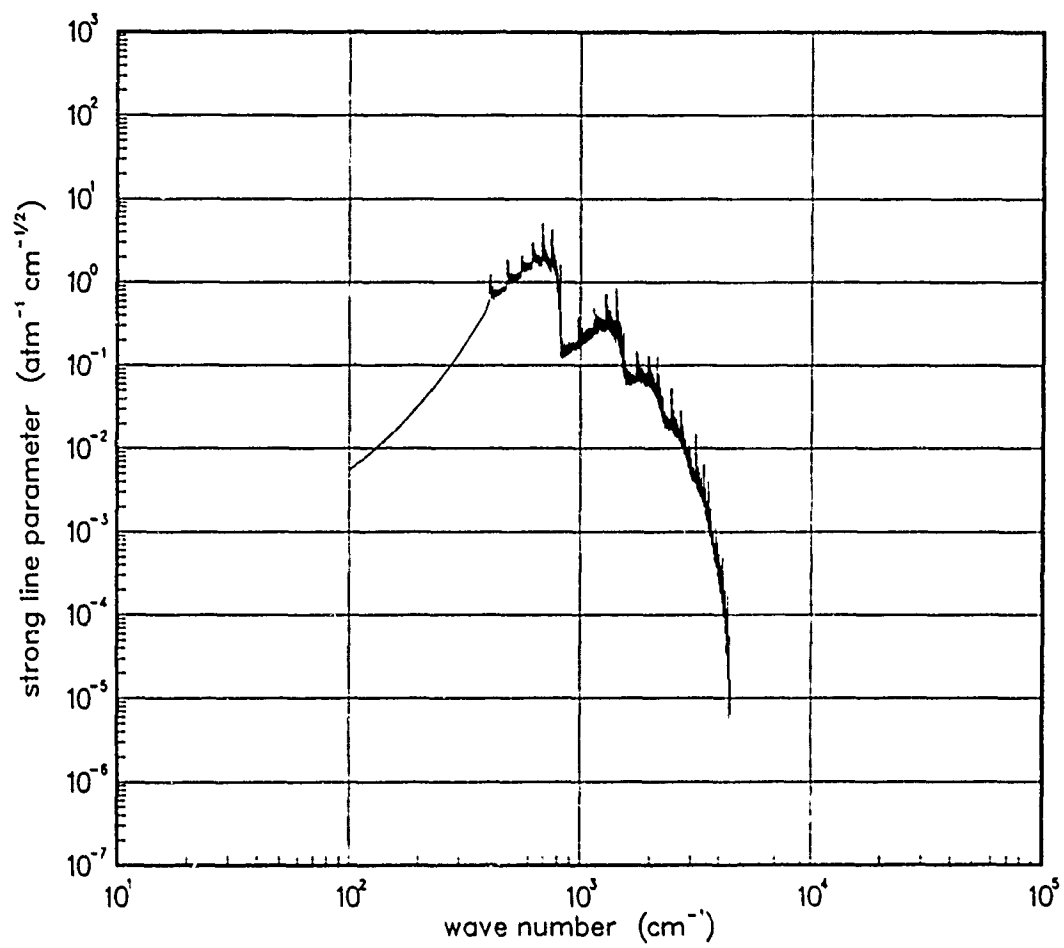


Figure 505. Strong-line parameter for UO at 5000°K.

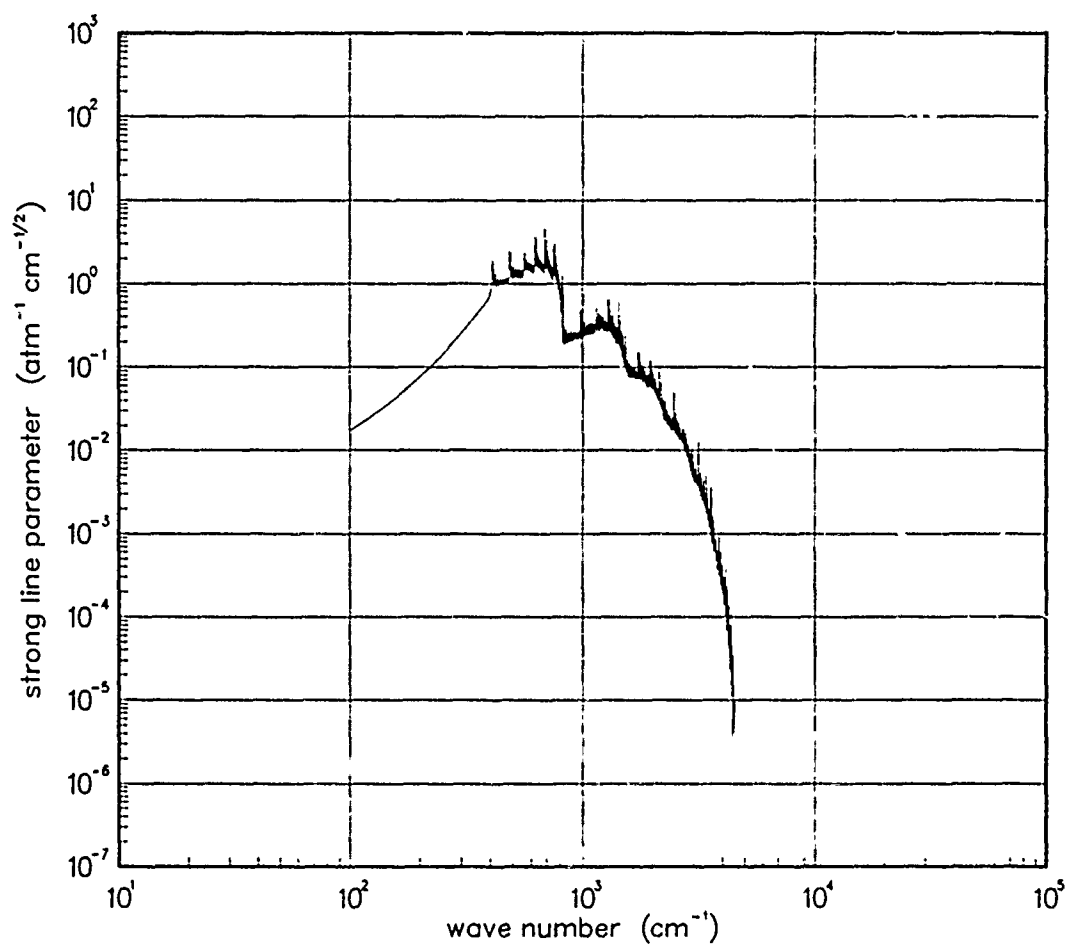


Figure 506. Strong-line parameter for UO at 7000°K.

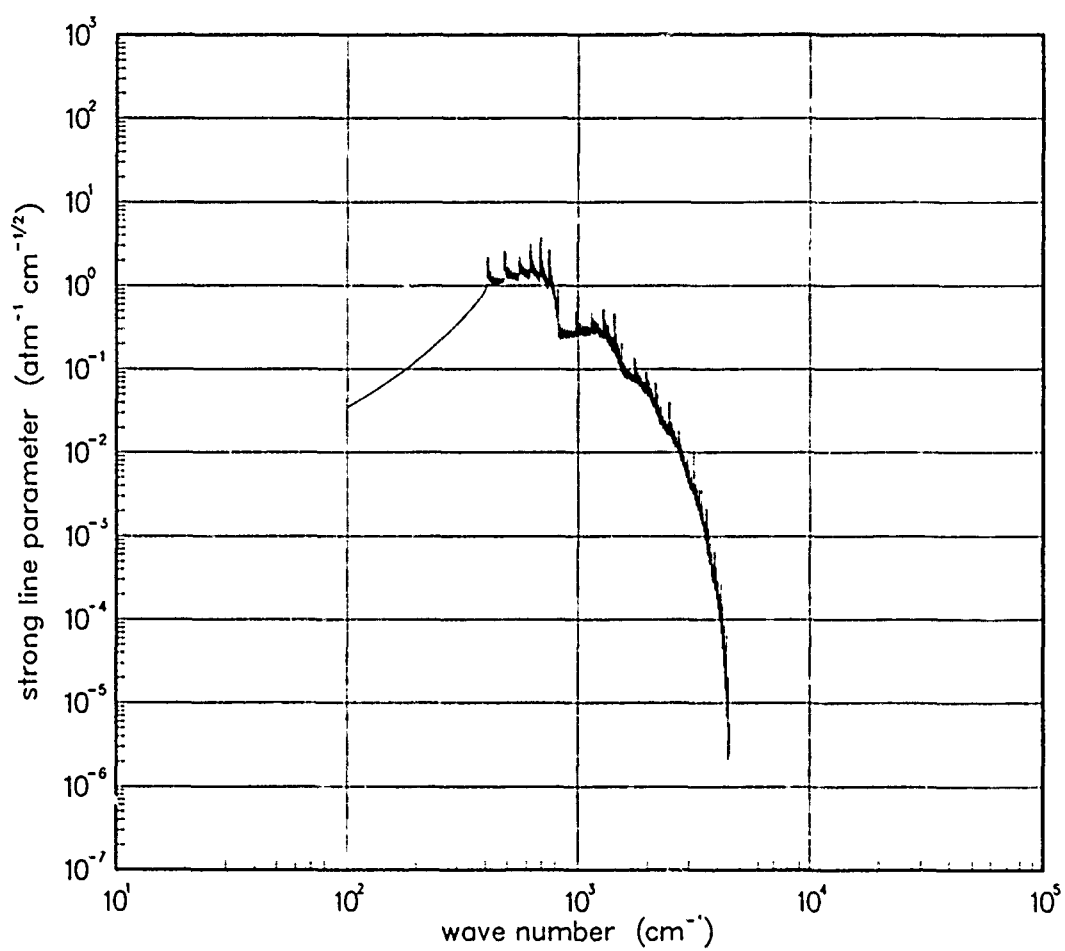


Figure 507. Strong-line parameter for UO at 10000°K.

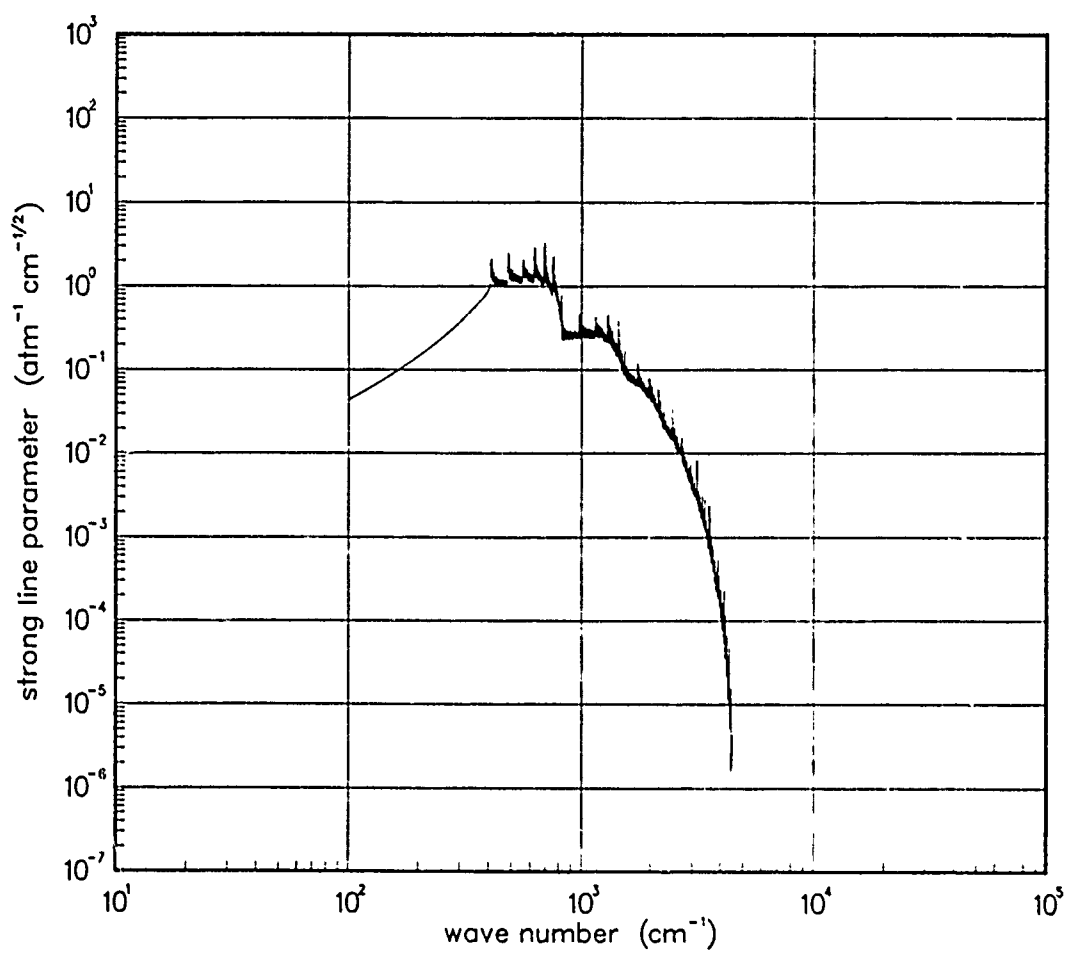


Figure 508. Strong-line parameter for UO at 12000°K.

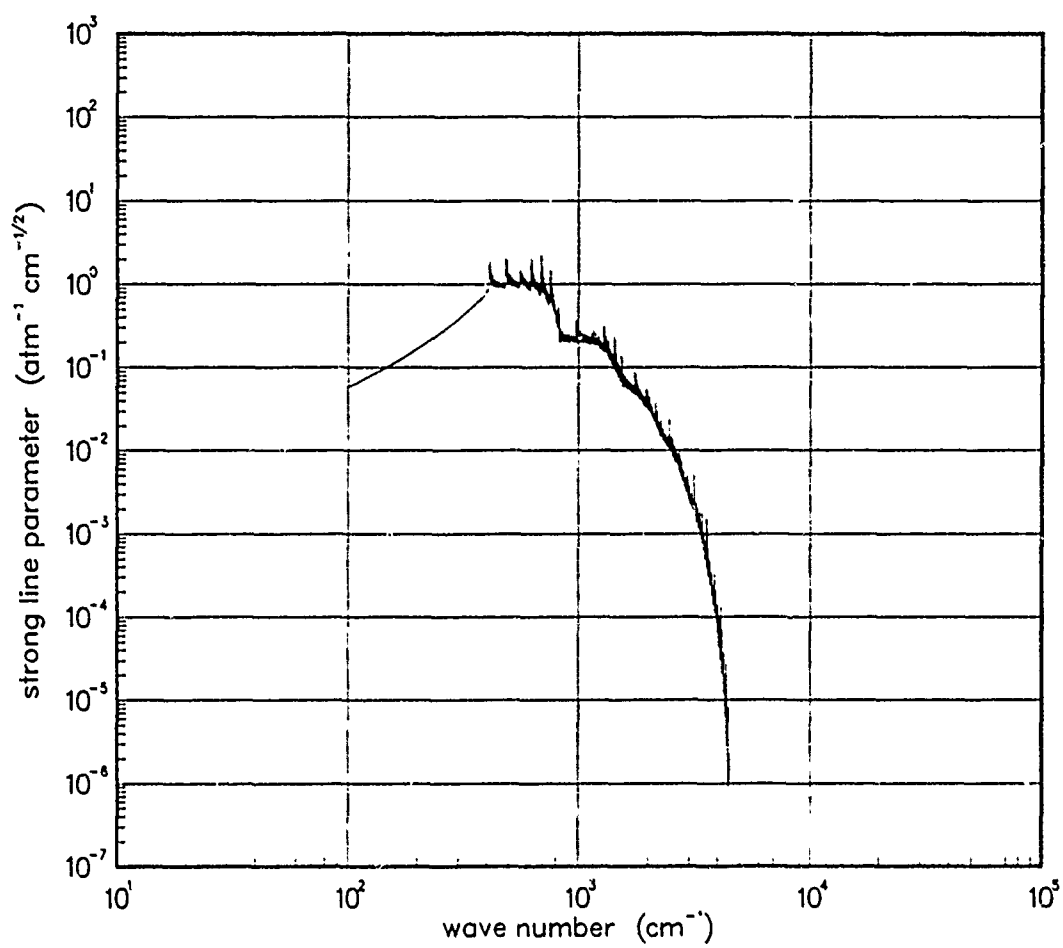


Figure 509. Strong-line parameter for UO at 18000°K.

The SOD and DEI's for UO^+ were calculated in 1985. The source of the molecular constants that were used in these calculations is unknown.

Table 15. Spectroscopic data for UO^+ .

Ground Electronic State

$$\begin{array}{ll} \omega_e = 925.00 & \omega_e x_e = 2.70 \\ \alpha_e = .0020 & B_e = 0.330 \end{array}$$

$$S_{10} = 1190.0$$

$$\gamma_t(300^\circ\text{K}) = 0.04^*$$

Data Source:

*Estimate.

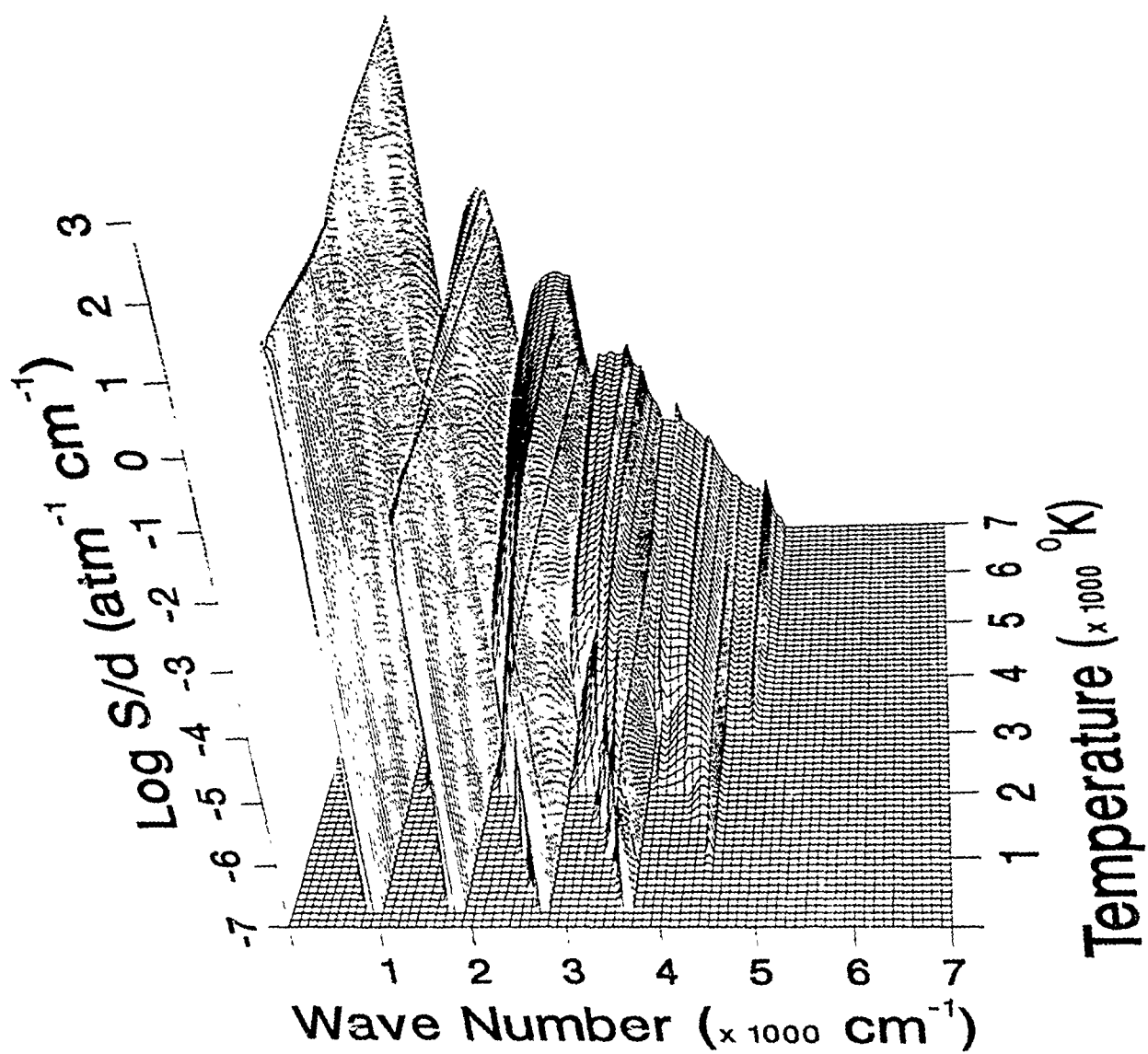


Figure 510. Weak-line parameter for UO^+ .

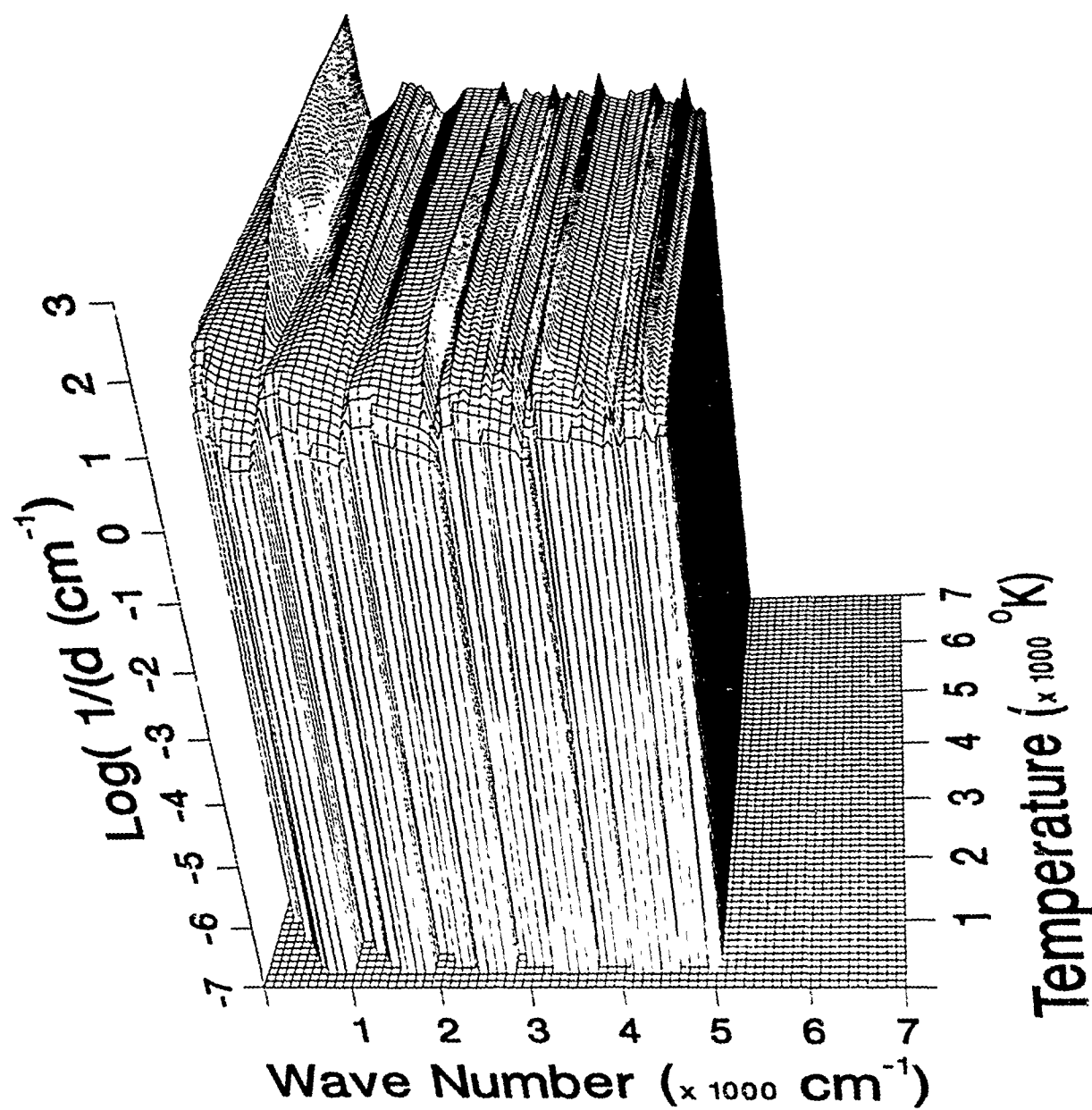


Figure 511. Inverse line spacing for UO^+ .

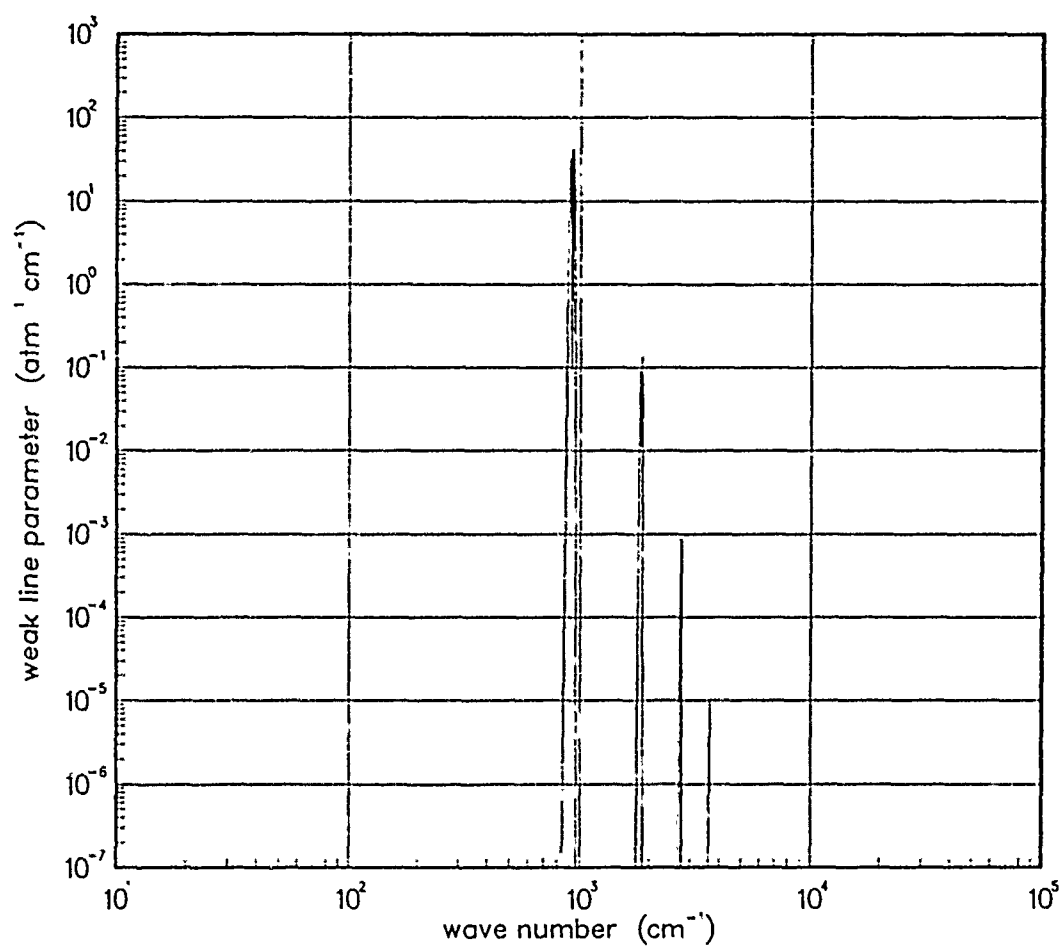


Figure 512. Weak-line parameter for UO⁺ at 200°K.

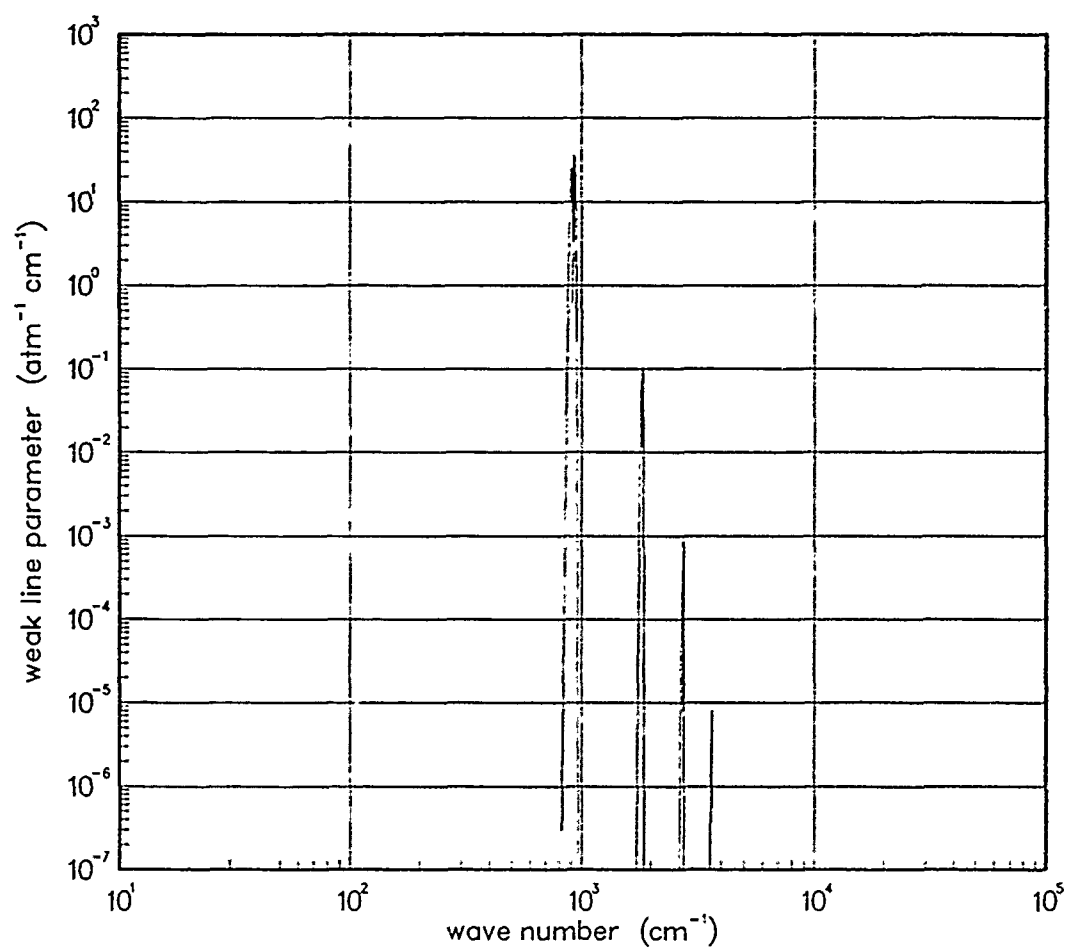


Figure 513. Weak-line parameter for UO^+ at 300°K .

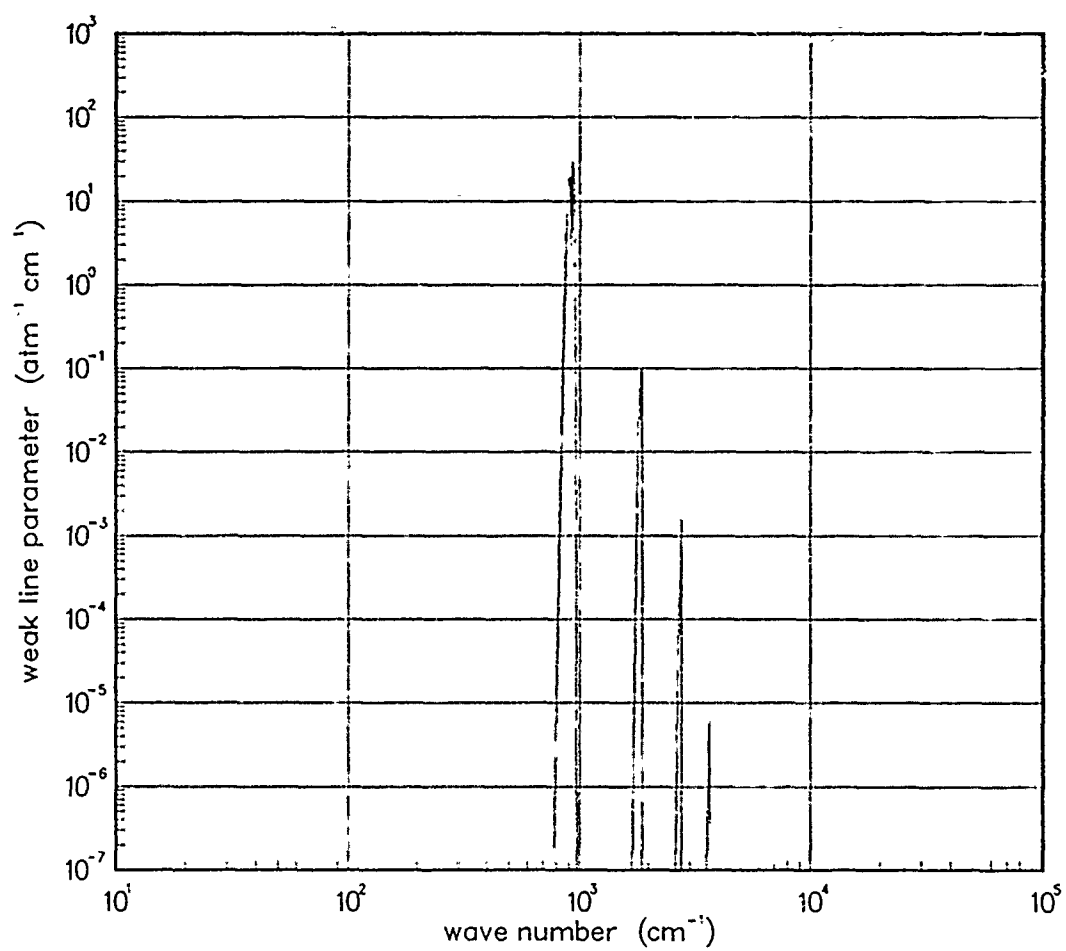


Figure 514. Weak-line parameter for UO^+ at 500°K .

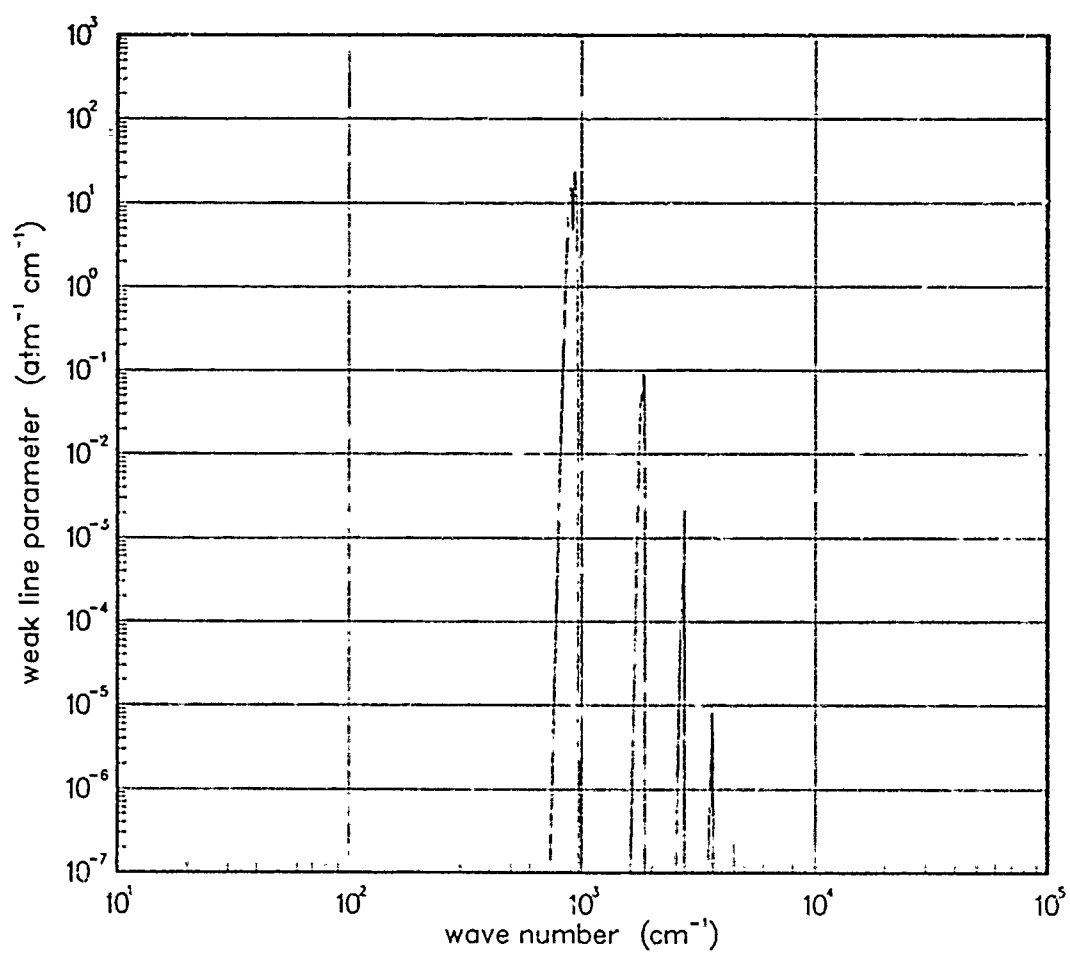


Figure 515. Weak-line parameter for UO⁺ at 750°K.

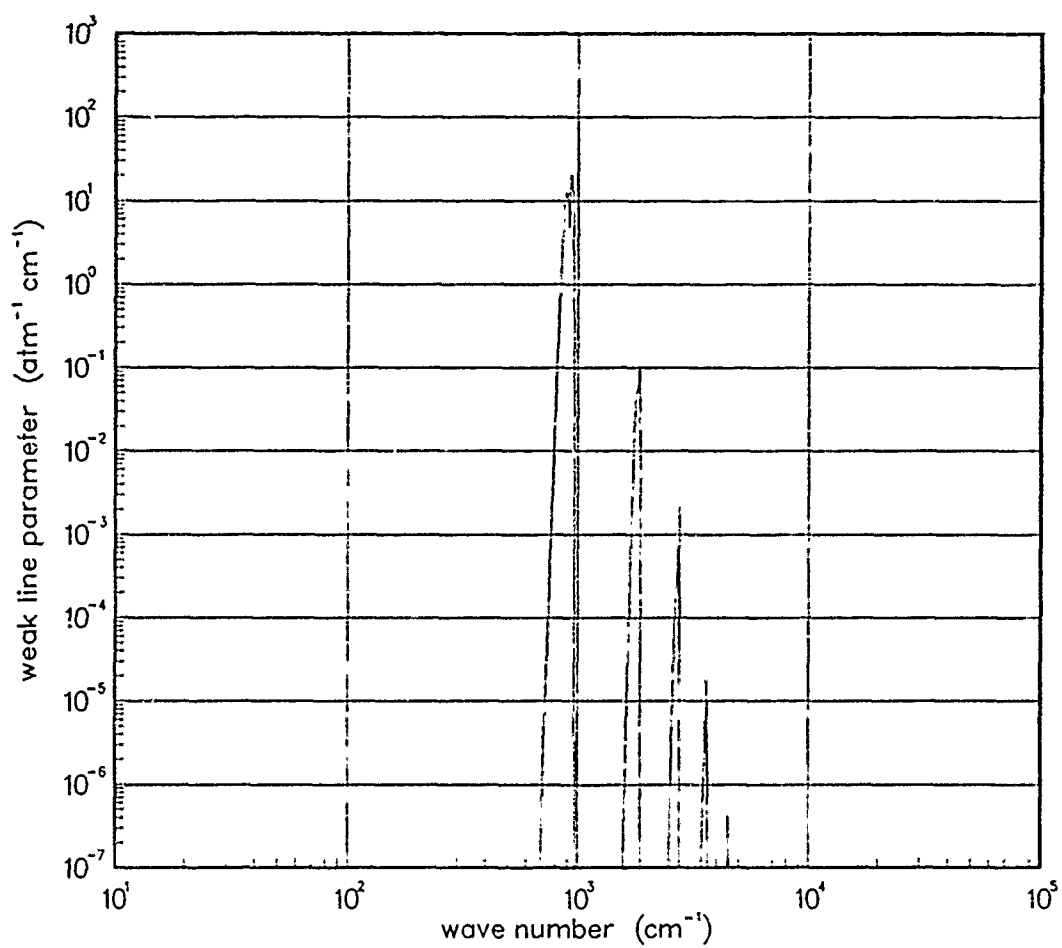


Figure 516. Weak-line parameter for UO^+ at 1000°K .

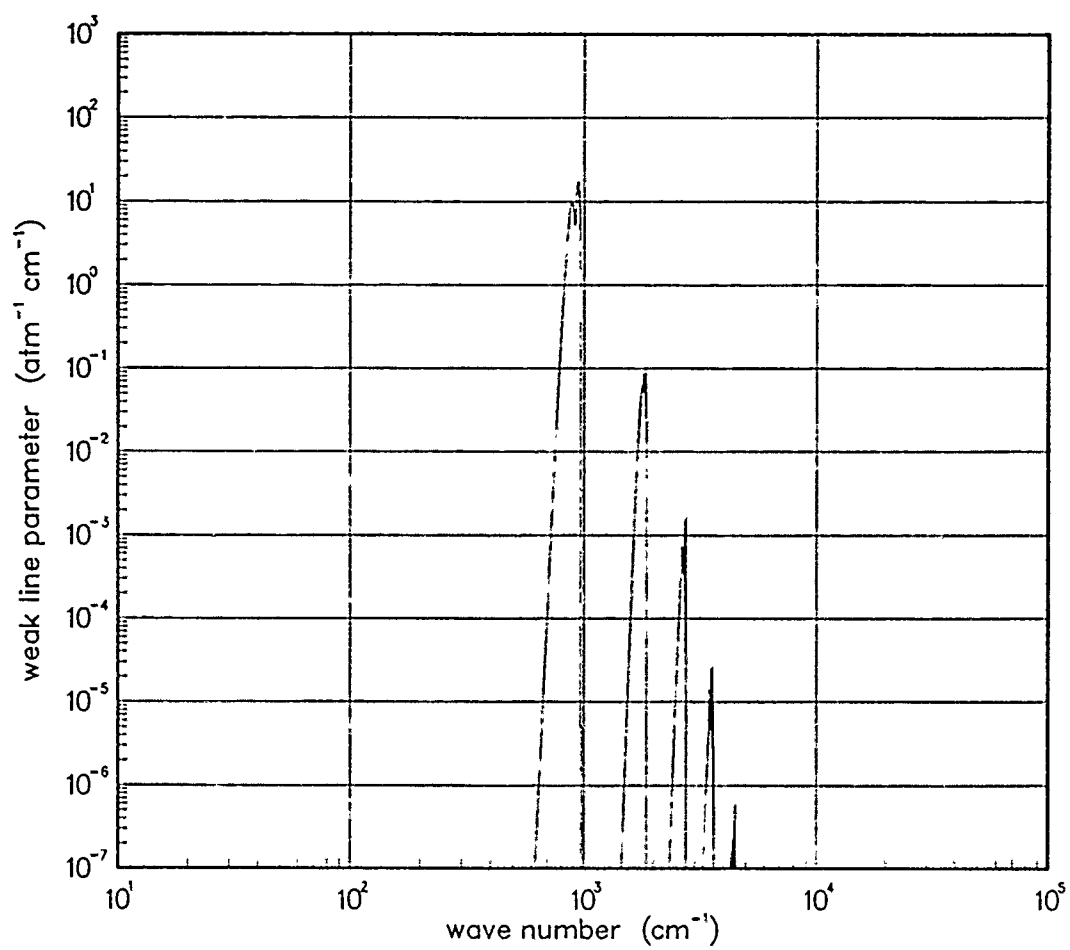


Figure 517. Weak-line parameter for UO^+ at 1500°K .

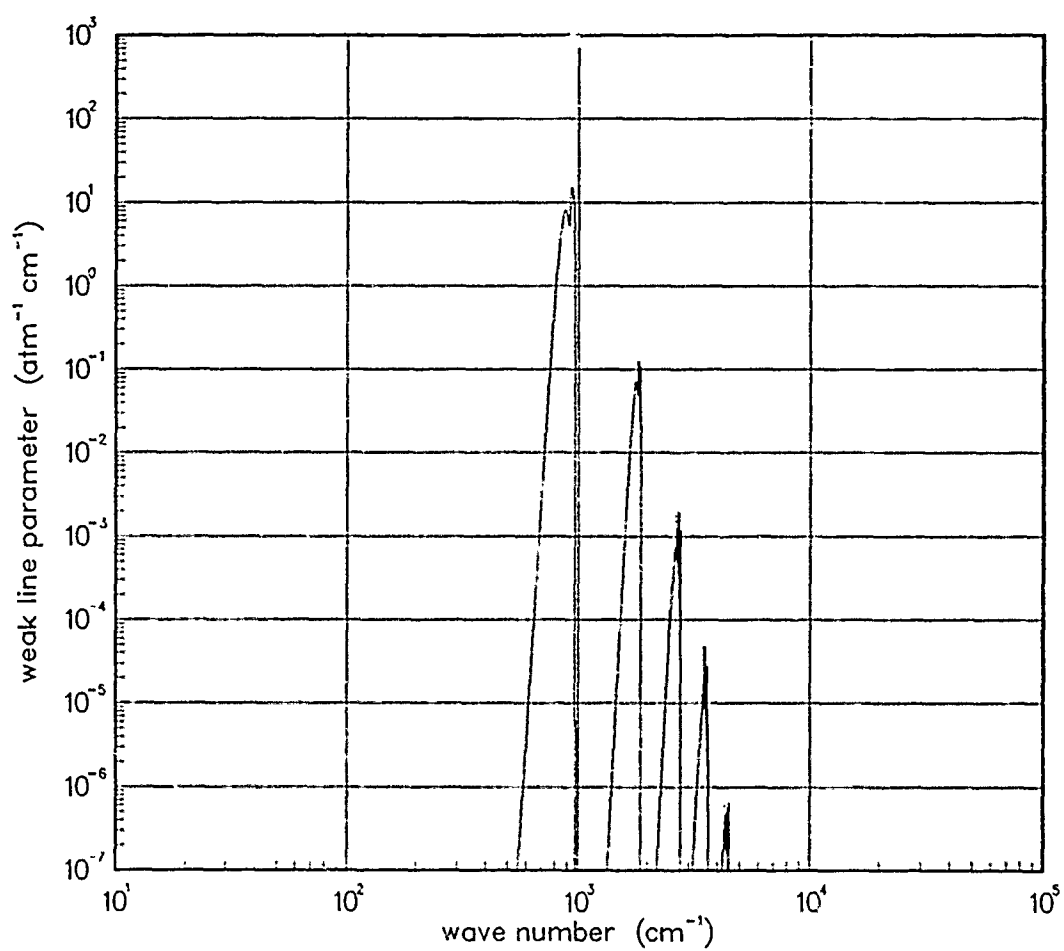


Figure 518. Weak-line parameter for UO⁺ at 2000°K.

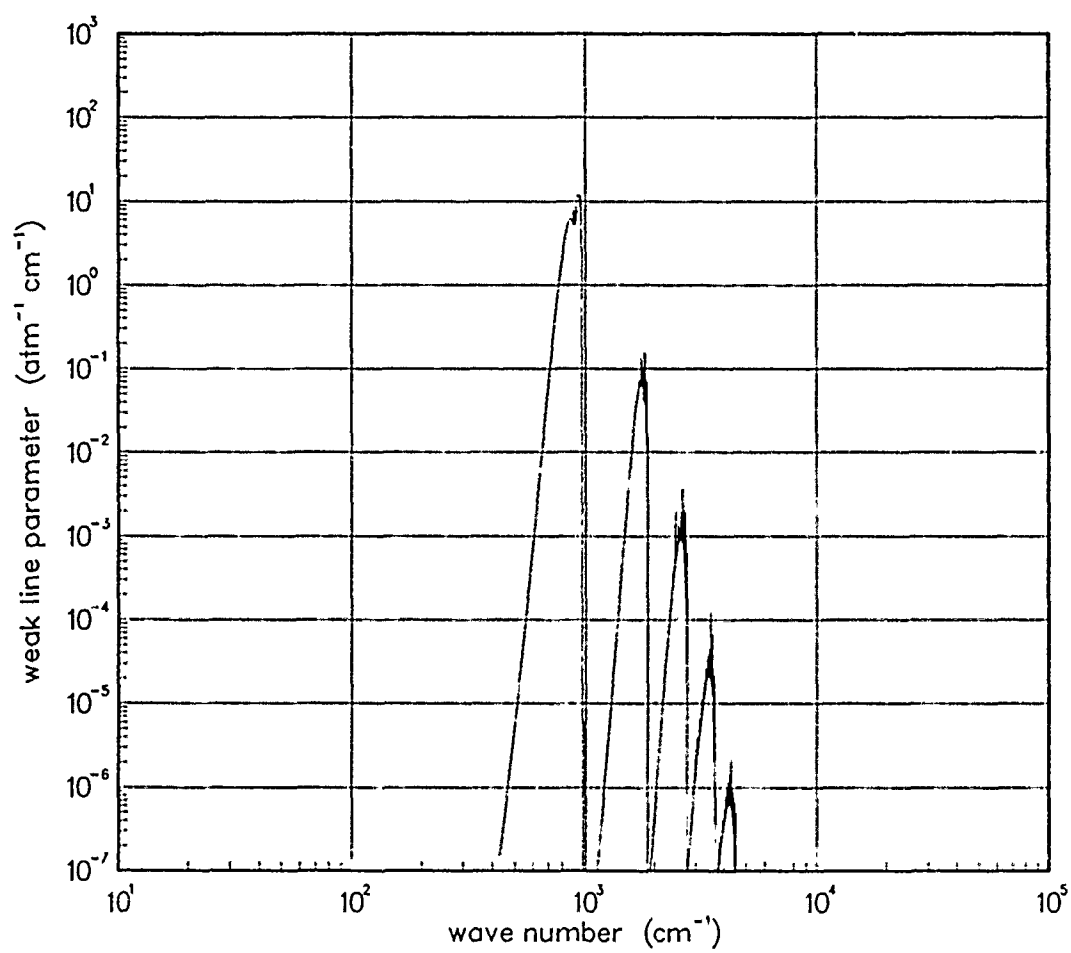


Figure 519. Weak-line parameter for UO^+ at 3000°K .

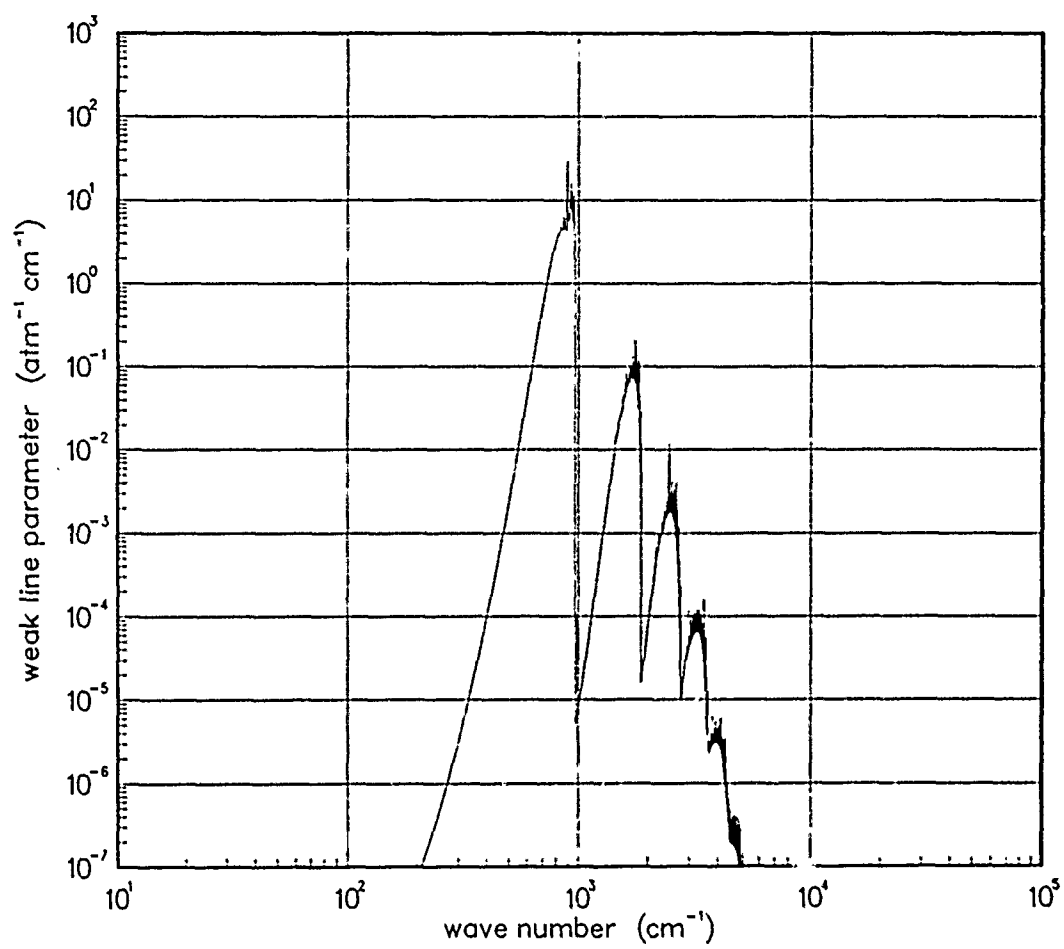


Figure 520. Weak-line parameter for UO^+ at 5000°K .

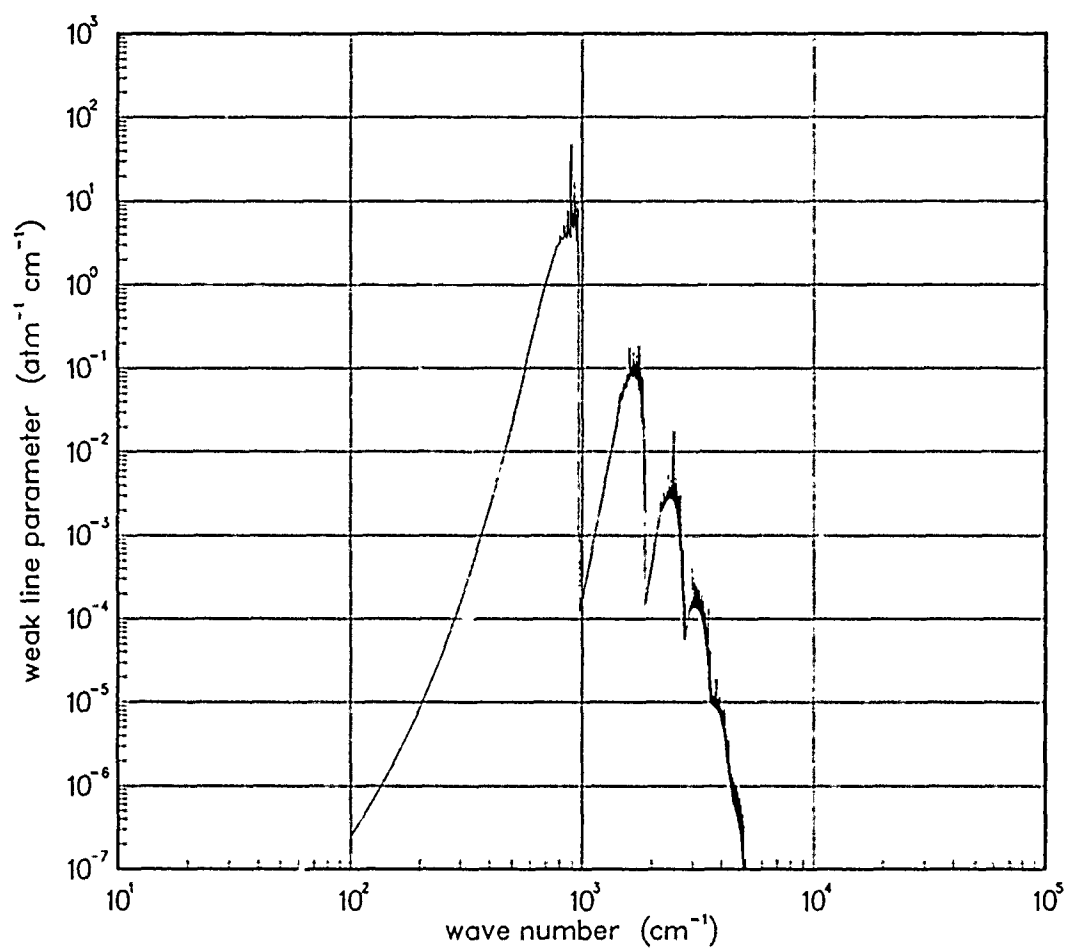


Figure 521. Weak-line parameter for UO^+ at 7000°K .

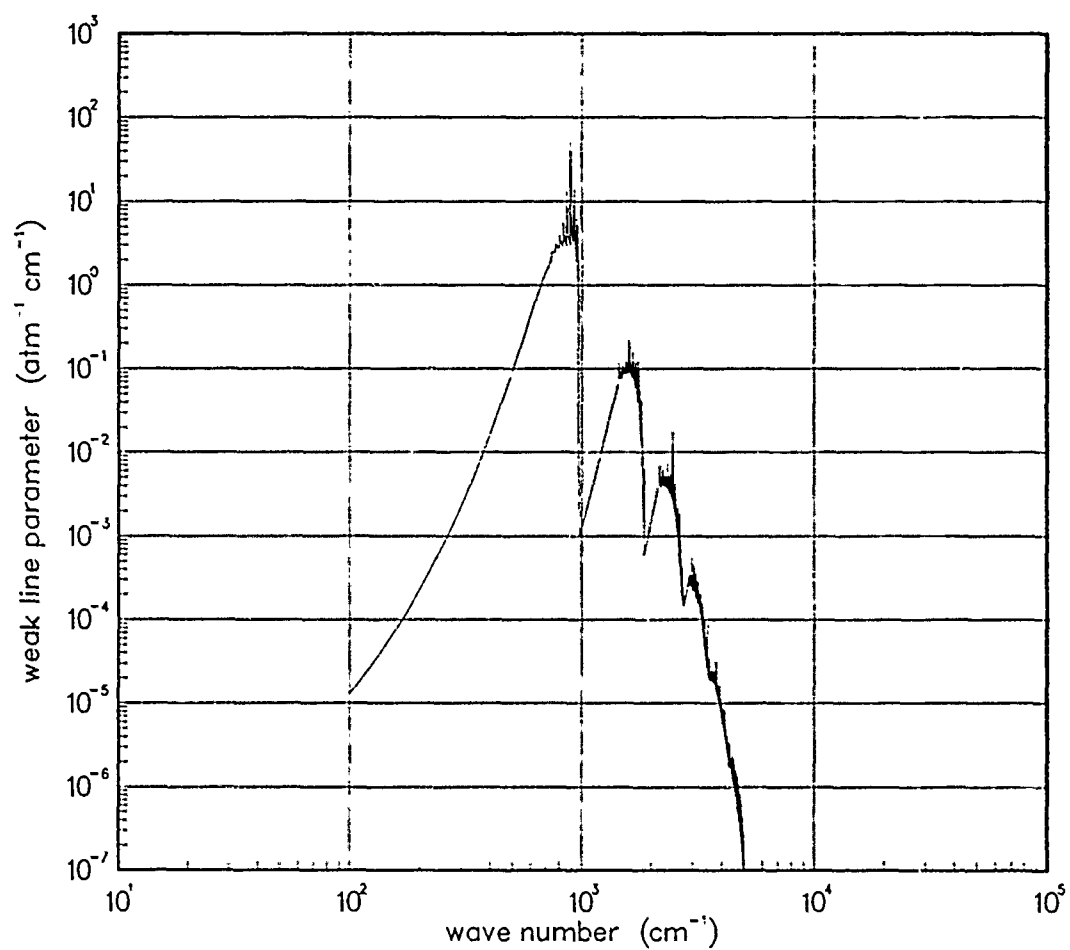


Figure 522. Weak-line parameter for UO^+ at 10000°K .

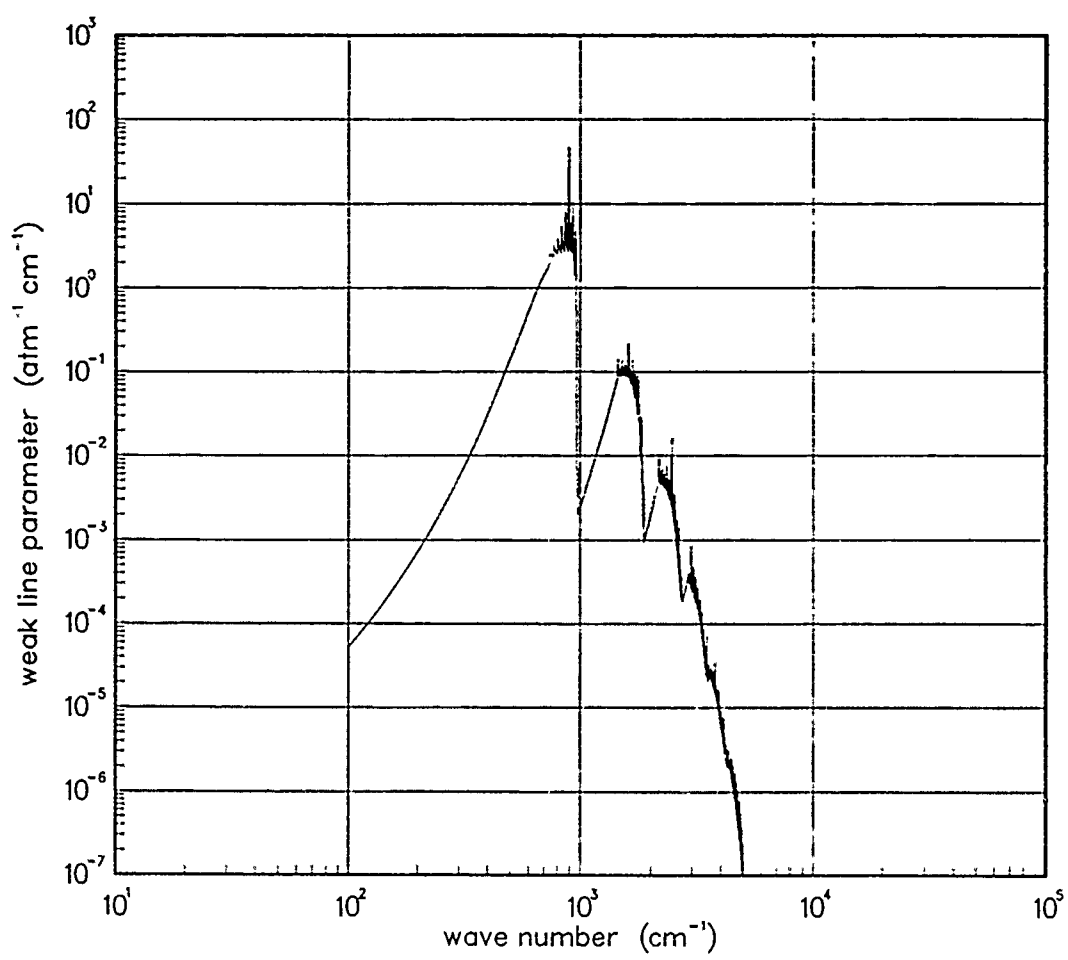


Figure 523. Weak-line parameter for UO^+ at 12000°K .

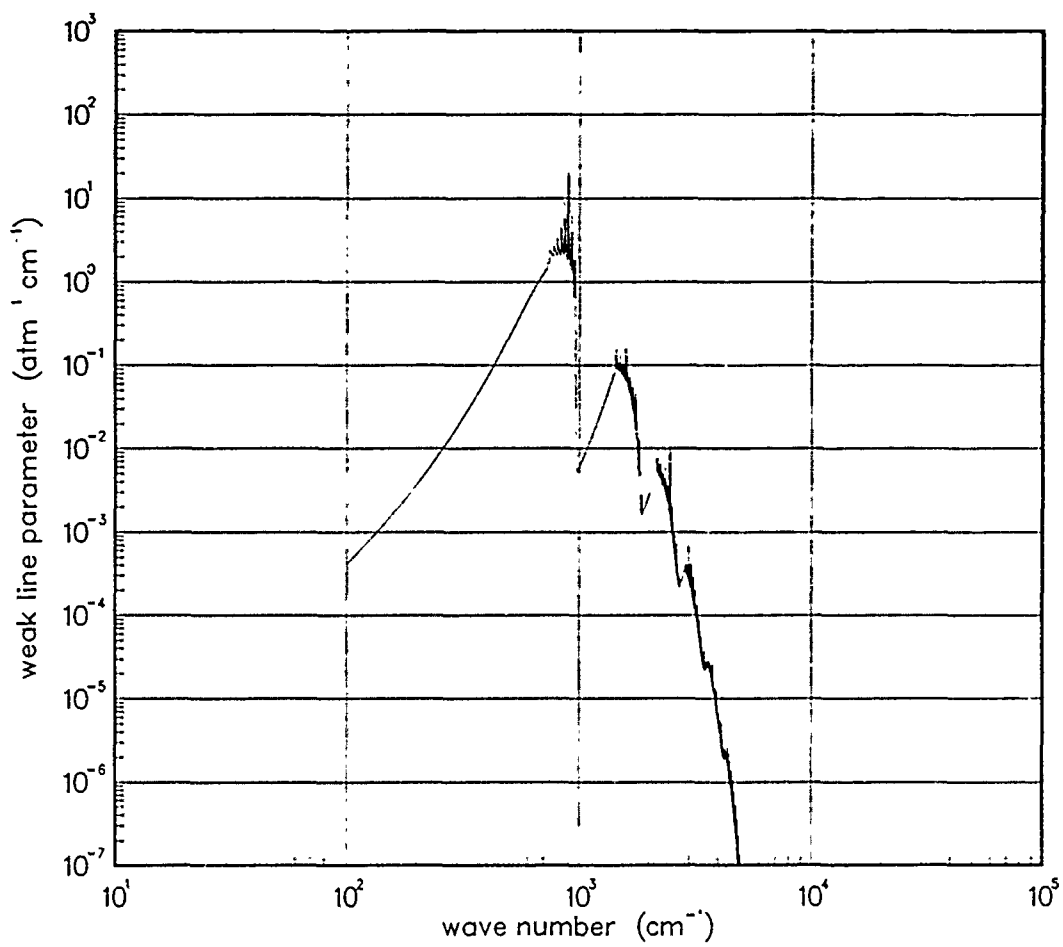


Figure 524. Weak-line parameter for UO^+ at 18000°K .

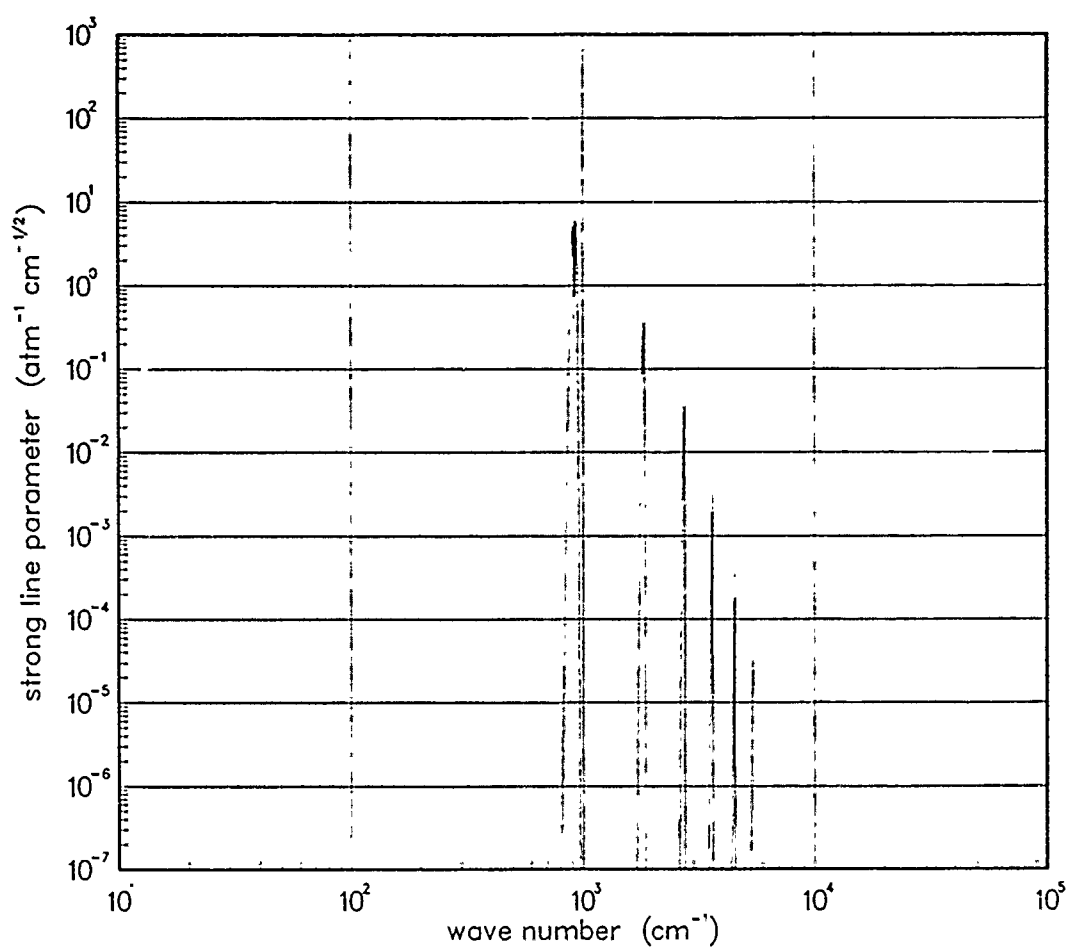


Figure 525. Strong-line parameter for UO^+ at 200°K .

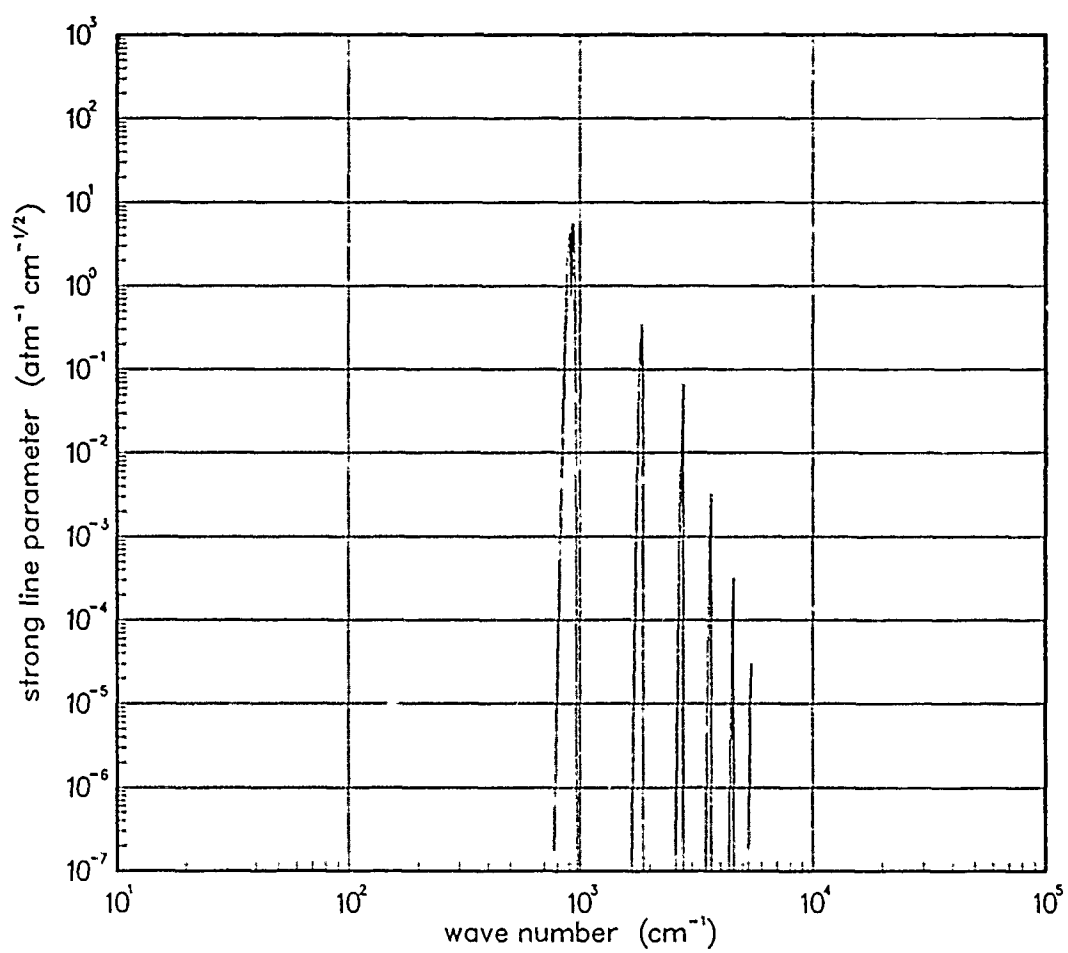


Figure 526. Strong-line parameter for UO^+ at 300°K .

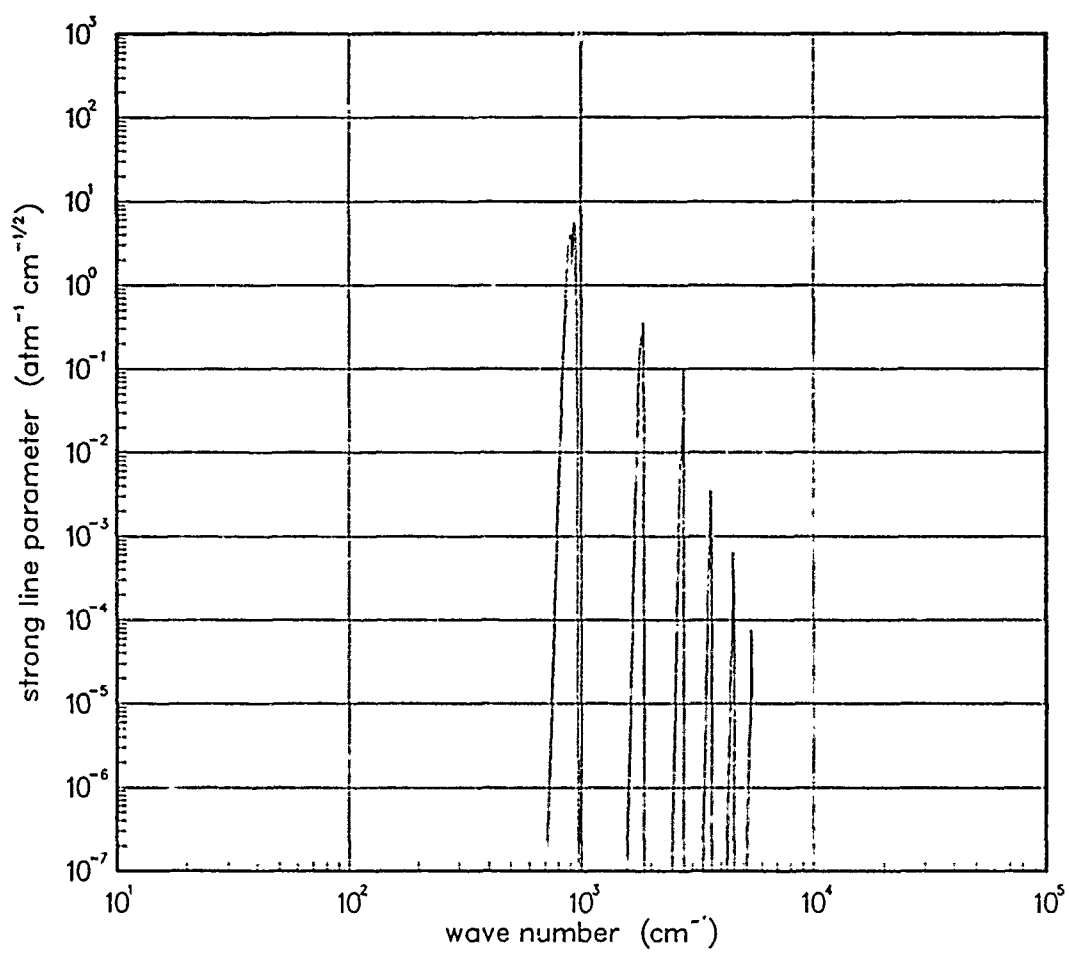


Figure 527. Strong-line parameter for UO^+ at 500°K .

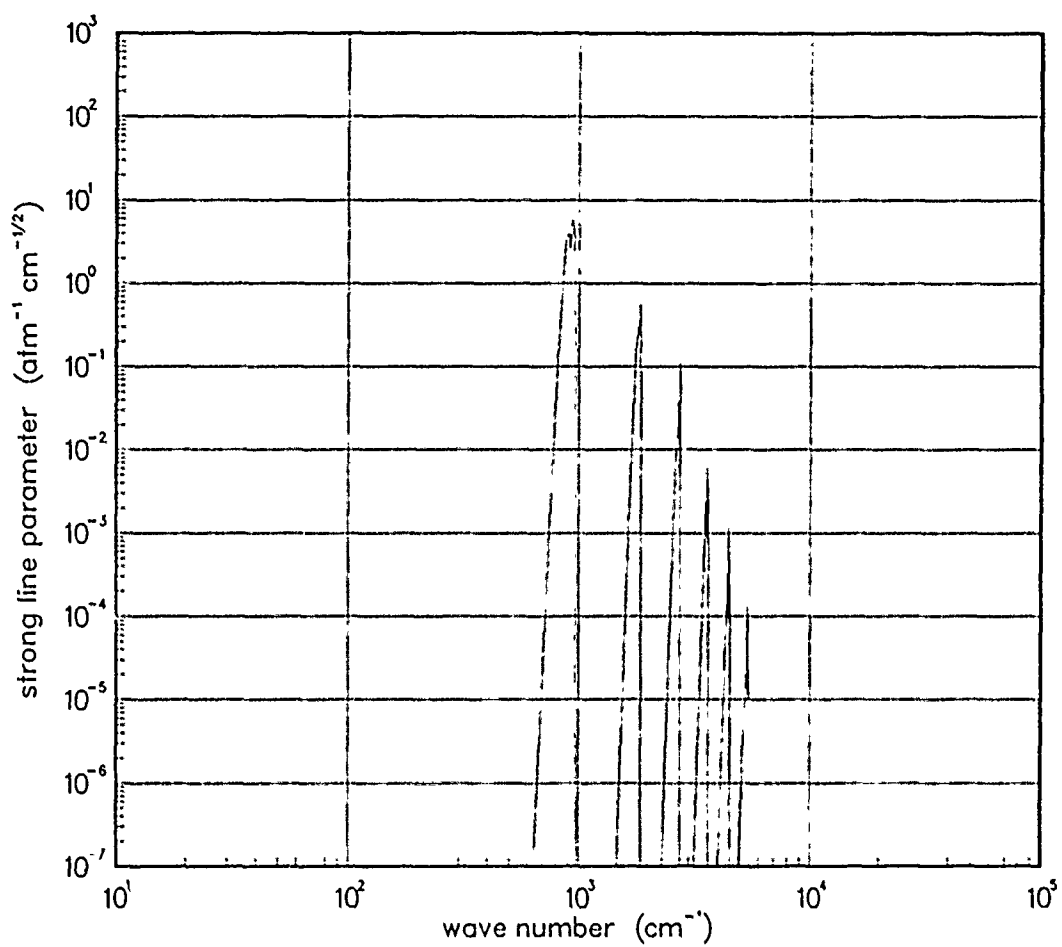


Figure 528. Strong-line parameter for UO^+ at 750°K .

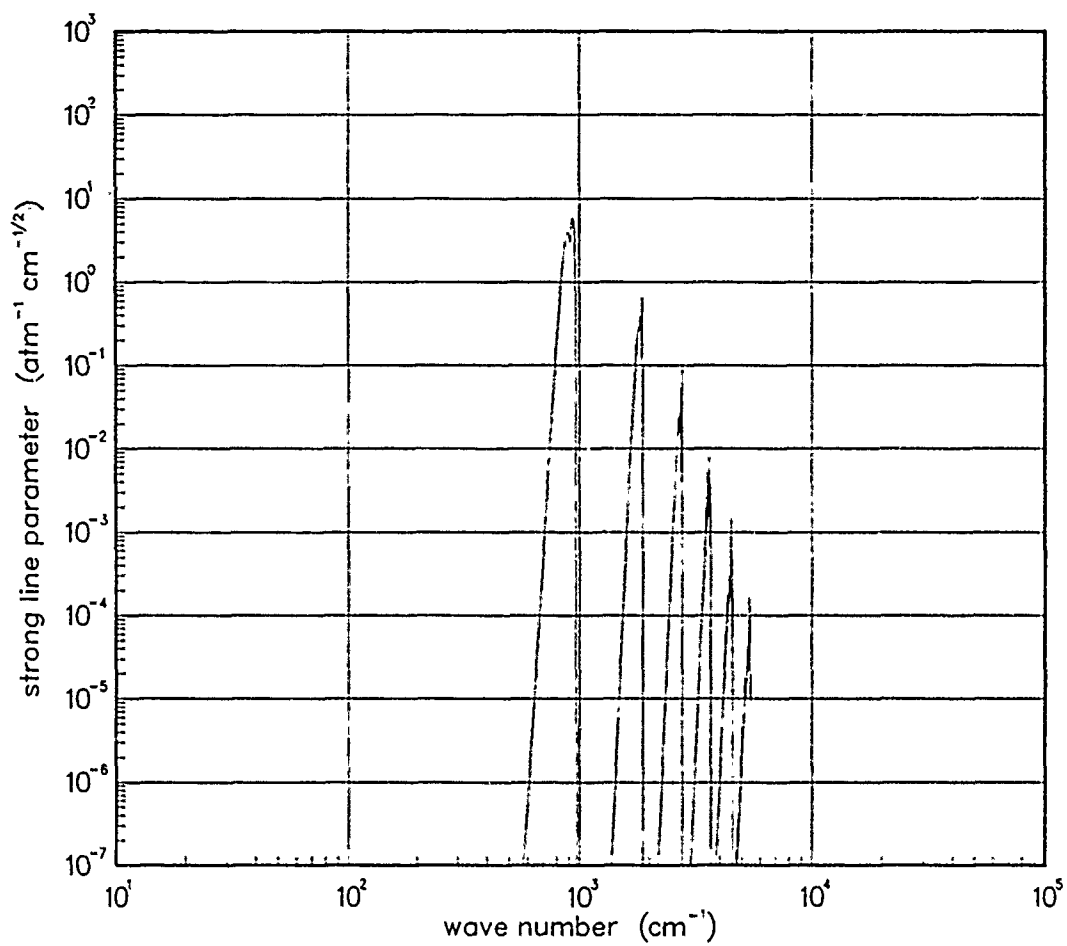


Figure 529. Strong-line parameter for UO^+ at 1000°K .

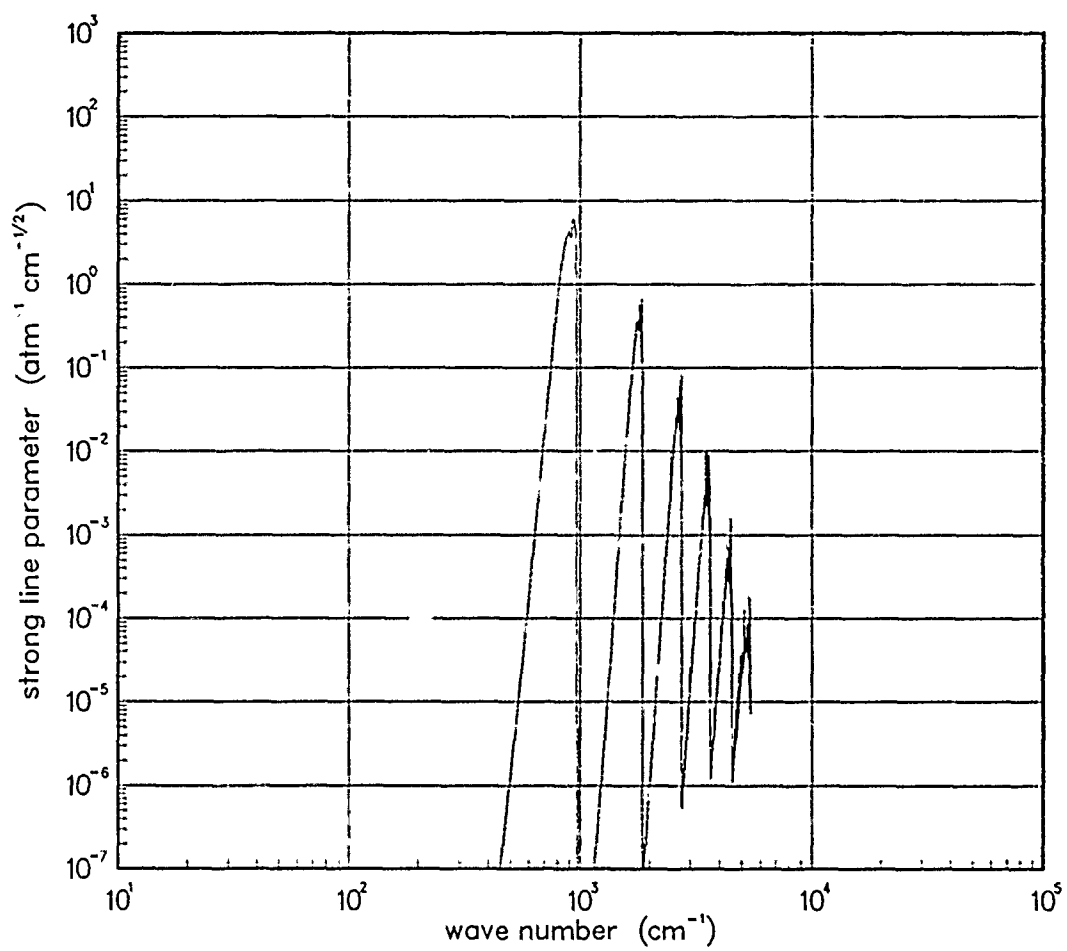


Figure 530. Strong-line parameter for UO^+ at 1500°K .

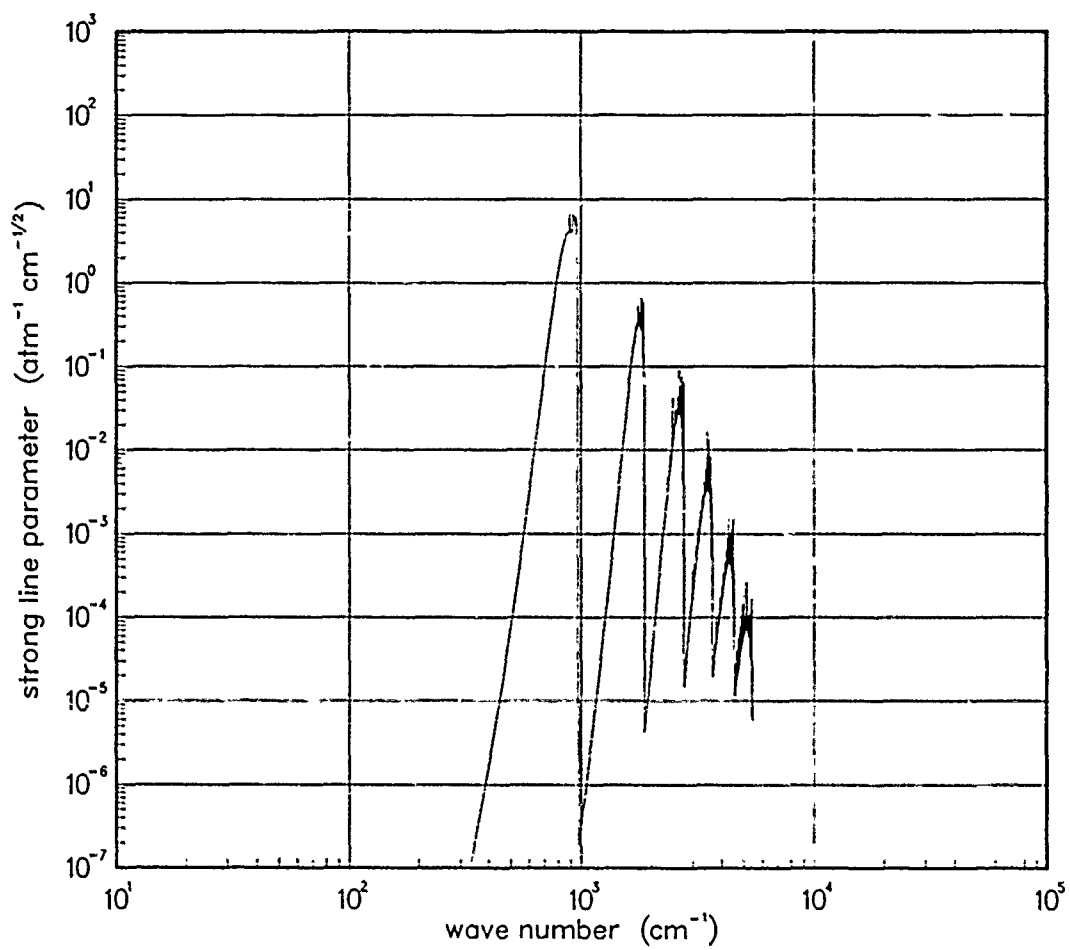


Figure 531. Strong-line parameter for UO^+ at 2000°K .

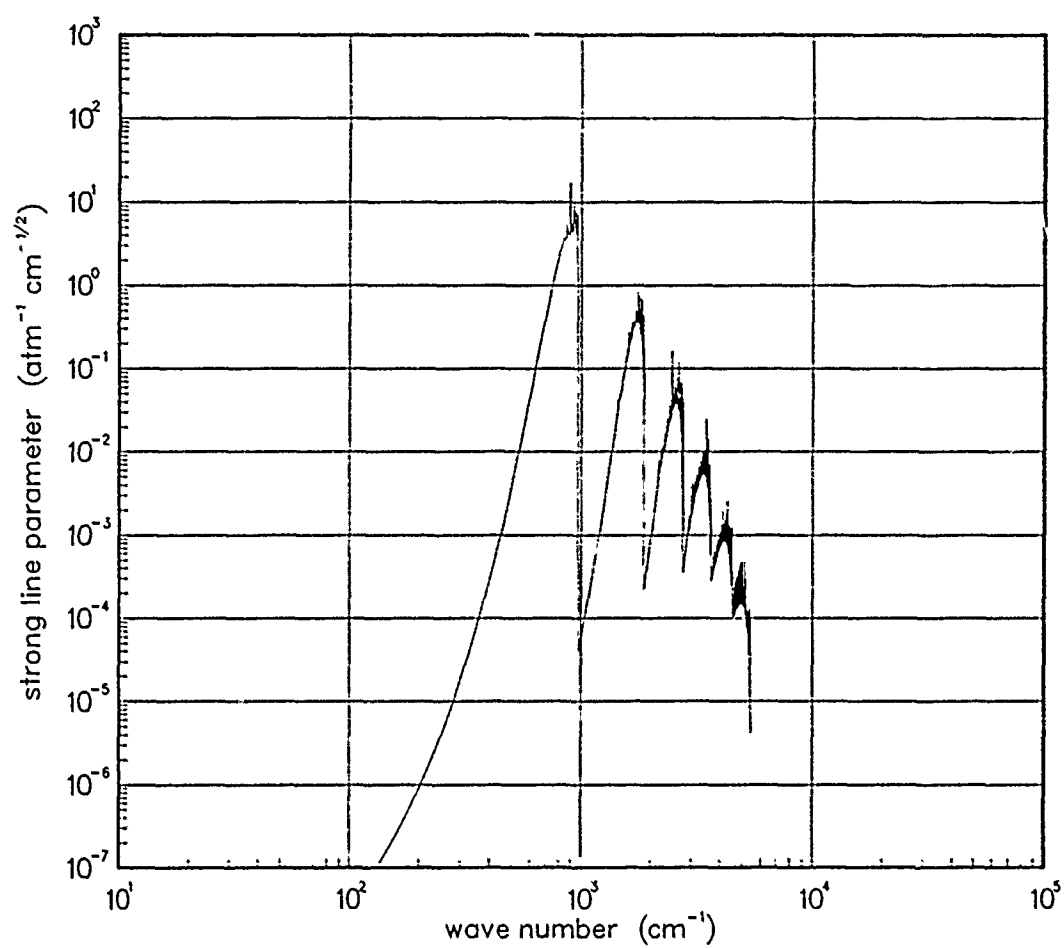


Figure 532. Strong-line parameter for UO^+ at 3000°K .

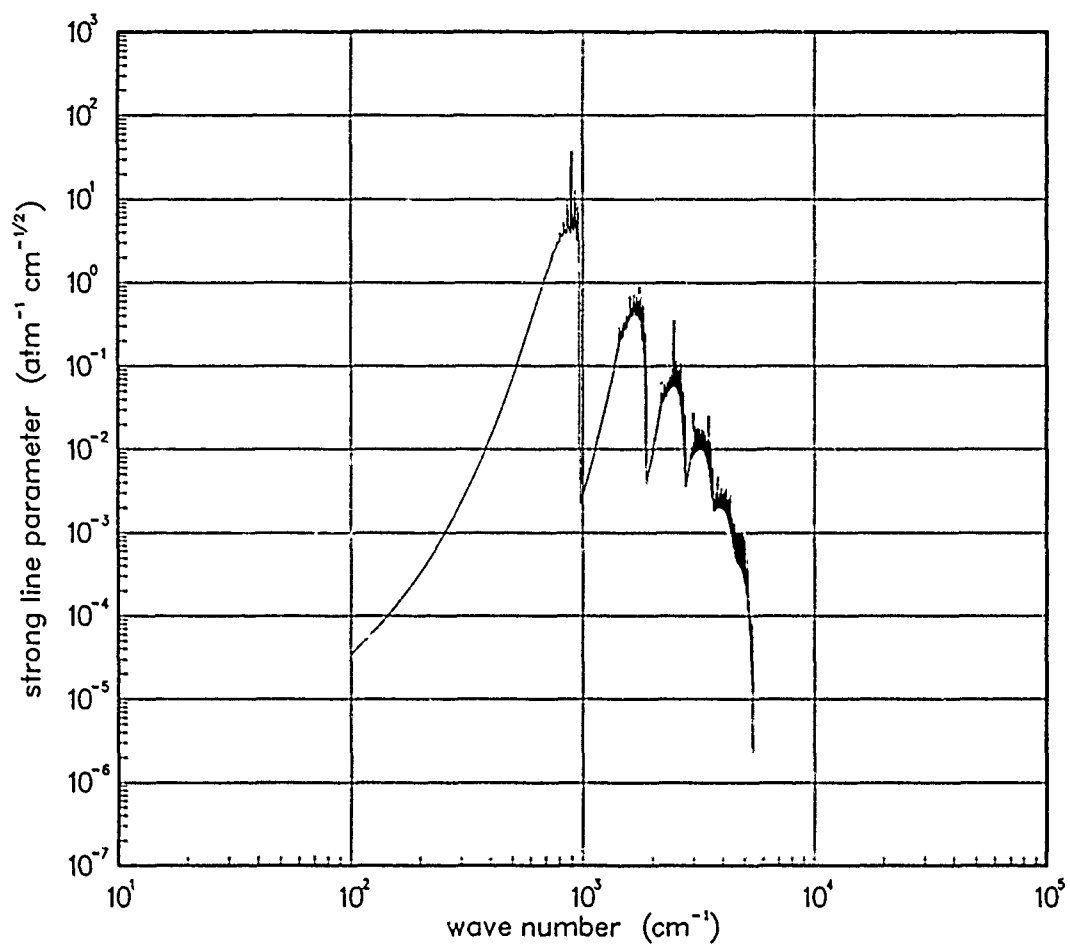


Figure 533. Strong-line parameter for UO^+ at 5000°K .

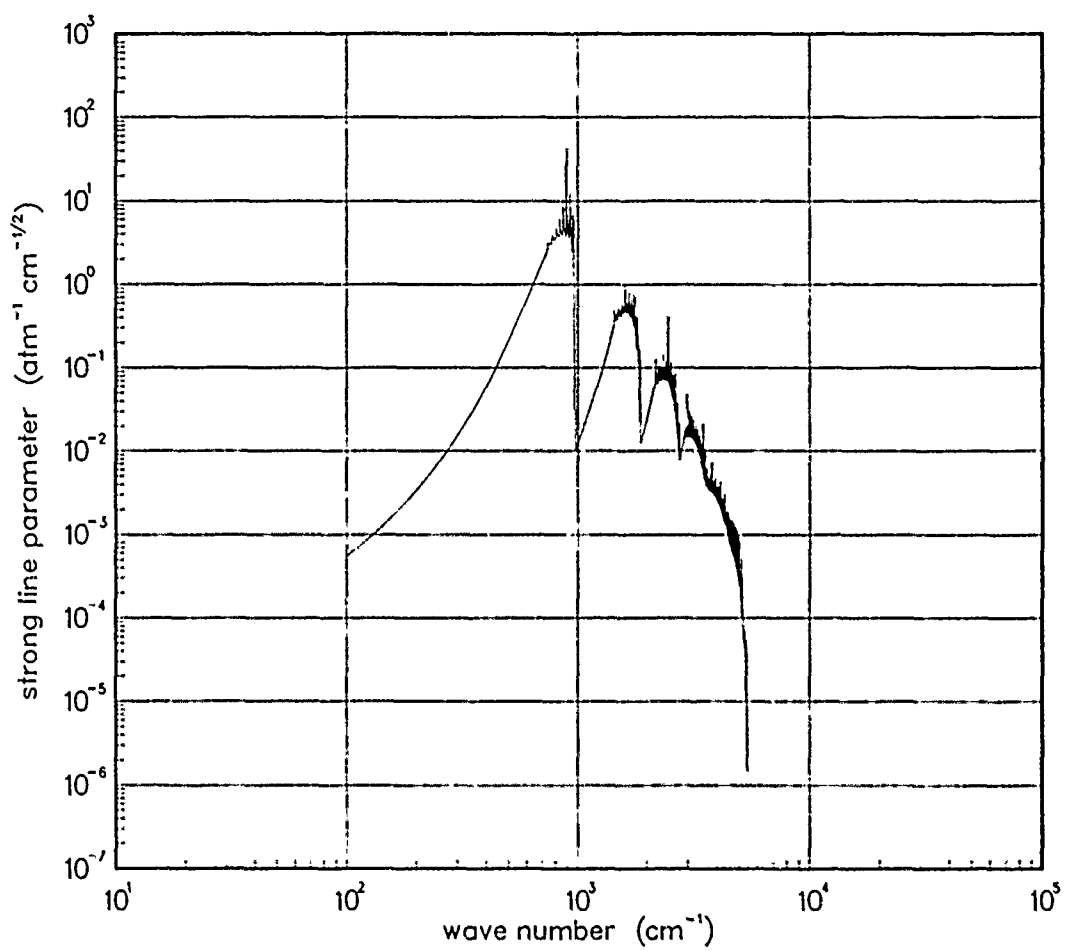


Figure 534. Strong-line parameter for UO^+ at 7000°K .

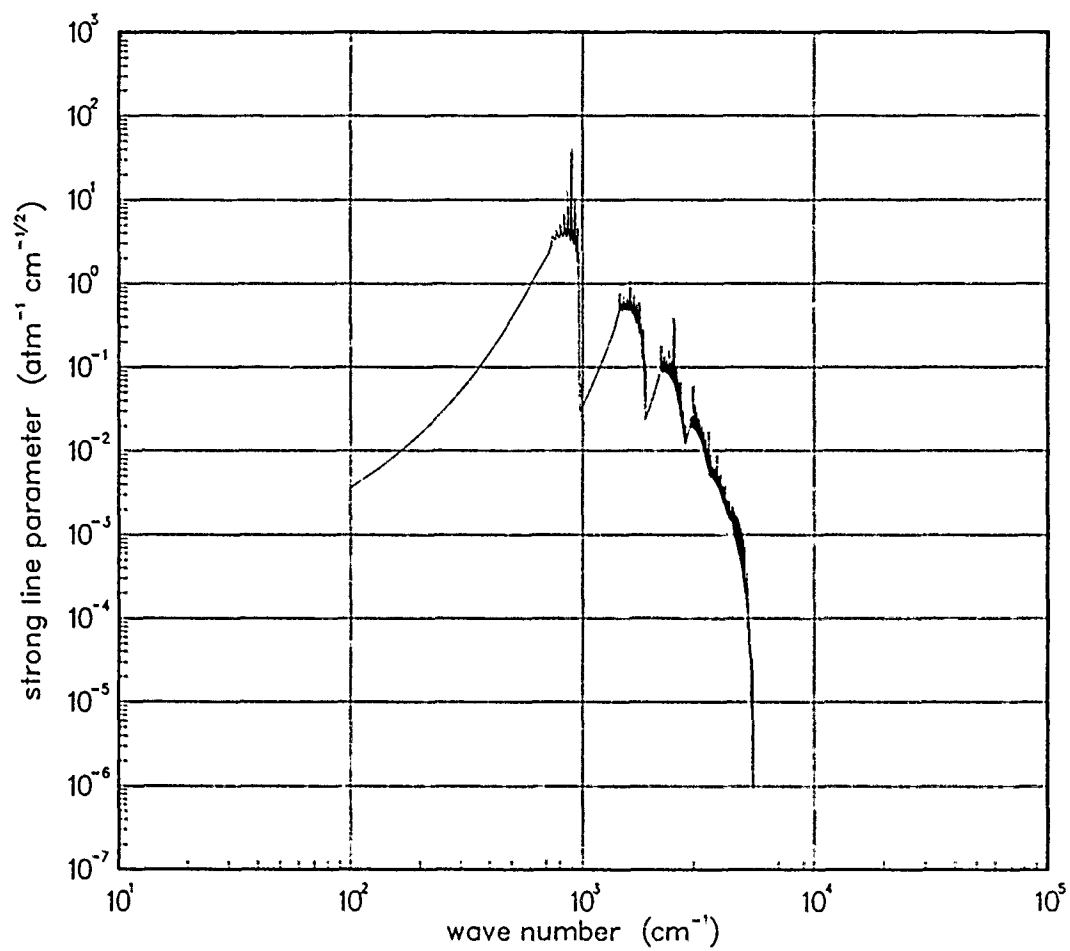


Figure 535. Strong-line parameter for UO^+ at 10000°K .

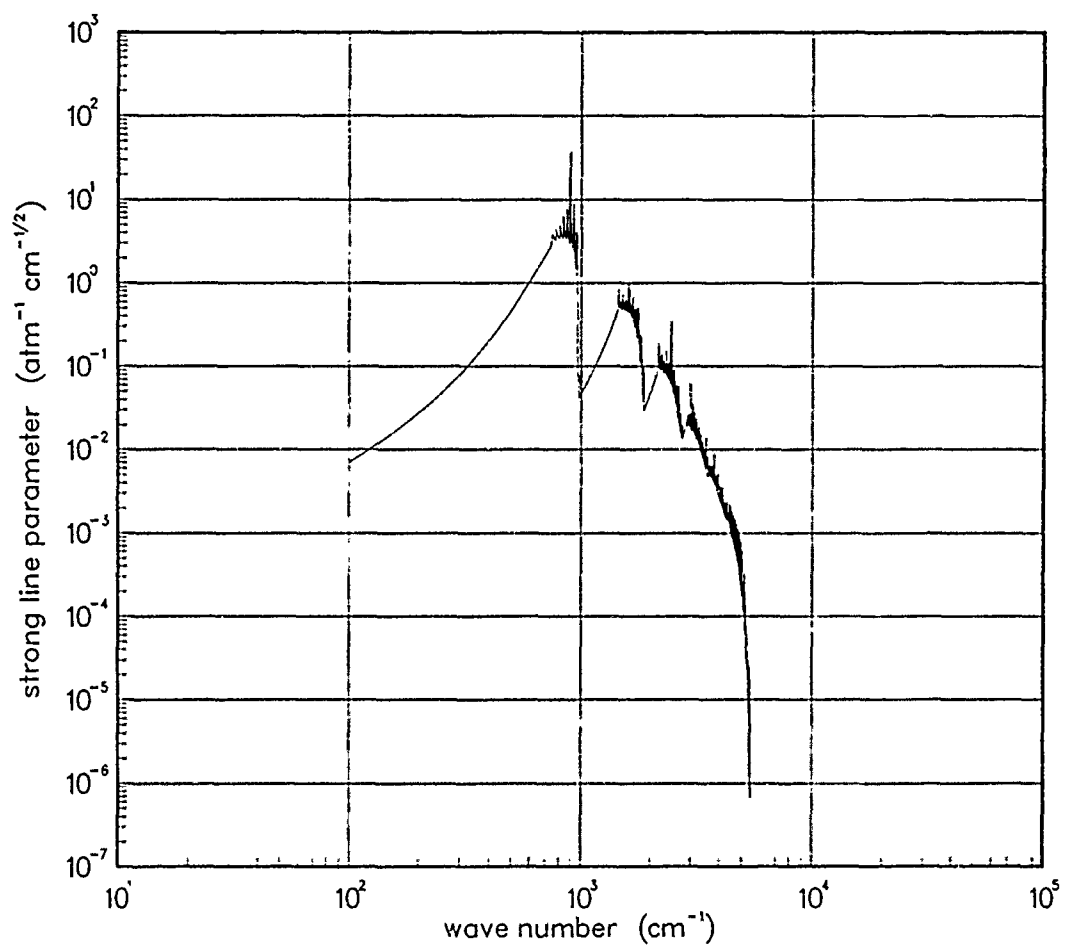


Figure 536. Strong-line parameter for UO^+ at 12000°K .

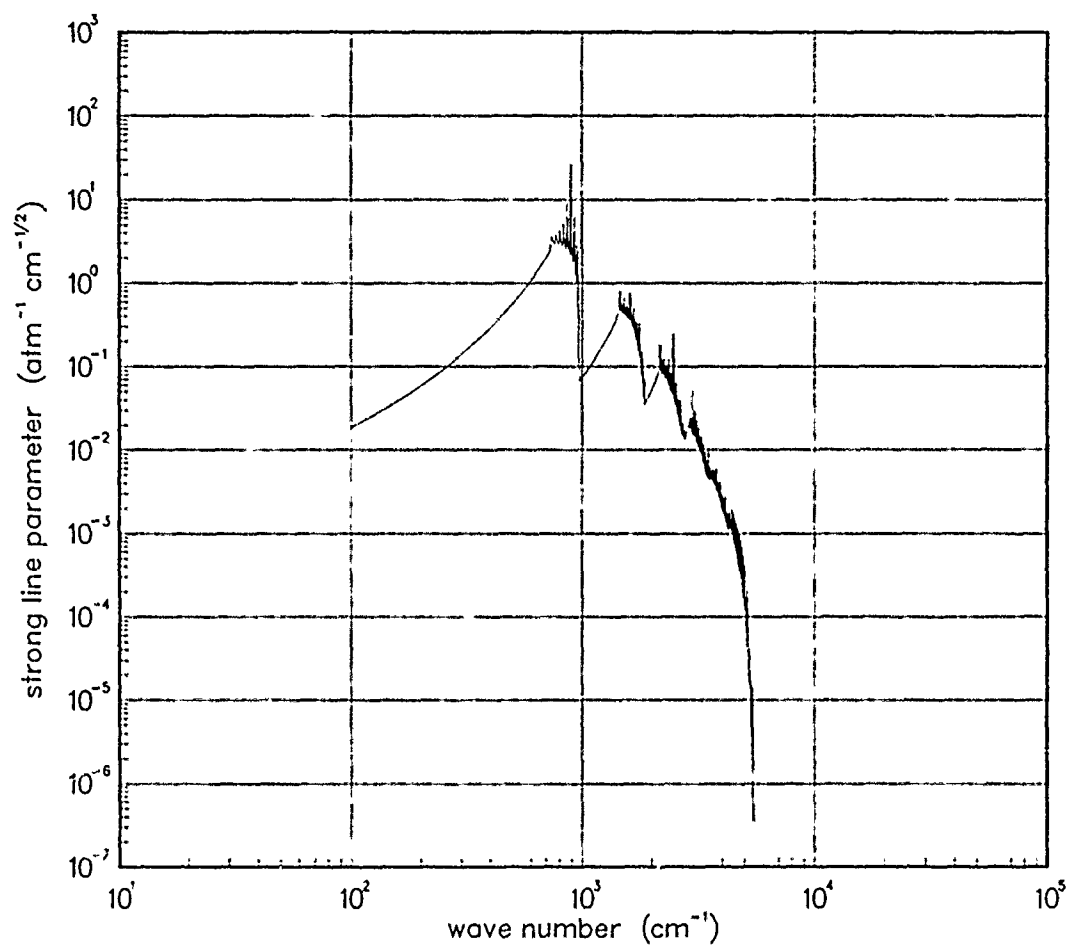


Figure 537. Strong-line parameter for UO^+ at 18000°K .

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APPENDIX A
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APPENDIX B

GLOSSARY

NORSE	<u>N</u> uclear and <u>O</u> ptical <u>R</u> adar and <u>S</u> ystems <u>E</u> ffects code.
LTE	<u>L</u> ocal <u>T</u> hermal <u>E</u> quilibrium.
DEI	Inverse line spacing.
SOD	<u>S</u> trength <u>O</u> ver line spacing (<u>D</u> istance).
RADFLO	<u>R</u> ADiation <u>F</u> LOW Code.
LINTRA	<u>L</u> INear <u>T</u> RIAtomic smeared band model.
WOE	<u>W</u> eapons <u>O</u> ptical <u>E</u> ffects code.
TATE	<u>T</u> RIAtomic <u>T</u> hermal <u>E</u> missions code.
STP	<u>S</u> tandard <u>T</u> emperature and <u>P</u> ressure.

APPENDIX C

LIST OF SYMBOLS

A	Area
A	Malkmus strong-line parameter
A_L	Effective band width
$\bar{A}_{ij}$	Effective line width
a_ν	Line absorption coefficient
$a_{\nu ij}$	Line absorption coefficient where ij indicates the upper and lower levels involved in the line transition
b_{ij}	Line profile
E_a	Energy absorbed
E_e	Energy emitted
I_ν	Intensity at energy ν
I_ν^b	Blackbody emission intensity, at energy ν
P	Pressure
$P(S)$	Probability distribution function
T	Temperature, Absolute
s	Path length
u	Adjusted path length
x	Mole fraction
γ_d	Doppler width
γ_L	Lorentzian width
ν	Energy
Ω	Solid angle

LIST OF SYMBOLS (Continued)

ω_e	Spectroscopic constant
$\omega_e x_e$	Spectroscopic constant
α_e	Spectroscopic constant
B_e	Spectroscopic constant
A_e	Spectroscopic constant
S_{10}	Band Strength 1-0 transition
S_{20}	Band Strength 1-0 transition
S_{30}	Band Strength 1-0 transition
γ_e	Lorentz Line Width

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