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THE ROSCOE MANUAL, VOLUME 28-1. MOLECULAR BAND MODEL PARAMETERS--ETC(U)

JAN 81 T L STEPHENS; A L KLEIN

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# THE ROSCOE MANUAL

## Volume 28-1-Molecular Band Model Parameters For Thermal Emissions: Expanded Wavelength Coverage

Kaman Tempo  
816 State Street (P.O. Drawer QQ)  
Santa Barbara, California 93102

31 January 1981

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)			
Band Model	Nitrous Oxide	Carbon Monoxide	Metal Oxides
Infrared	Nitrogen Dioxide	Methane	ROSCOE Code
Absorption	Ozone	Water Vapor	
Nitric Oxide	Carbon Dioxide	Hydroxyl	
20. ABSTRACT (Continue on reverse side if necessary and identify by block number)  The spectral range of band model parameters for the ROSCOE thermal emission has been extended to cover the 2- to 100-micron region. Sources for the new parameter compilation are documented, and graphical representations of the parameters at selected temperatures are presented.			

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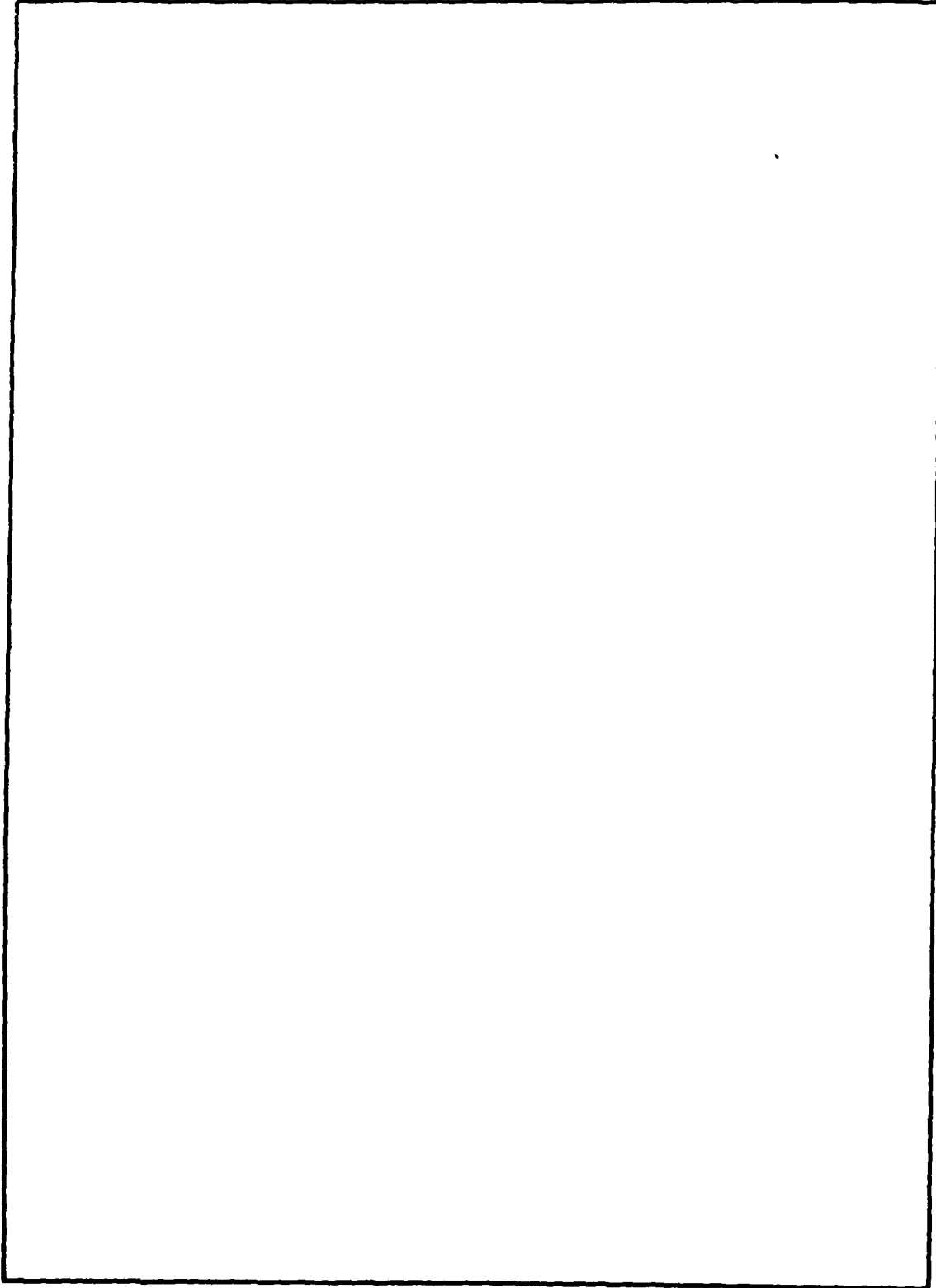
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SECTION 1  
INTRODUCTION

The molecular thermal emission model in ROSCOE is documented in Volume 28, *Molecular Band Models for Thermal and Optically Pumped Emissions*. Thermal emissions arise under conditions of local thermodynamic equilibrium (LTE). These conditions occur when collisions are sufficiently frequent to maintain equilibrium. The use of Kirchhoff's law to obtain emission from absorption, which applies in this situation, is discussed in Volume 31, *Sight Path Integration*.

The original model covered only the 2- to 5-micron region (SWIR). The present work expands the data base used by the model to LWIR wavelengths. Band model parameters are now provided for the 2- to 100-micron spectral range. In addition parameters for metal oxides have been added and parameters for certain other molecules have been upgraded.

Section 2 documents the sources used for the revised parameter set as a function of species, wavelength and temperature. In addition the weak line and strong line parameters (describing absorption in optically thin and thick regions respectively) are shown graphically at temperatures of 300 and 3000 K.

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## SECTION 2 LTE MOLECULAR BAND SHAPES

### MODEL IMPLEMENTATION IN ROSCOE

The ROSCOE model for LTE (local thermodynamic equilibrium) molecular band emission and absorption is documented in Reference 2-1. In its original form the model was developed only for the SWIR spectral region between 2000 and 5000  $\text{cm}^{-1}$  (2 to 5 microns). In the present effort, the spectral coverage of the model was extended to the LWIR. This was accomplished primarily by augmenting the data base containing weak line and strong line parameters for the molecular species of interest.

The revised data tape contains parameters for the species listed in Table 2-1. The spectral coverage now extends from 100 to 5000  $\text{cm}^{-1}$  (2 to 100 microns). The data base, however, does not contain contributions from pure rotational bands of several species, which are important at wavelengths beyond 25 microns. (The pure rotational contributions of  $\text{H}_2\text{O}$  are included in the data base; these are important at wavelengths shorter than 25 microns.) Therefore, the revised data base can be used with confidence in the wavelength region between 2 and 25 microns. Other aspects of the data tape, such as the 5  $\text{cm}^{-1}$  wave number resolution and the 200 to 7000 K temperature coverage, remain unchanged from Reference 2-1.

Although band model parameters have been provided for 19 species in the new data set, thermal emission and absorption in ROSCOE are still calculated only for the 10 species originally included in the code (denoted by "a" in the last column of Table 2-1). Since the parameters for other species (primarily metal oxides) were available on the WOE II data tape (Reference 2-2), they were incorporated into ROSCOE for use at a future time when concentrations of these additional species may be calculated.

The Lorentz half-width for pressure-broadened molecular lines is required by the ROSCOE LTE band model. The Lorentz half-width used in the revised model,  $\alpha_L^i(\text{STP})$  on page 12 of Reference 2-1, can be determined from Table 2-1 according to the relation

$$\alpha_L^i(\text{STP}) = \alpha_L^i(T_{\text{ref}}) \sqrt{T_{\text{ref}}/273} \quad (2-1)$$

Values for  $\alpha_L^i(T_{\text{ref}})$  and  $T_{\text{ref}}$  are given in Table 2-1.

### MOLECULAR BAND SHAPE PARAMETERS

The development of the molecular band shape parameter data set used in the revised ROSCOE model has been described in Section 6 of Reference 2-2. Table 2-2, taken from Reference 2-2, summarizes the sources of data used in the model.

The revised parameters generated according to the procedure described in Reference 2-2 have not been previously published. Graphical representations of these parameters at two selected temperatures (300 and 3000 K) are therefore included

Table 2-1. Lorentz half-width parameters.

Species	$\alpha_L^i(T_{ref})$	$T_{ref}$	Source (See Notes)
AlO	0.04	300	b
CH <sub>4</sub>	0.06	273	a
CO	0.06	273	a
CO <sub>2</sub>	0.07	273	a
CuO	0.04	300	b
FeO	0.04	300	b
H <sub>2</sub> O	0.04	273	a
HNO <sub>3</sub>	0.05	273	c
LiO	0.04	300	b
MgO	0.04	300	b
NO	0.04	273	a
NO <sup>+</sup>	0.04	273	a
N <sub>2</sub> O	0.08	273	a
NO <sub>2</sub>	0.10	273	a
OH	0.06	273	a
O <sub>3</sub>	0.11	273	a
SiO	0.04	300	b
TiO	0.04	300	b
UO	0.04	300	b

Notes:  
<sup>a</sup>Unchanged from Reference 2-1.  
<sup>b</sup>See Section 5 of Reference 2-3.  
<sup>c</sup>Reference 2-4.

as Figures 2-1 to 2-38. The data compilation consists of the two parameters,

- SOD, the average line strength
- DEI, the reciprocal of the effective line spacing,

which are defined explicitly in Equations 2-7 and 2-8 of Reference 2-1.

Figures 2-1 through 2-38 show the weak line parameters

SOD

and the strong line parameters

Table 2-2. Sources of LTE band shape data.

Species	Spectral Range (cm <sup>-1</sup> )		
	400 - 2000	2000 - 5000	5000 +
Diatomics	D	D/R	D
Metal oxides	D	D	-
NO <sub>2</sub> , O <sub>3</sub>	T	T/R	-
N <sub>2</sub> O, CH <sub>4</sub> (T < 500 K)	A	A/R	-
N <sub>2</sub> O (T > 500 K)	B/WF	B/WF	-
CO <sub>2</sub> (T < 500 K)	T	T	A
CO <sub>2</sub> (T > 500 K)	T	T	-
H <sub>2</sub> O (T < 500 K)	A	A/R	A/WA
H <sub>2</sub> O (T > 500 K)	L/WF	L/R	L/WF
HNO <sub>3</sub> (T < 300 K)	G	-	-

Notes:

D = DATE (Diatomic Thermal Emission) code (Reference 2-3)  
R = Data same as ROSCOE-IR (Reference 2-1)  
T = TATE (Triatomic Thermal Emission) code (Reference 2-3)  
A = AFGL line-by-line data tape (Reference 2-5)  
B = Boxcar (rectangular) band shape  
WF = Retained old WOE fireball model (Reference 2-6)  
WA = Retained old WOE ambient model (Reference 2-7)  
L = Data obtained by Ludwig, et al (Reference 2-8)  
G = Data obtained by Goldman, et al (Reference 2-4).

$$2(\alpha_L^i \cdot \text{SOD} \cdot \text{DEI})^{1/2}$$

for each molecule for the temperatures 500 and 3000 K. In each case the curves labeled "1" represent the 500 K value, and the curves labeled "2" represent the 3000 K value. The Lorentz half-width  $\alpha_L^i$  is determined according to

$$\alpha_L^i = \alpha_L^i(\text{STP})\sqrt{273/T} \quad (2-2)$$

(The weak line parameter describes absorption for optically thin paths; the strong line parameter describes absorption for thick paths. In particular, the strong line parameter defines the square root region of the curve of growth for a statistical band.) Parameter values less than 10<sup>-7</sup> are not shown in the figures; horizontal lines at 10<sup>-7</sup> are artifacts of the plotting routine.

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- 2-1. Stephens, T.L., V.R. Stull, A.L. Klein, and J.D. Losse, *The AFOSR Manual, Volume 28—Molecular Band Models for Thermal and Optical Property Prediction*, Unpublished.
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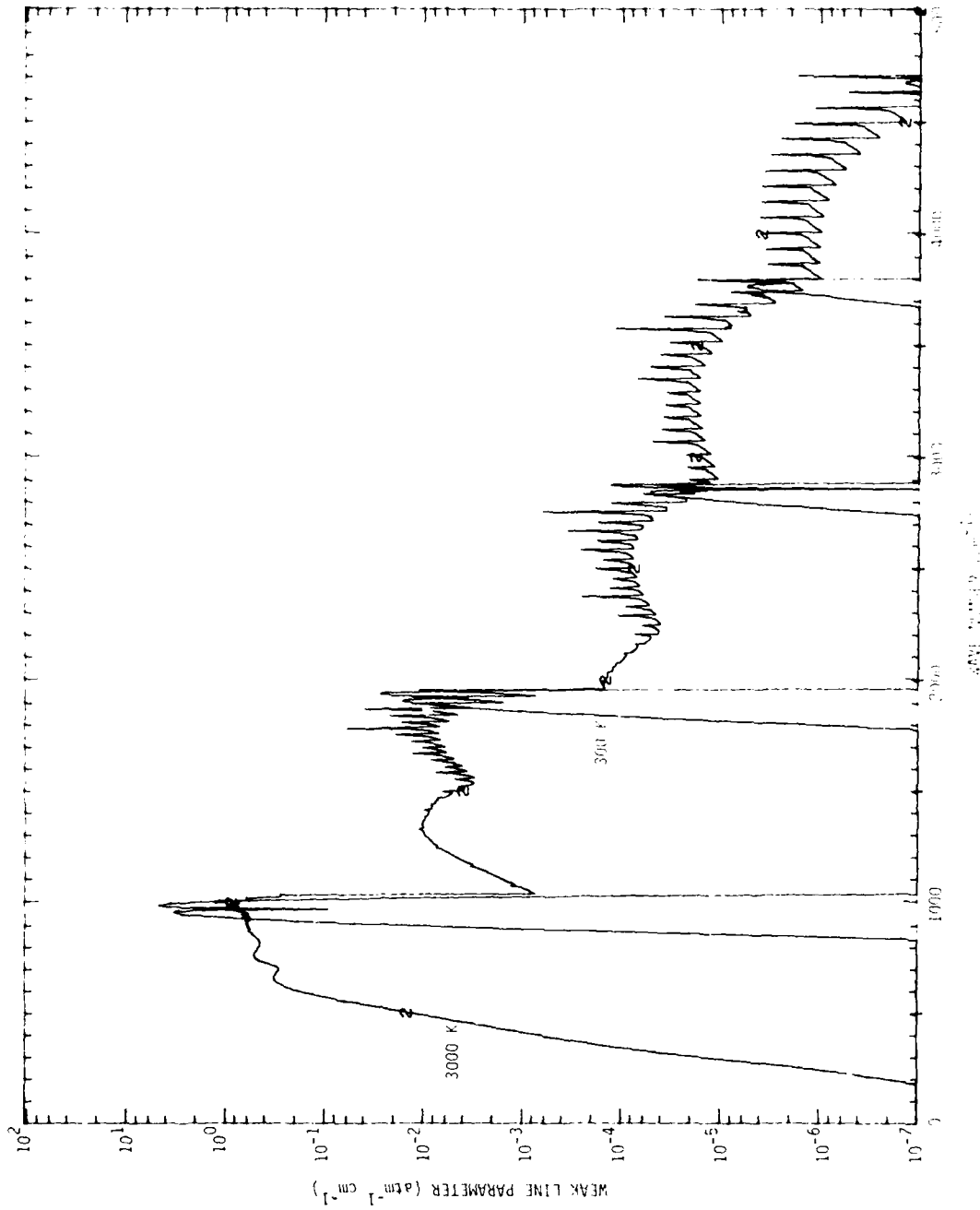


Figure 2-1. Weak line parameters for AsO.

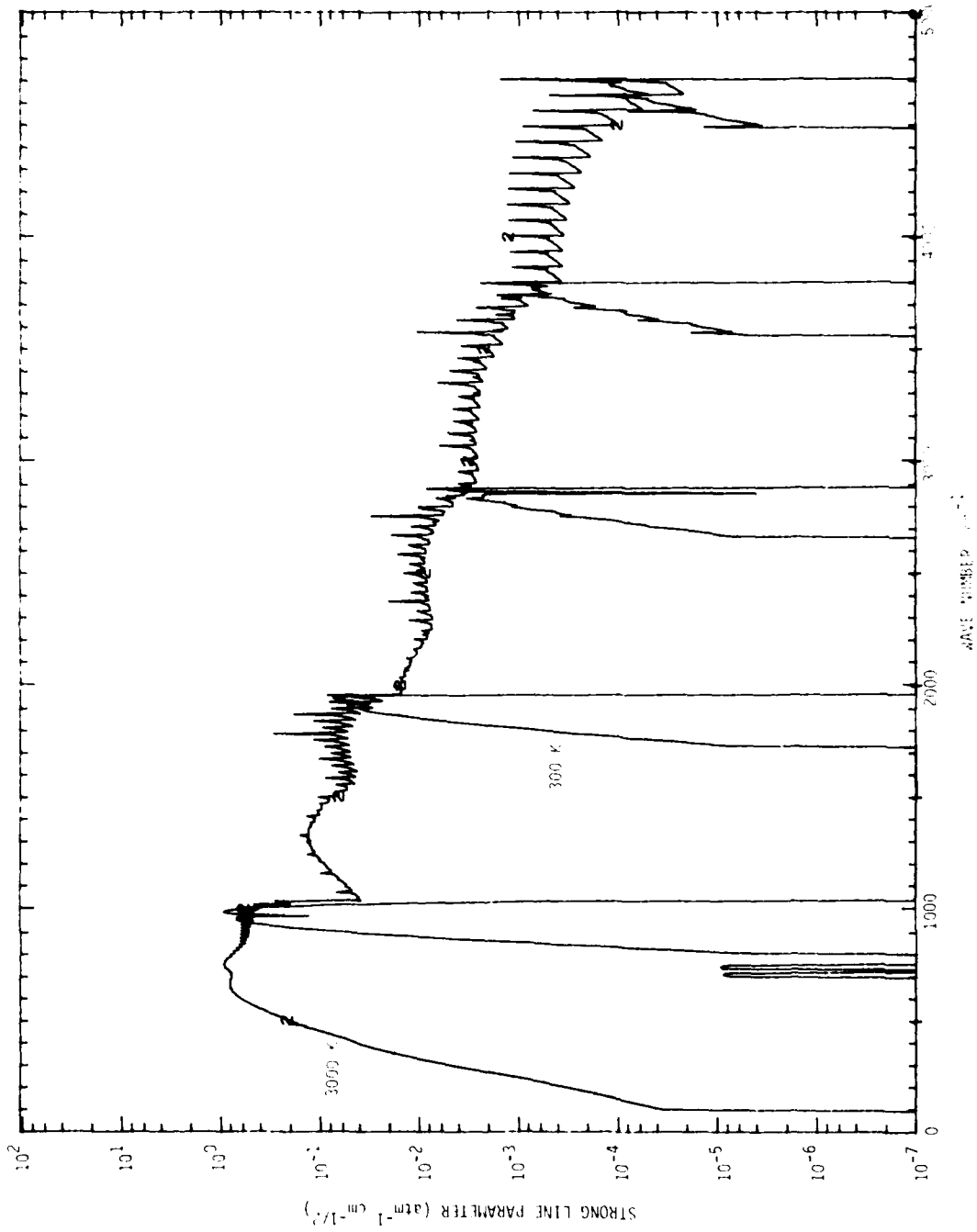


Figure 2-2. Strong line parameters for A00.

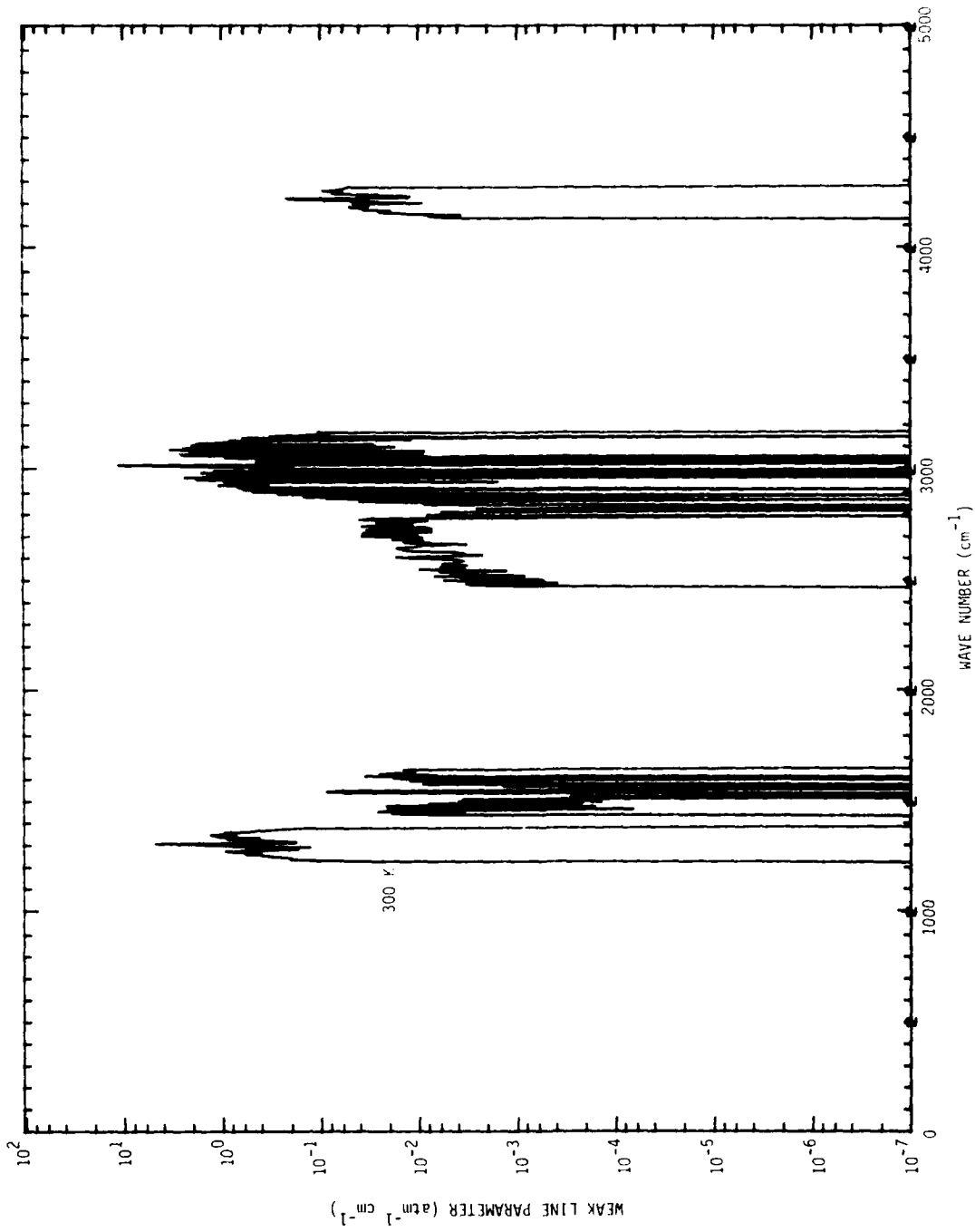


Figure 2-3. Weak line parameters for CH<sub>4</sub>.



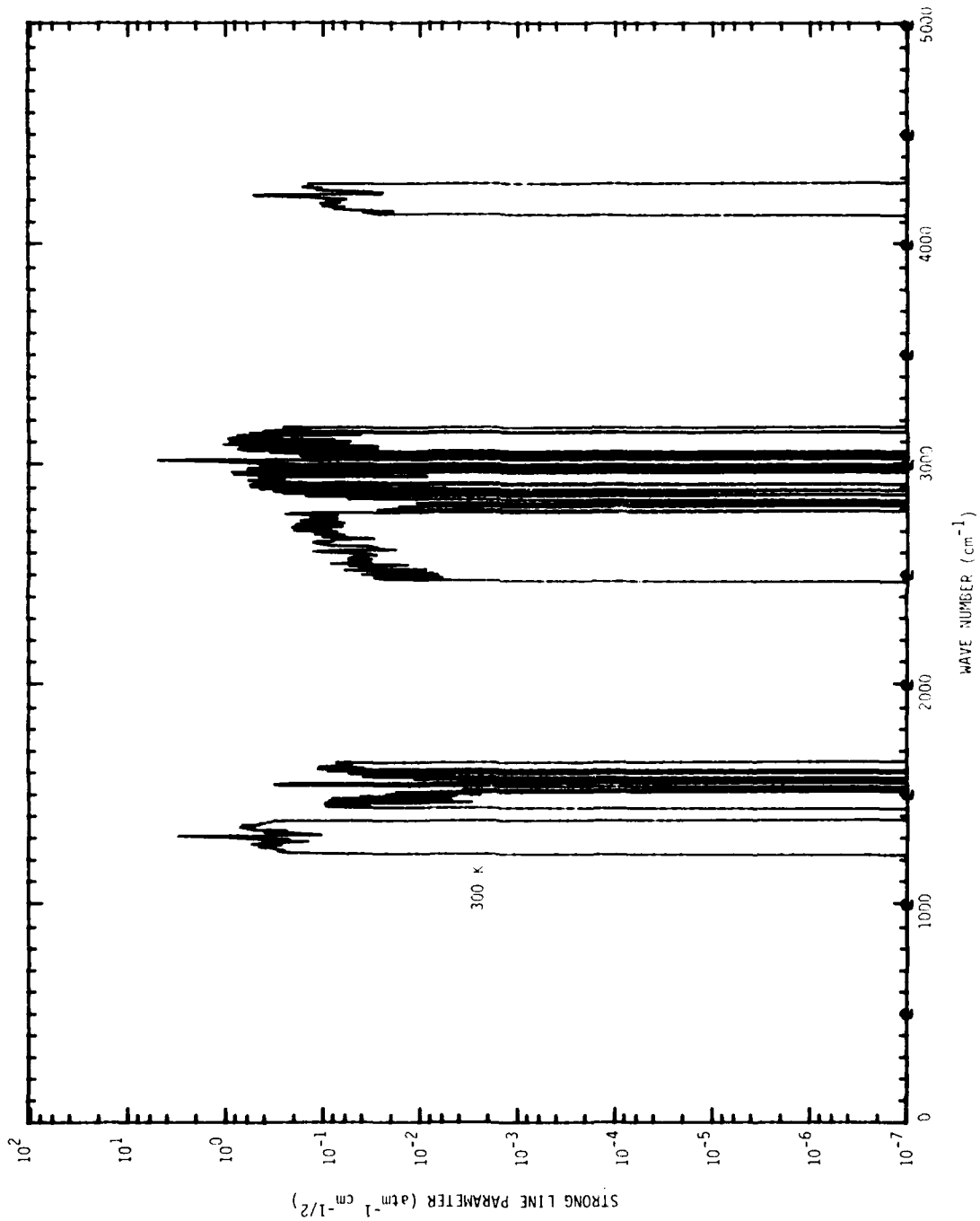


Figure 2-4. Strong line parameters for CH<sub>4</sub>.

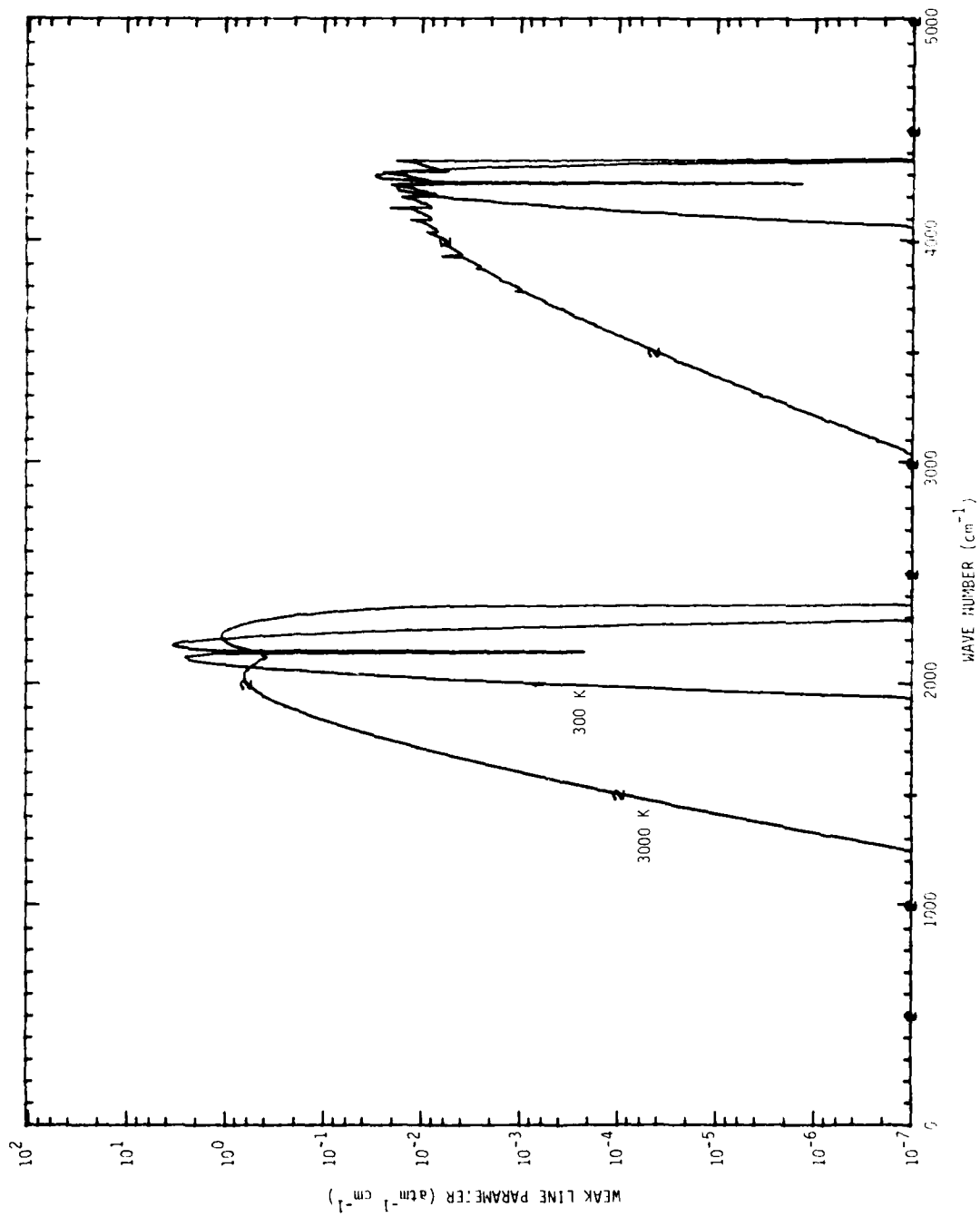


Figure 2-5. Weak line parameters for CO.

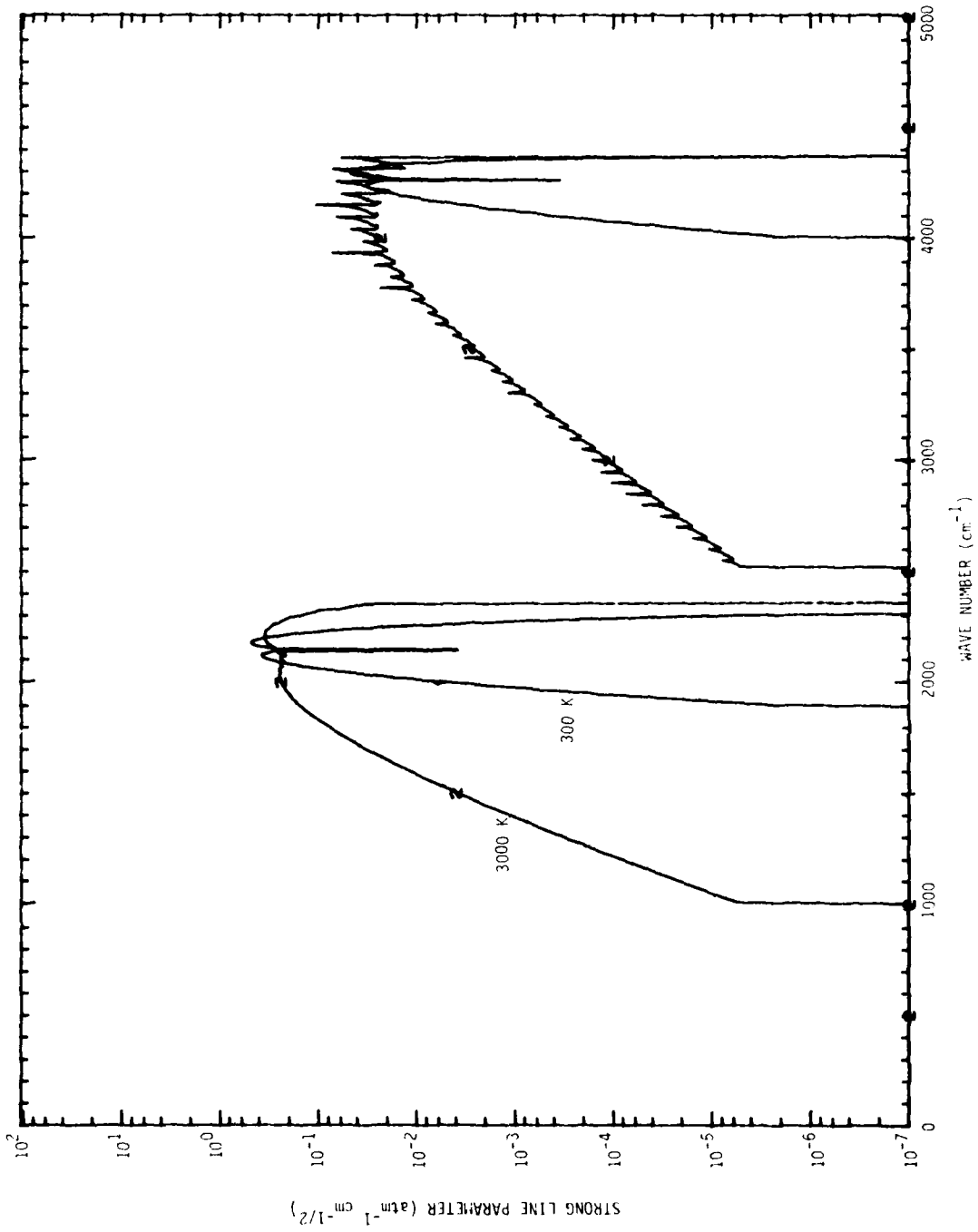


Figure 2-6. Strong line parameters for CO.

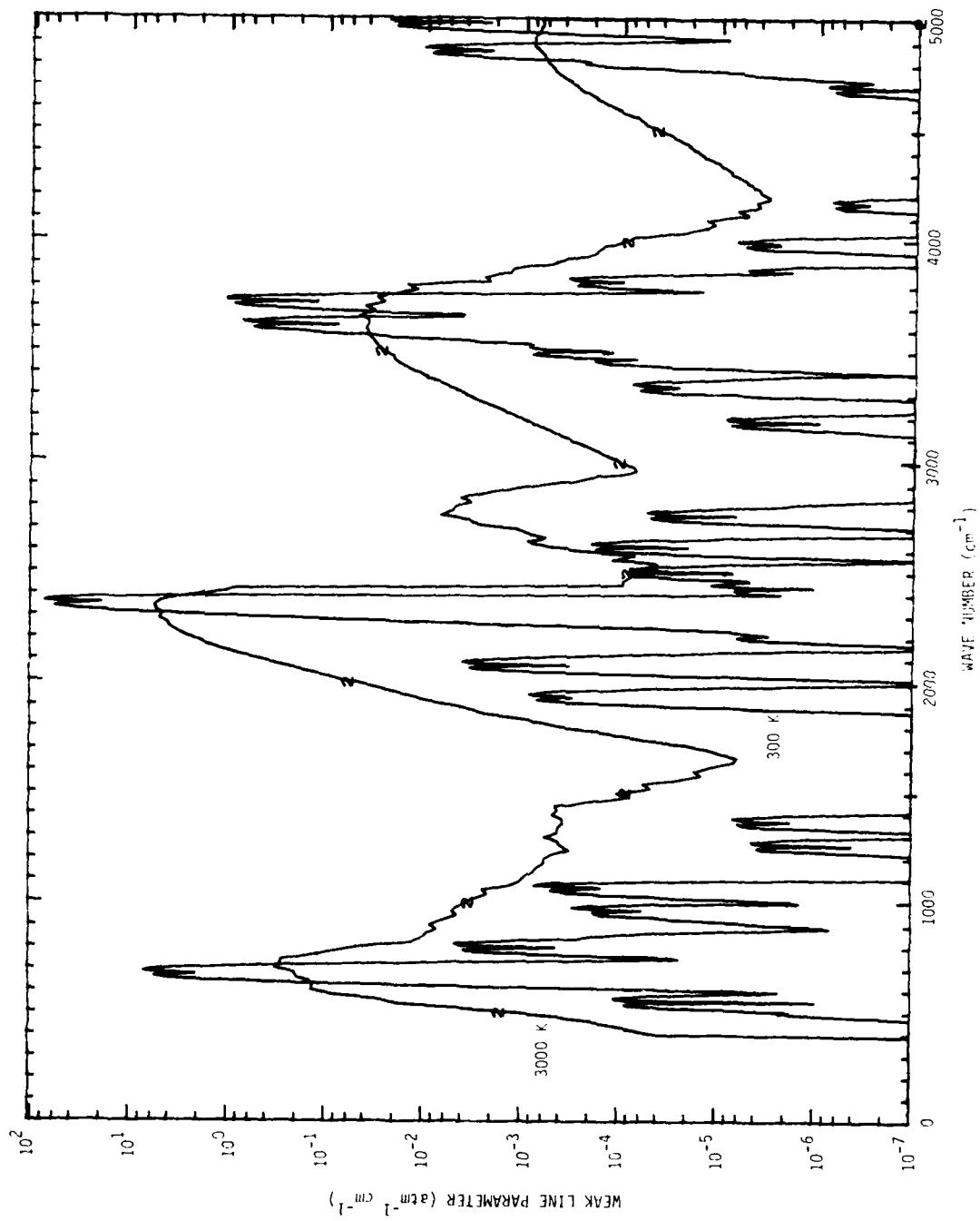


Figure 2-7. Weak line parameters for CO<sub>2</sub>.

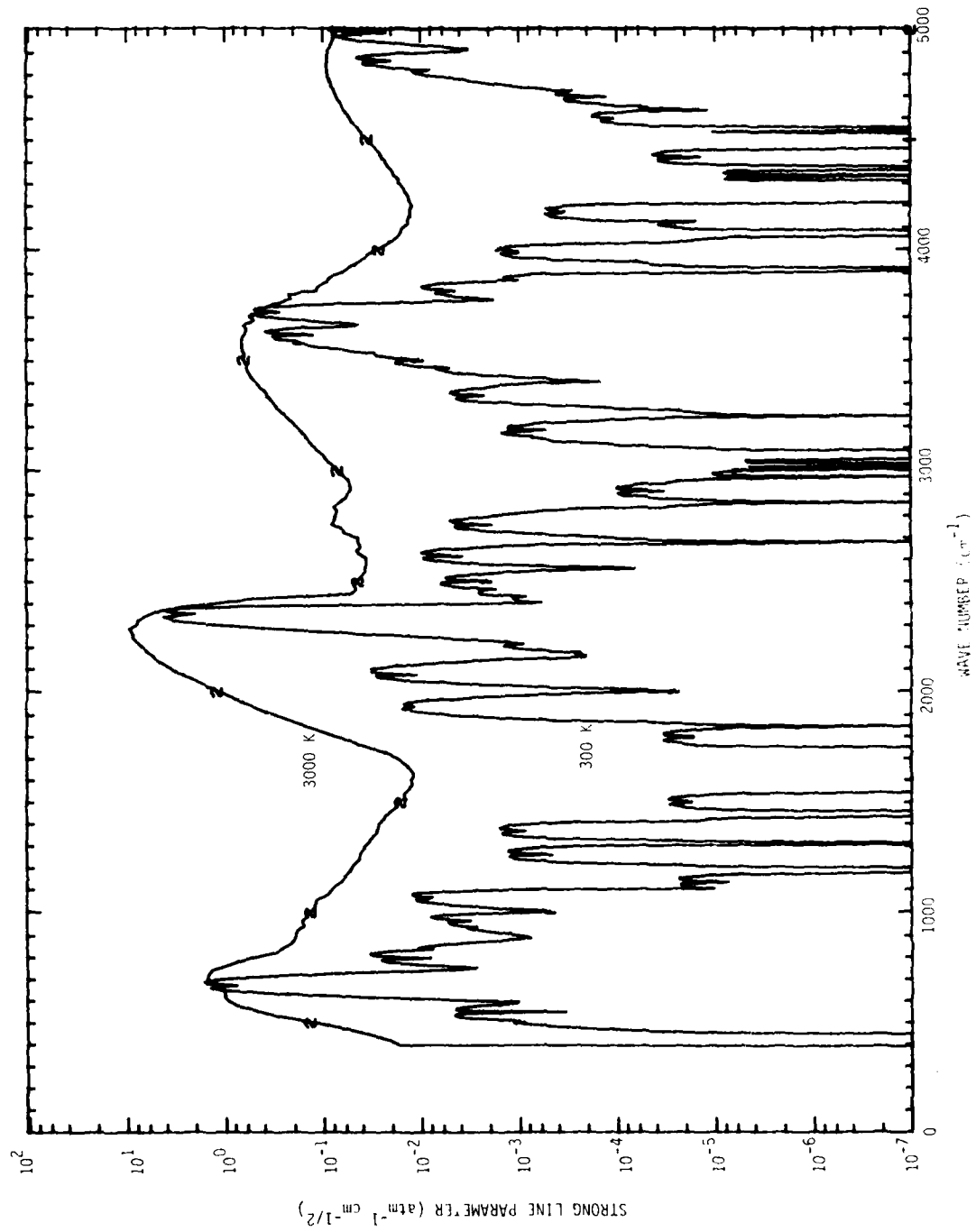


Figure 2-8. Strong line parameters for CO<sub>2</sub>.

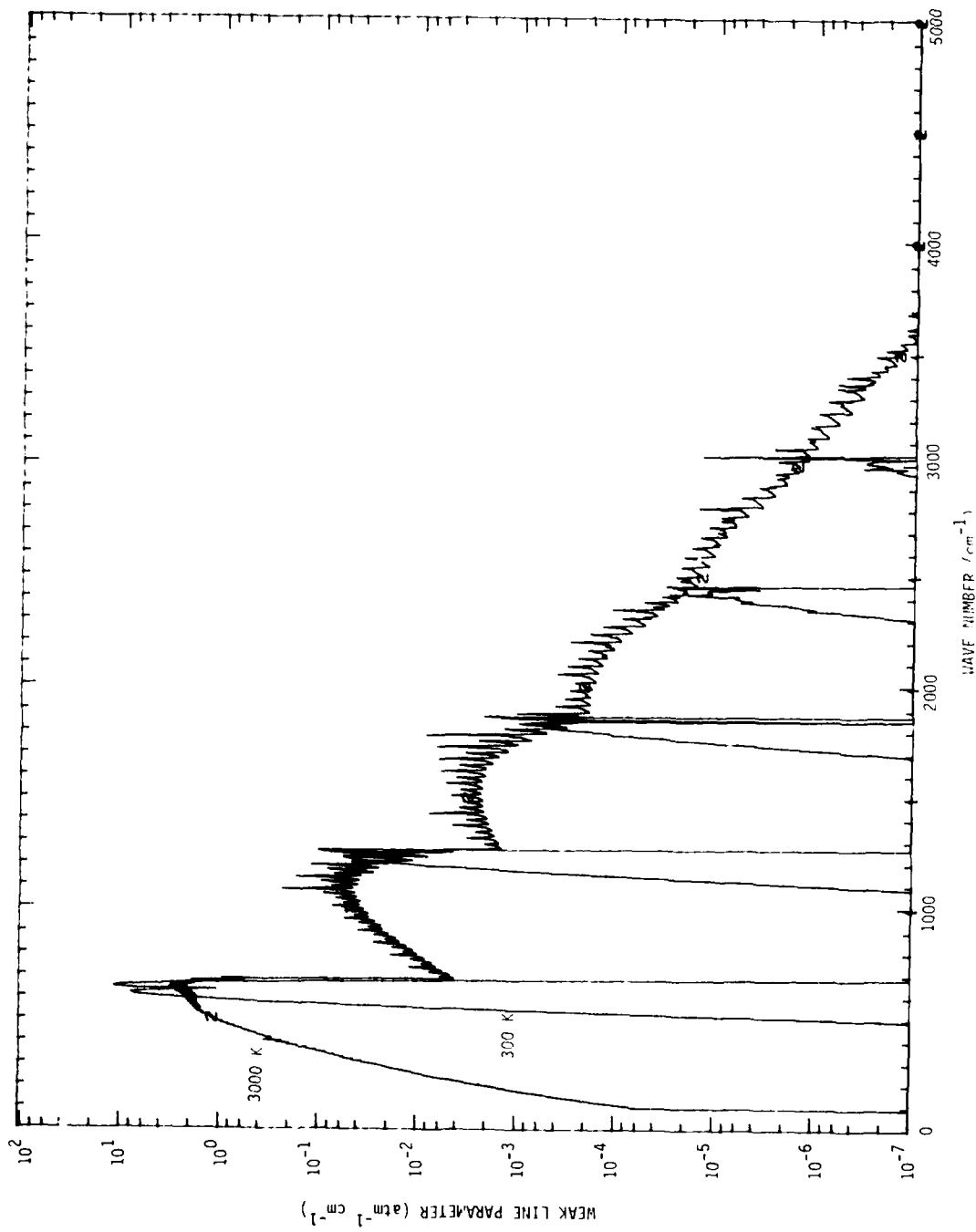


Figure 2-9. Weak Line parameters for CuO.

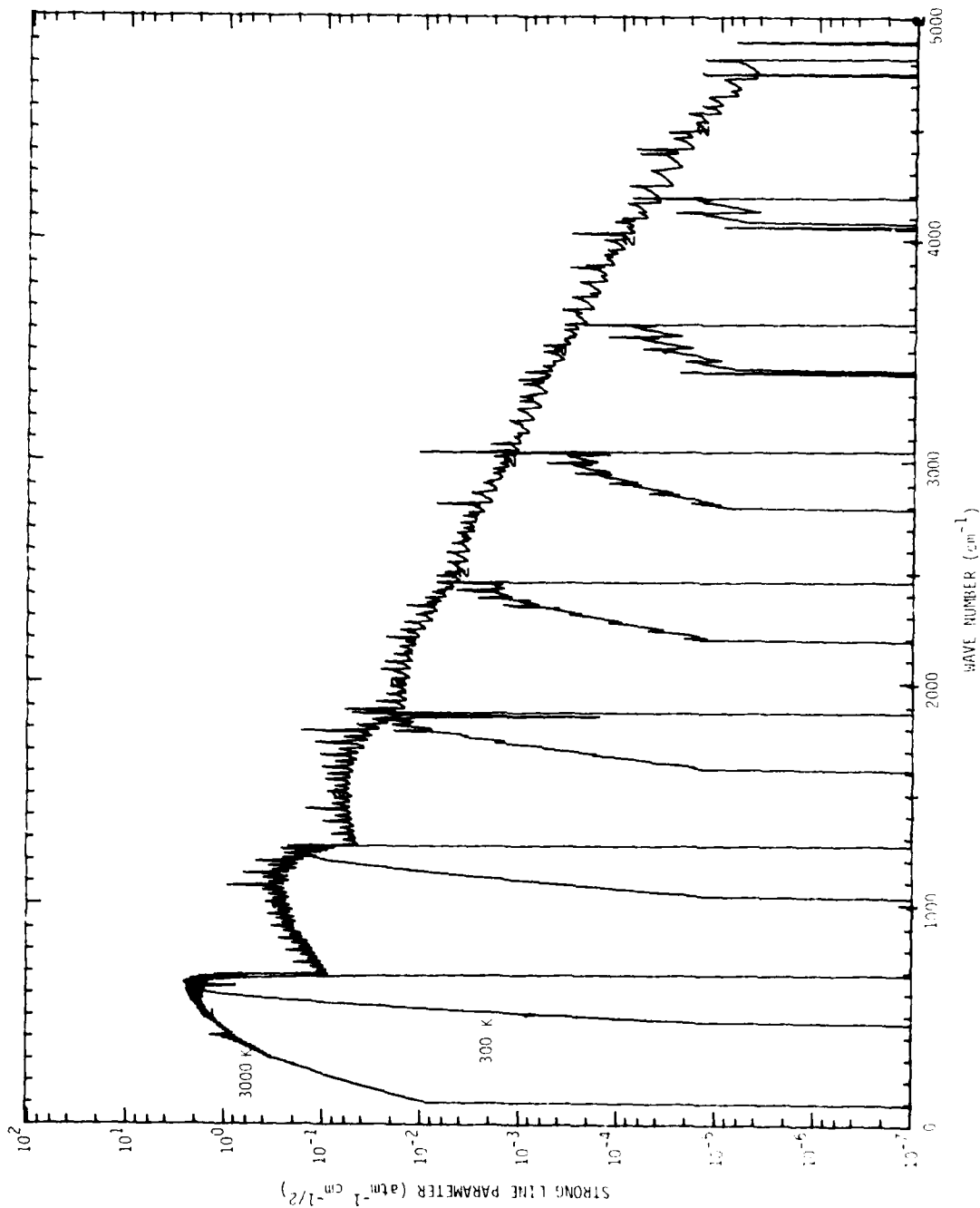


Figure 2-10. Strong line parameters for  $\text{CuO}$ .

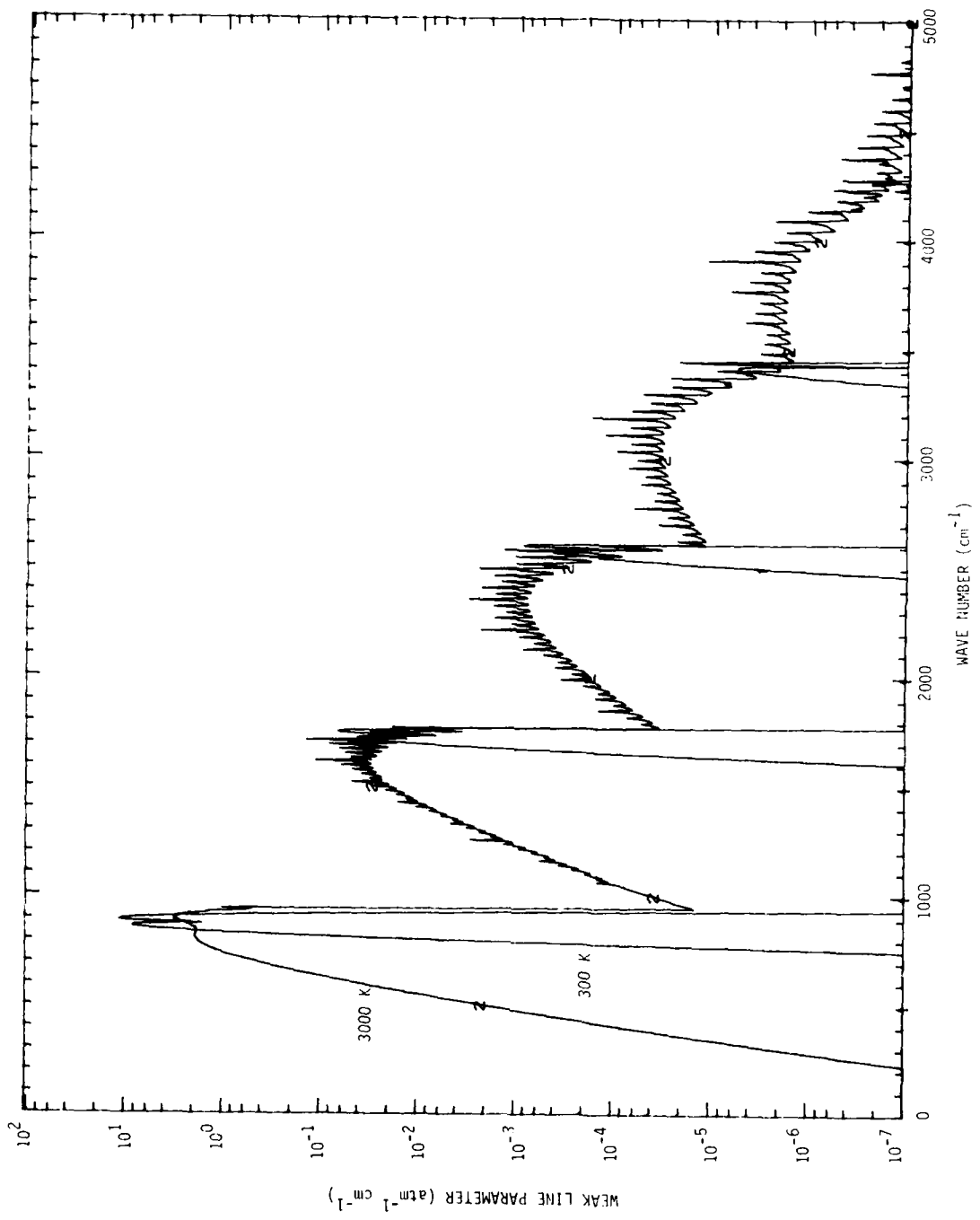


Figure 2-11. Weak line parameters for FeO.



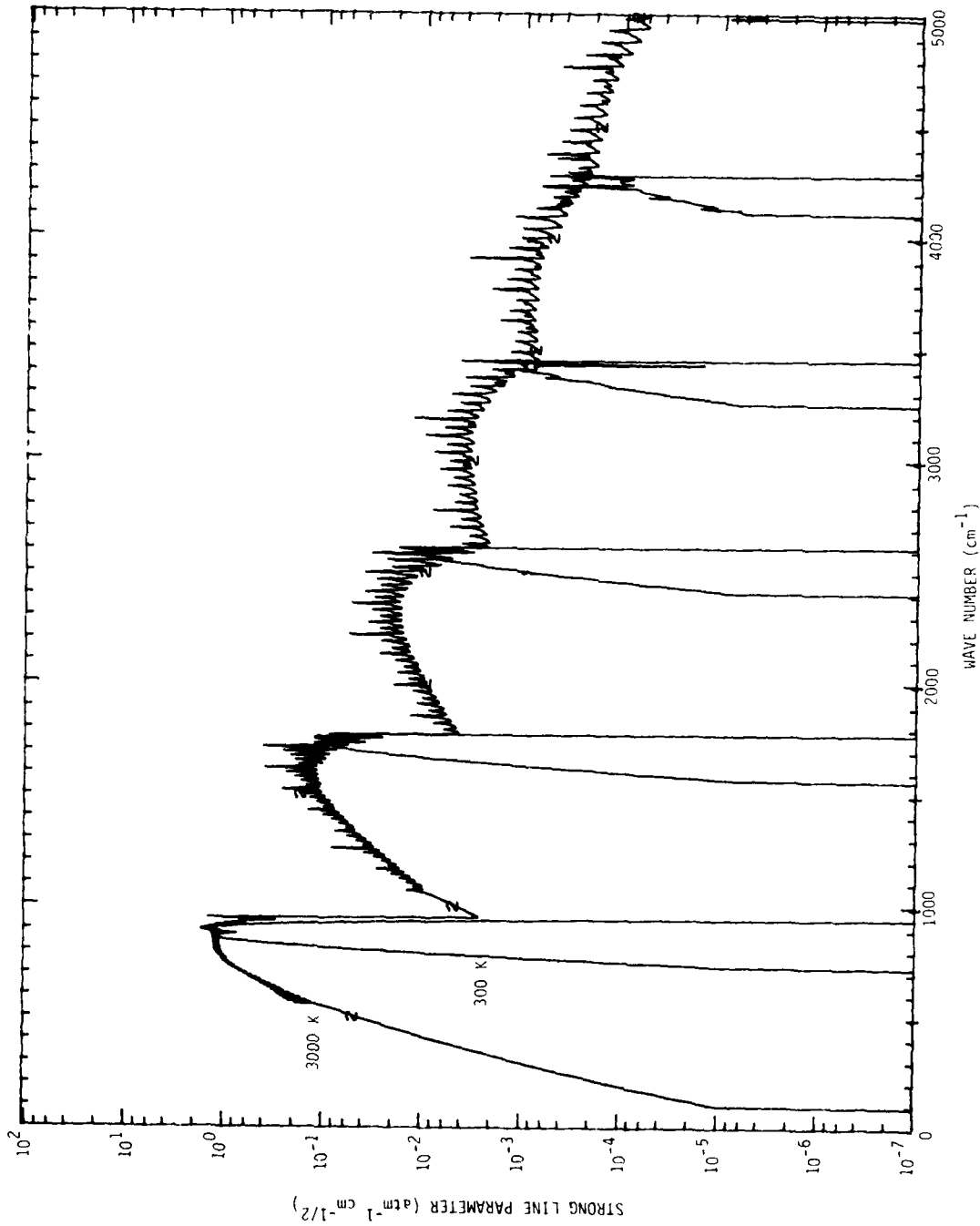


Figure 2-12. Strong line parameters for FeO.

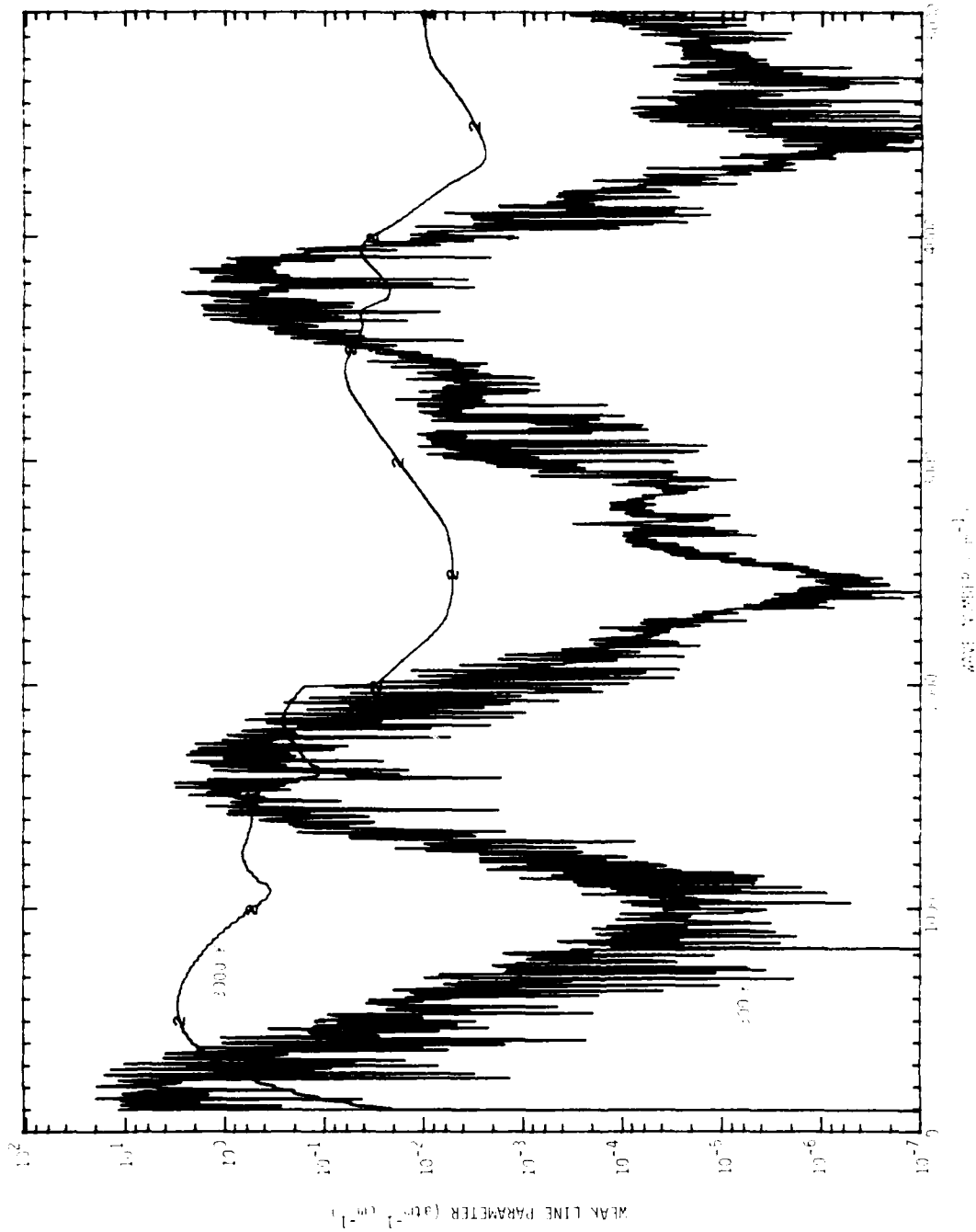


Figure 2-13. Weak line parameters for H<sub>2</sub>O.

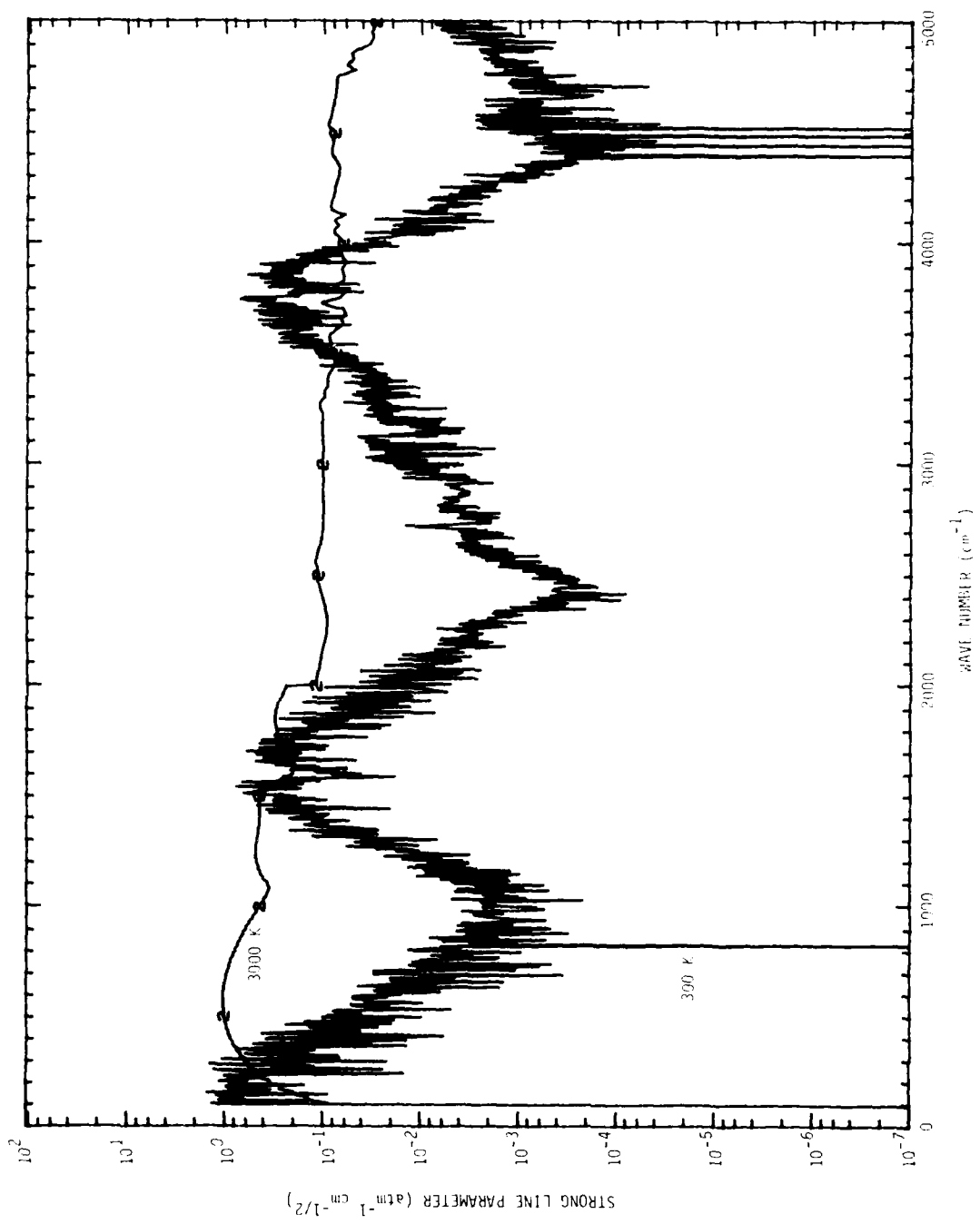


Figure 2-14. Strong line parameters for H<sub>2</sub>O.

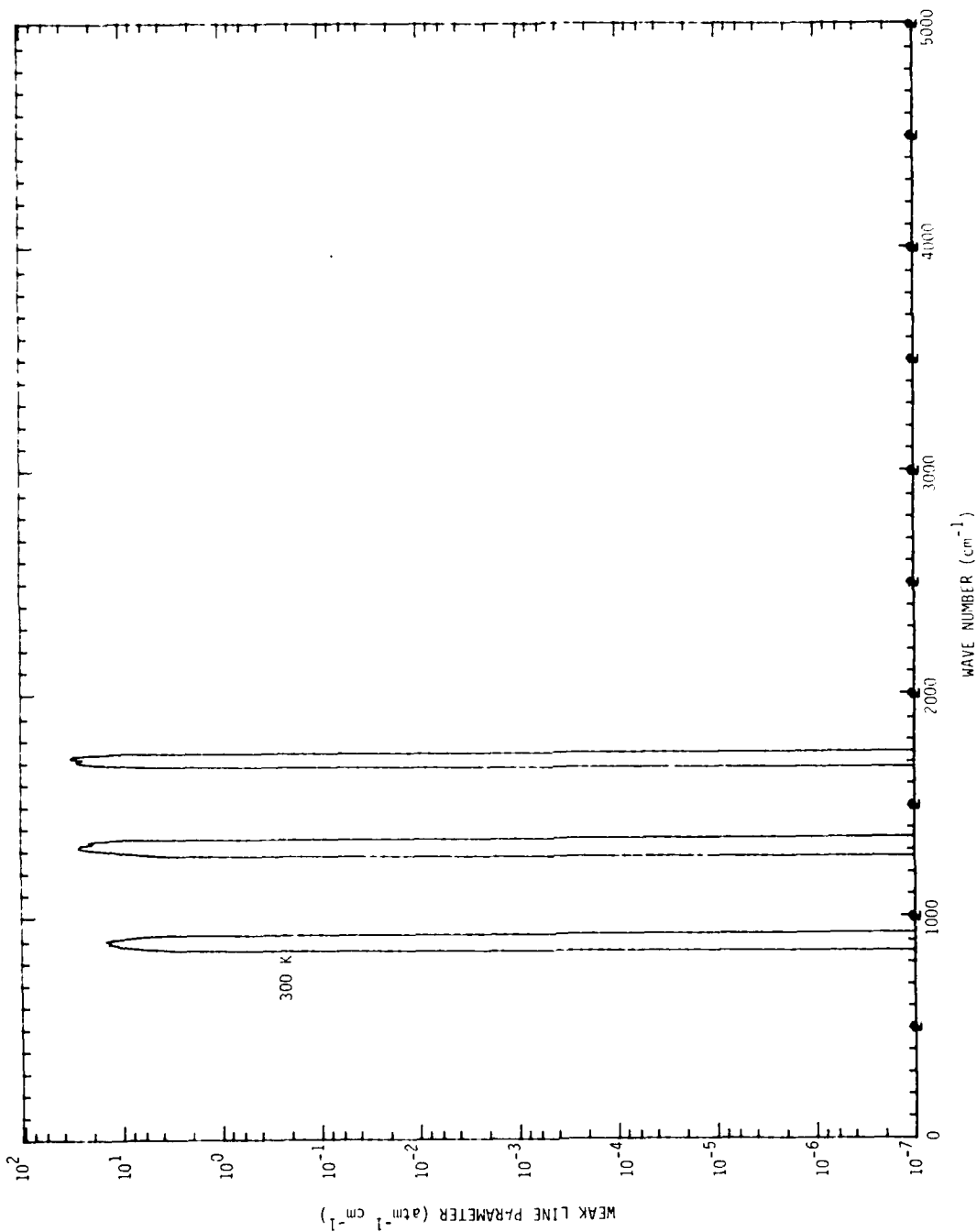


Figure 2-15. Weak line parameters for HNO<sub>3</sub>.

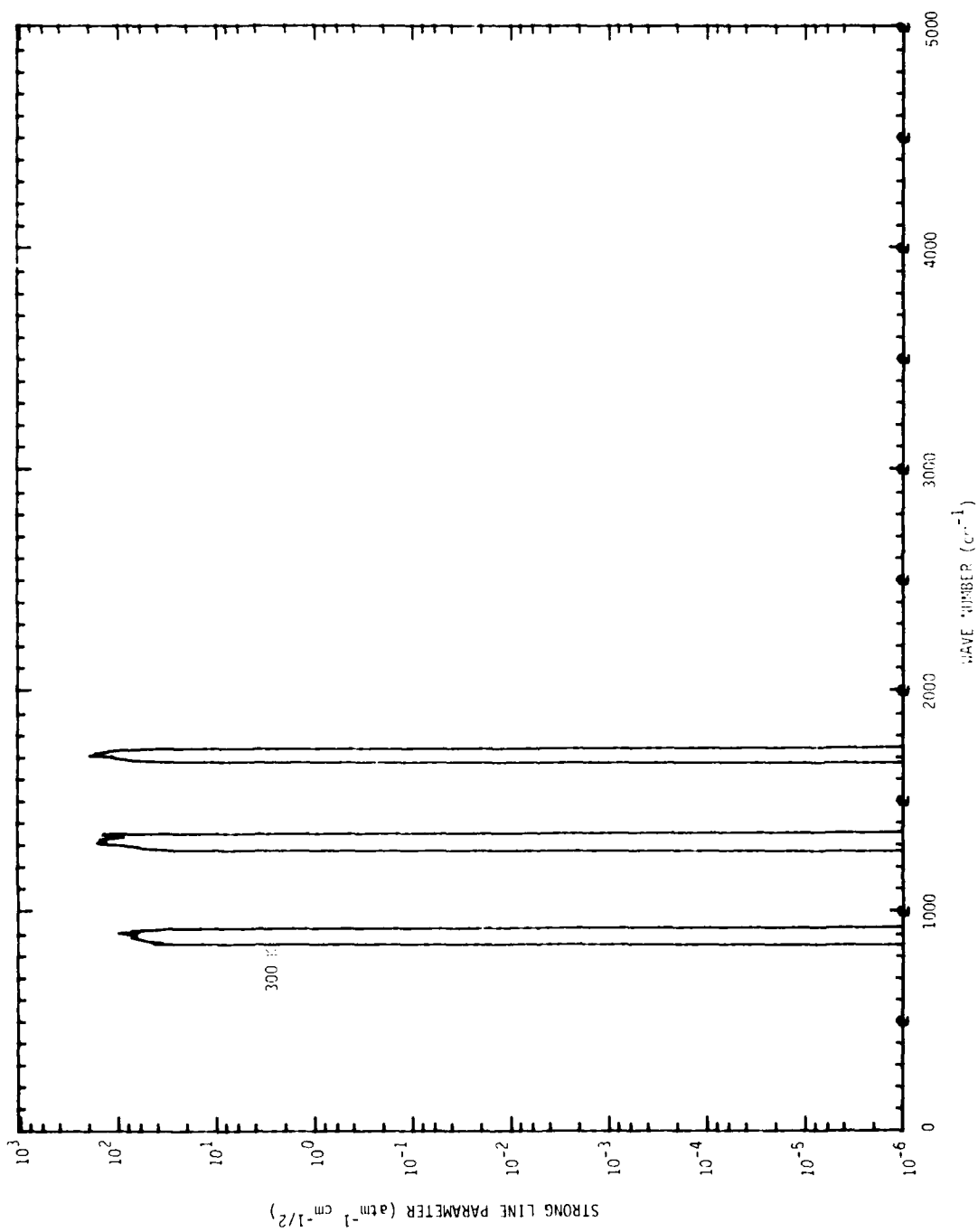


Figure 2-16. Strong line parameters for HNO<sub>3</sub>.

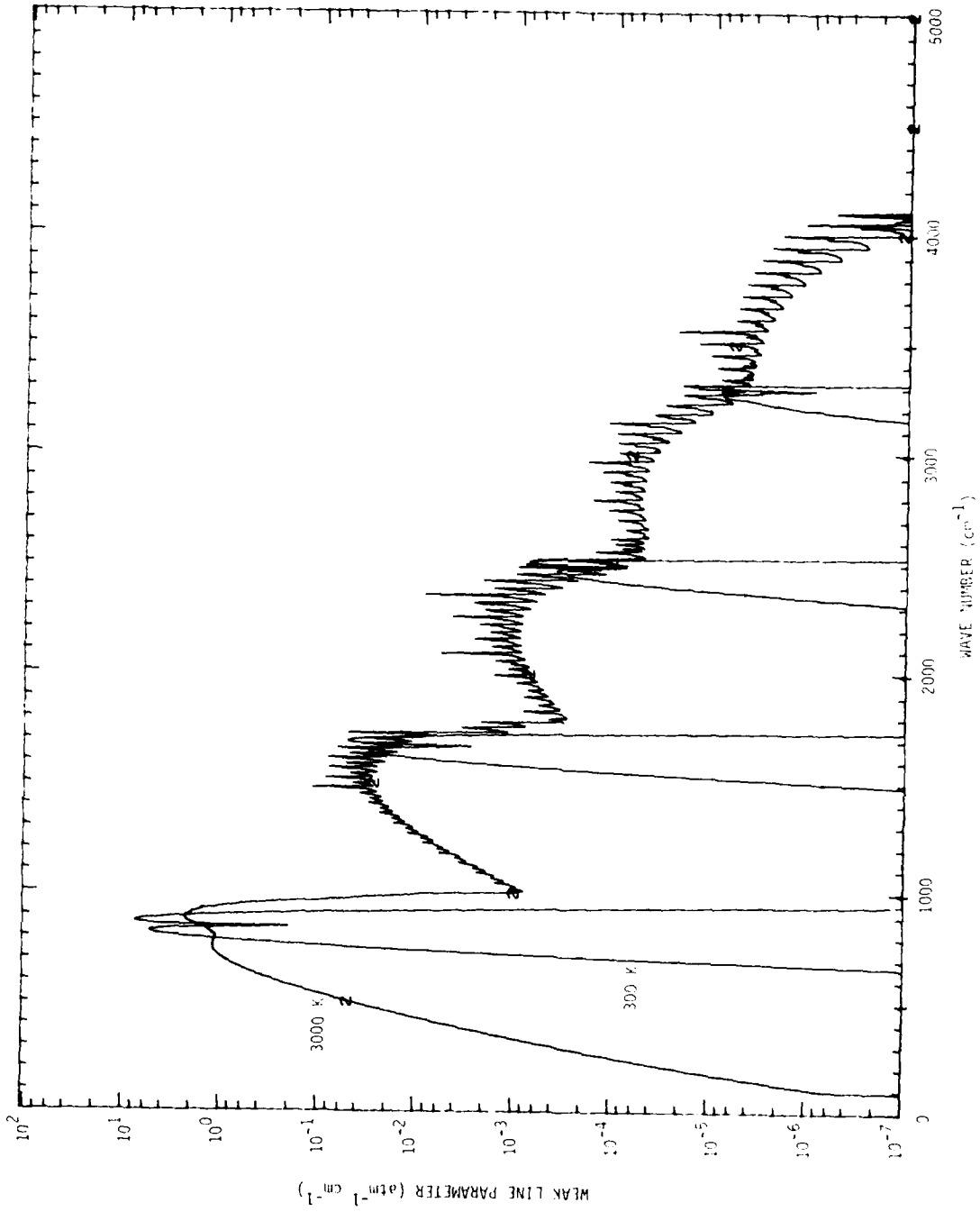


Figure 2-17. Weak line parameters for LiO.

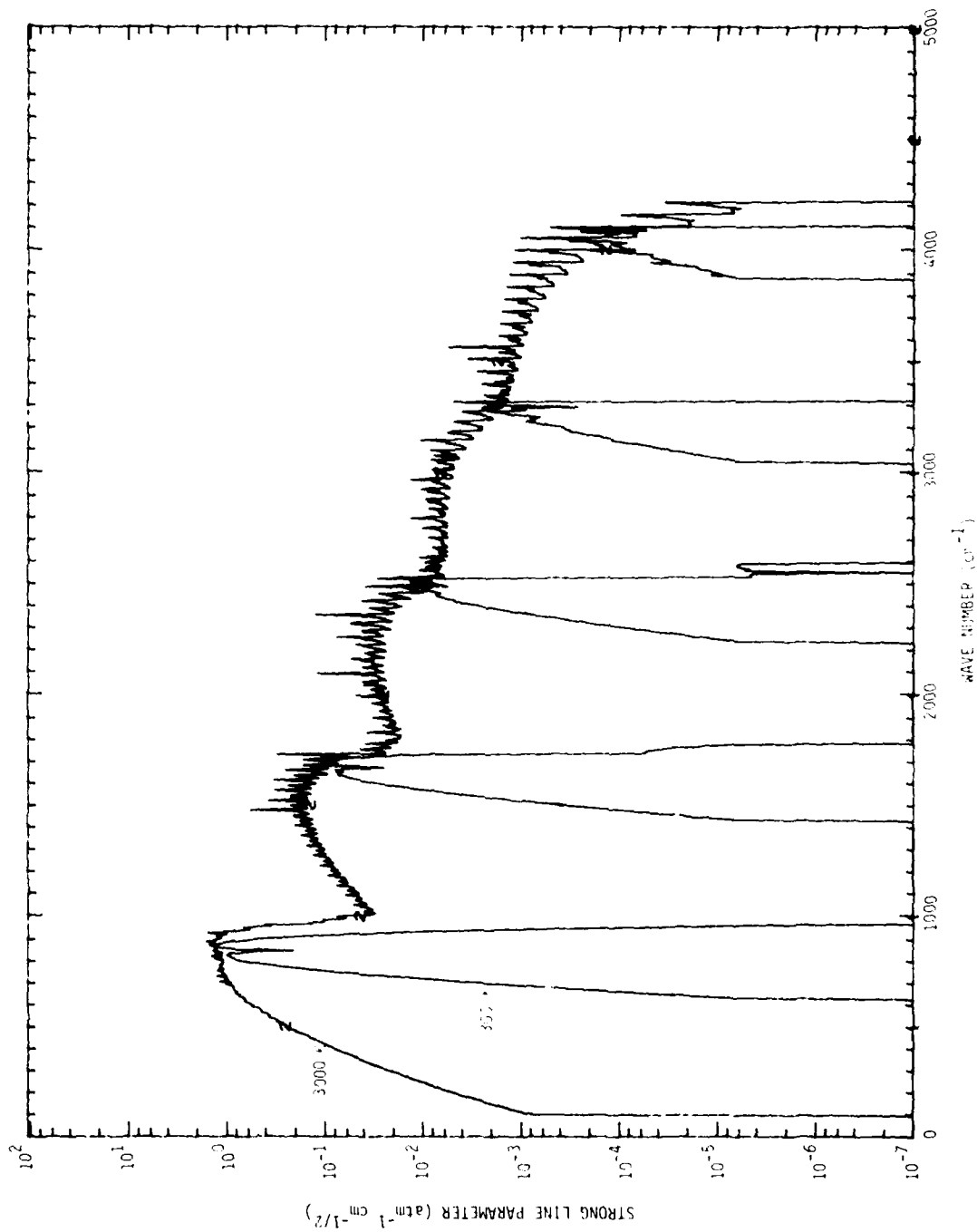


Figure 2-18. Strong line parameters for LiO.

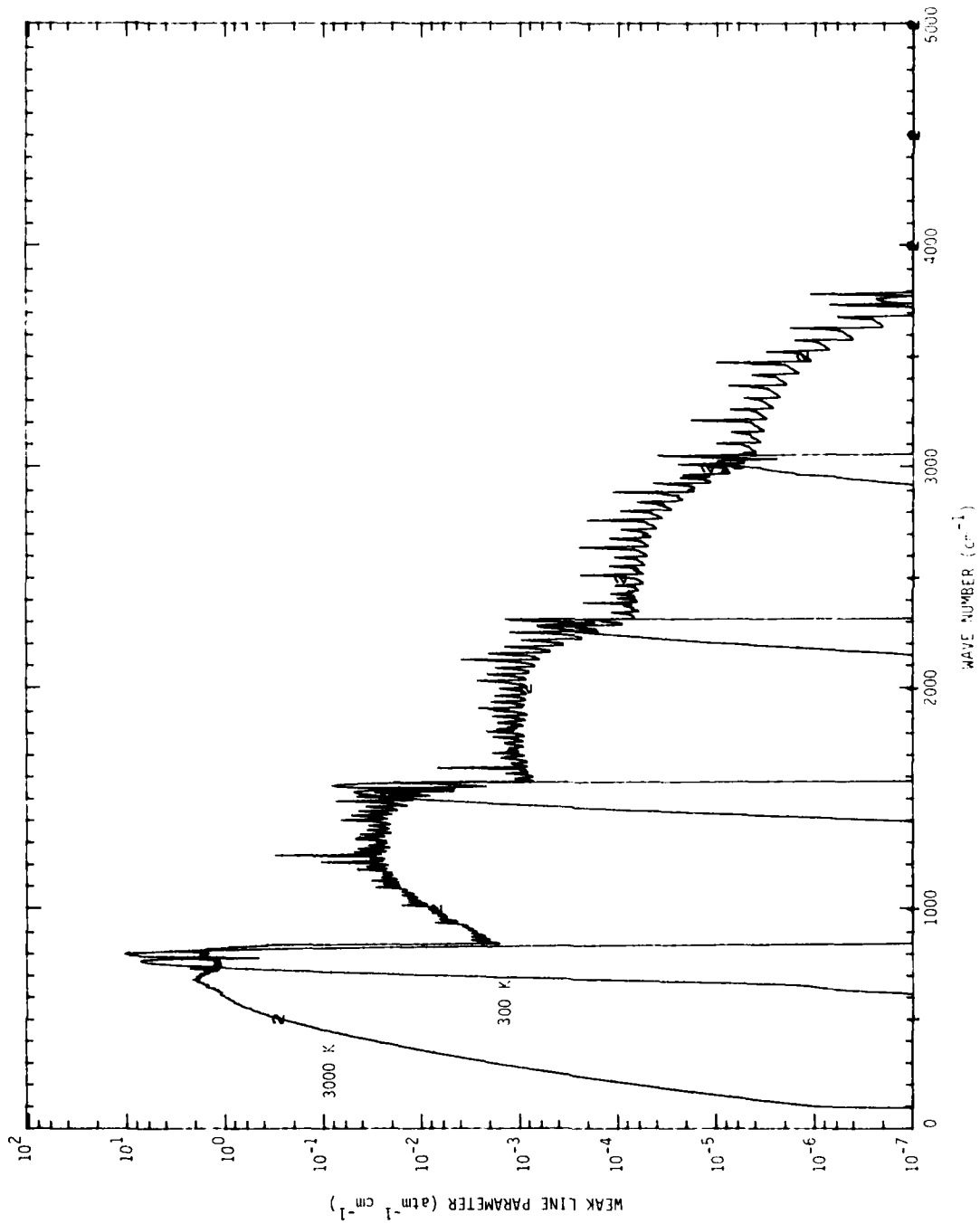


Figure 2-19. Weak line parameters for MgO.



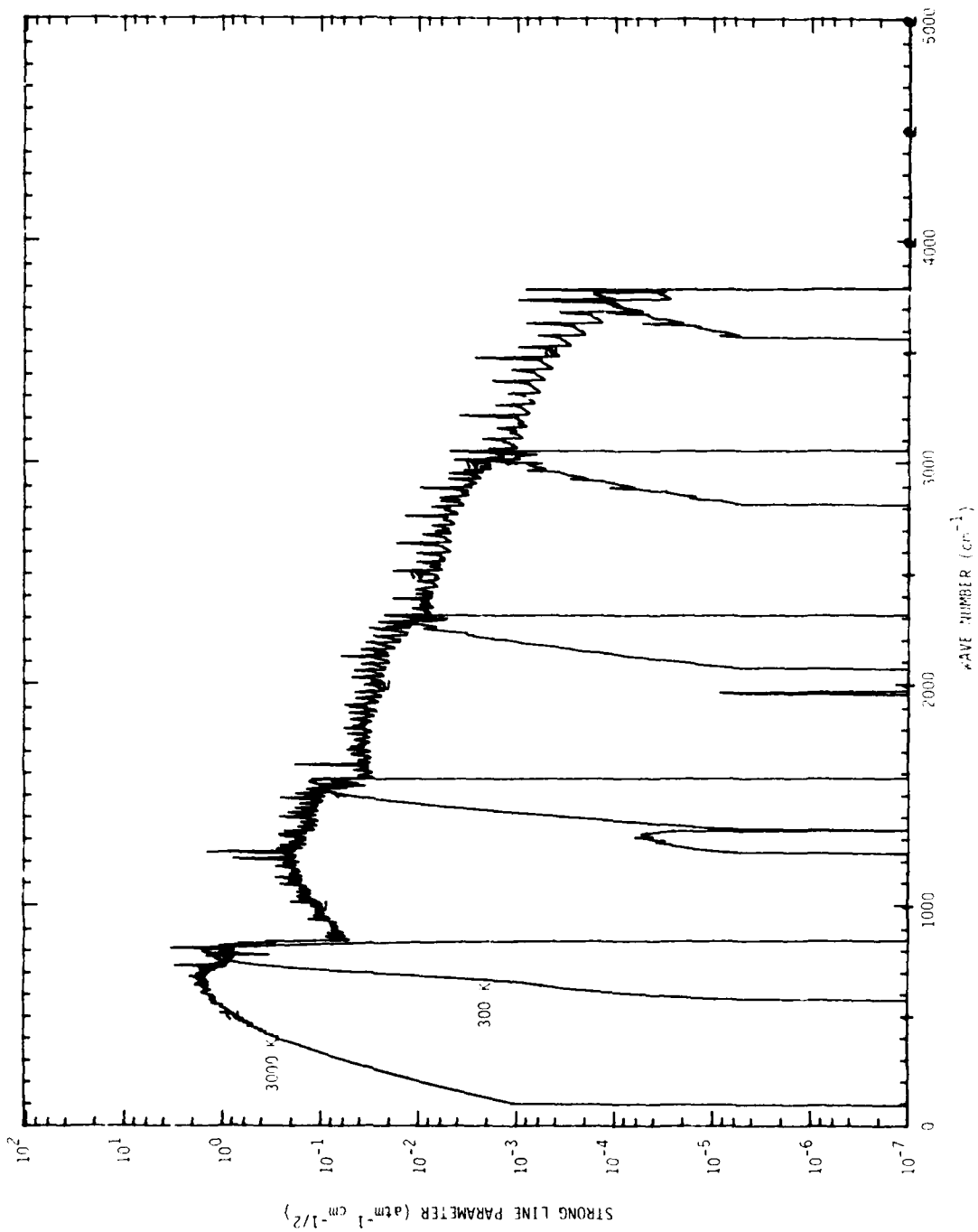


Figure 2-20. Strong line parameters for MgO.

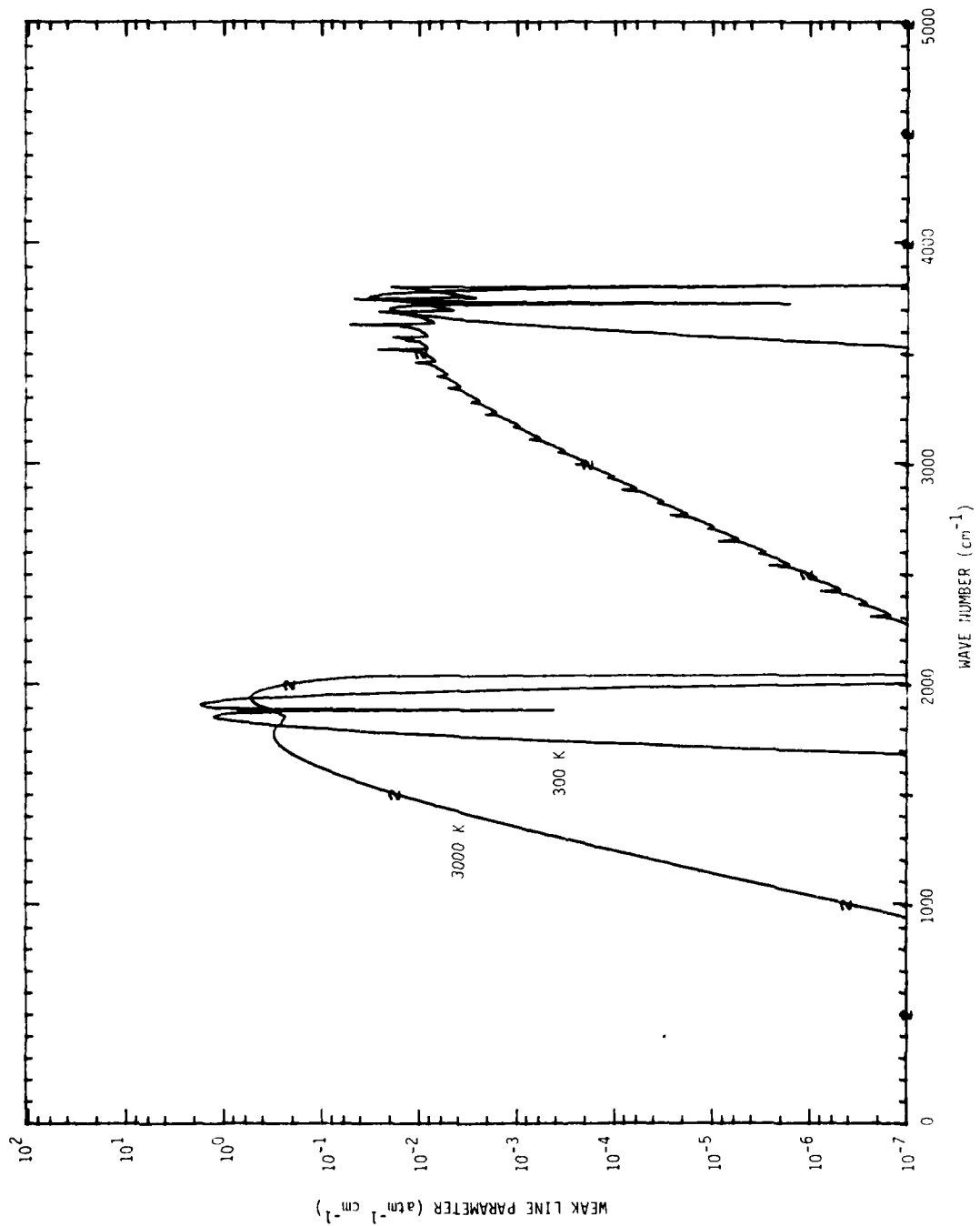


Figure 2-21. Weak line parameters for NO.

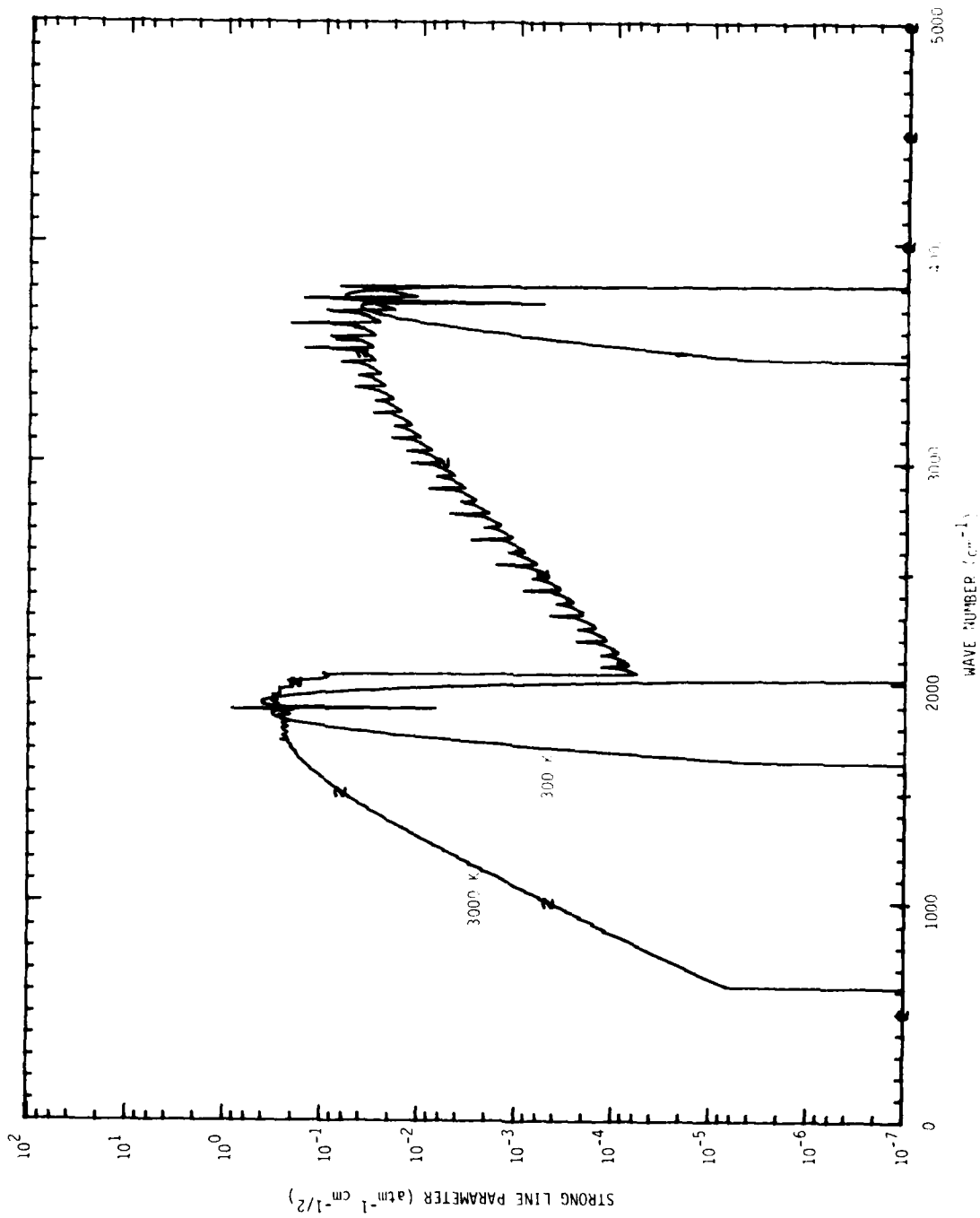


Figure 2-22. Strong line parameters for NO.

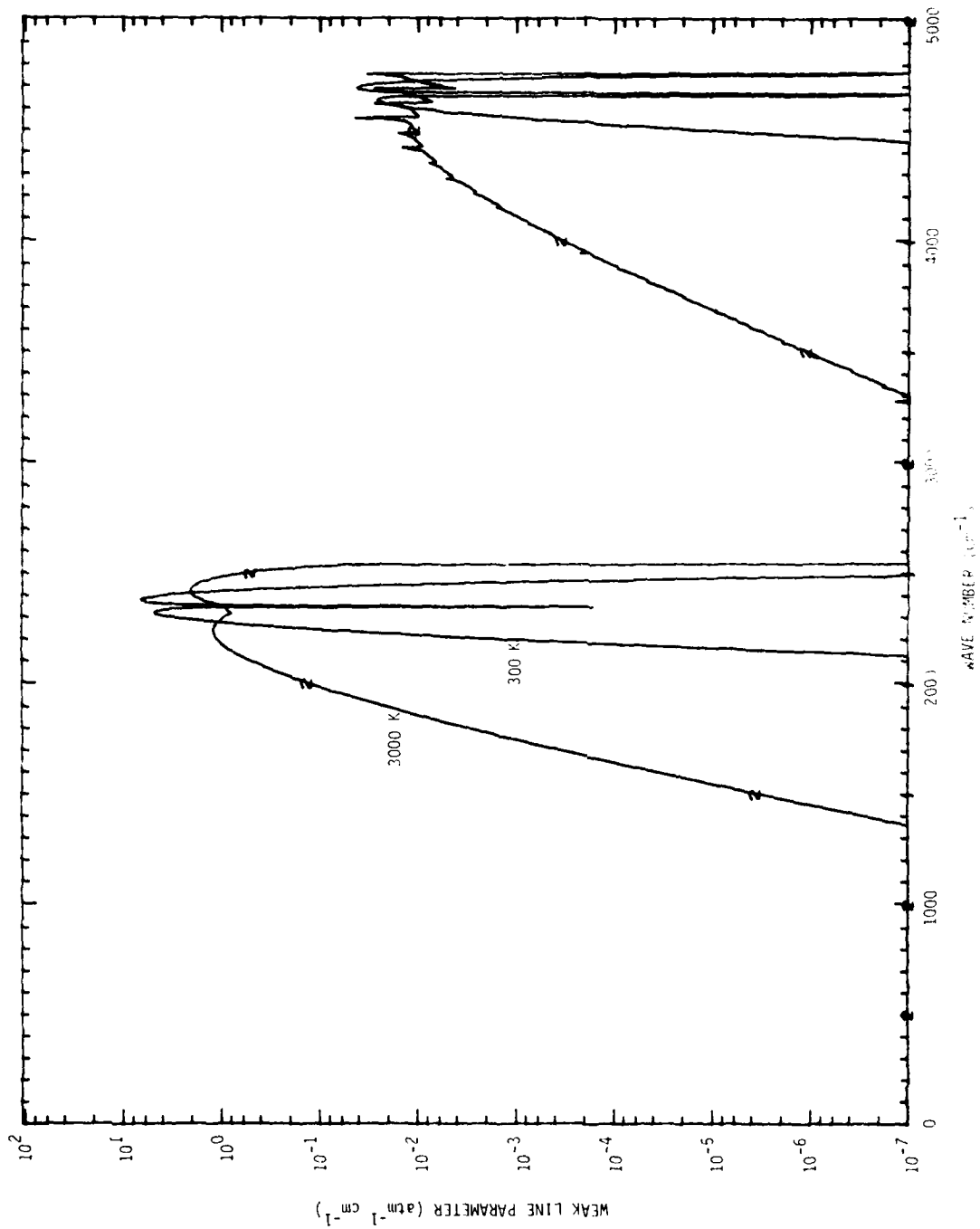


Figure 2-23. Weak line parameters for NO<sup>+</sup>.

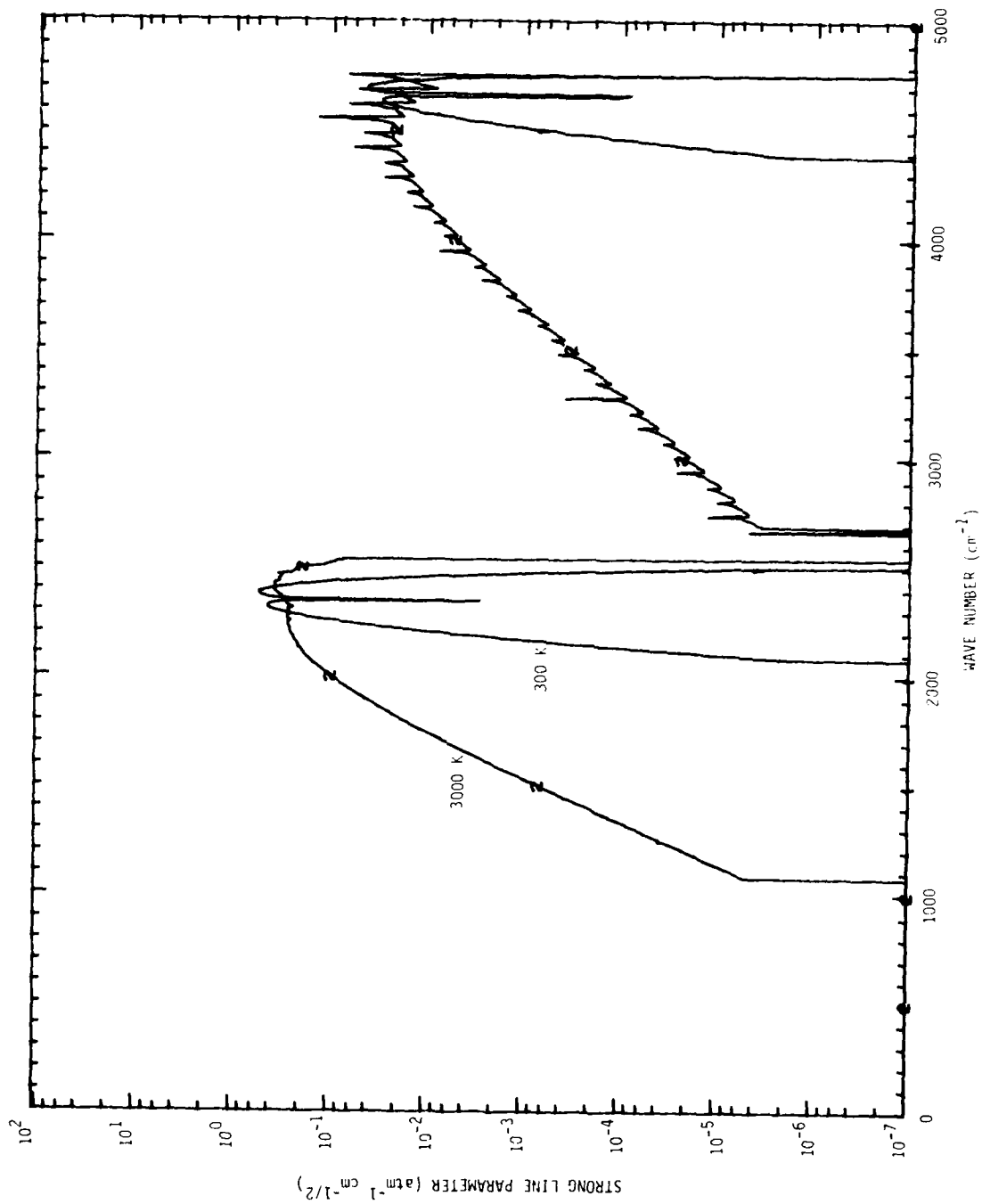


Figure 2-24. Strong line parameters for NO<sup>+</sup>.

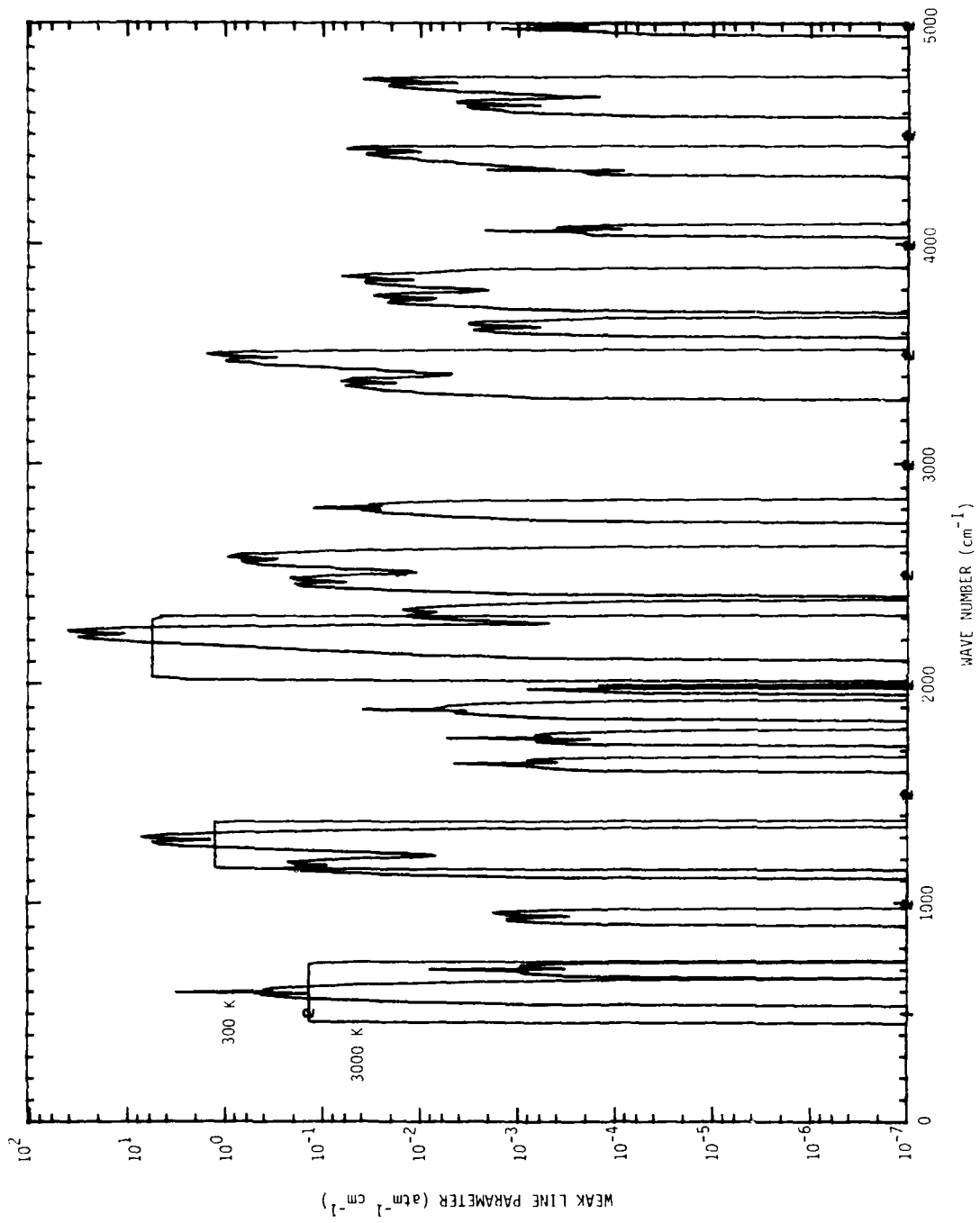


Figure 2-25. Weak line parameters for N<sub>2</sub>O.

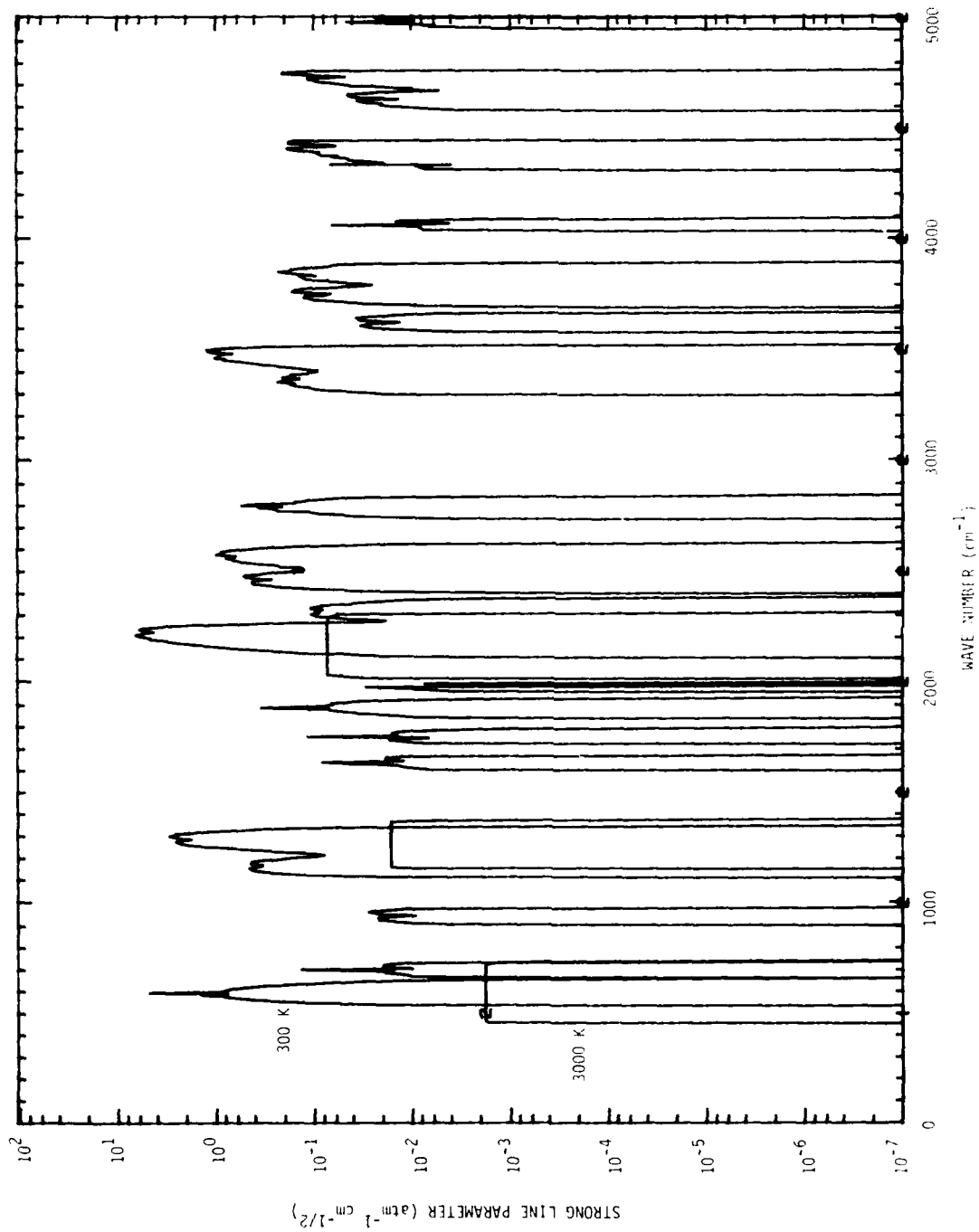


Figure 2-26. Strong line parameters for N<sub>2</sub>O.

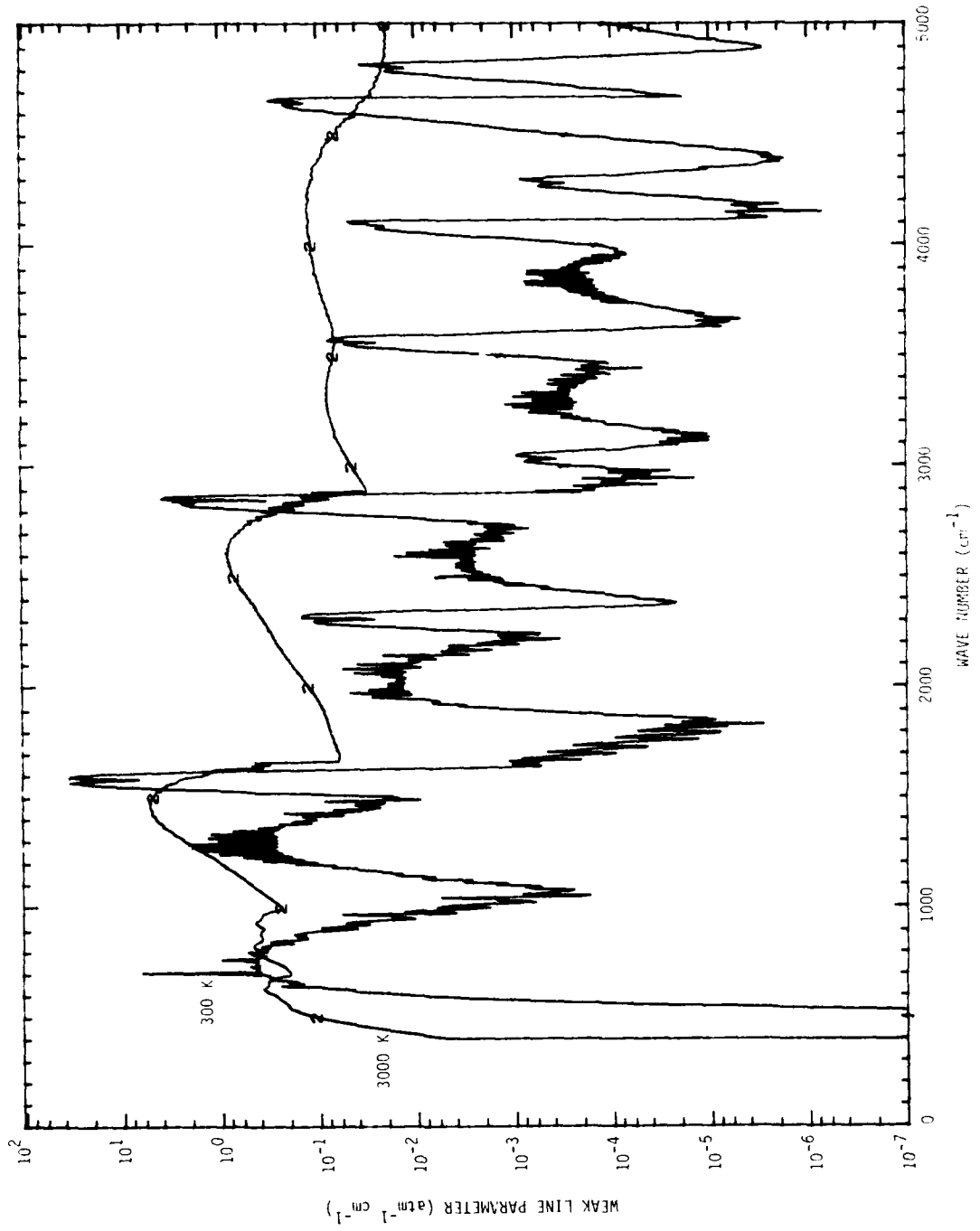


Figure 2-27. Weak line parameters for NO<sub>2</sub>.



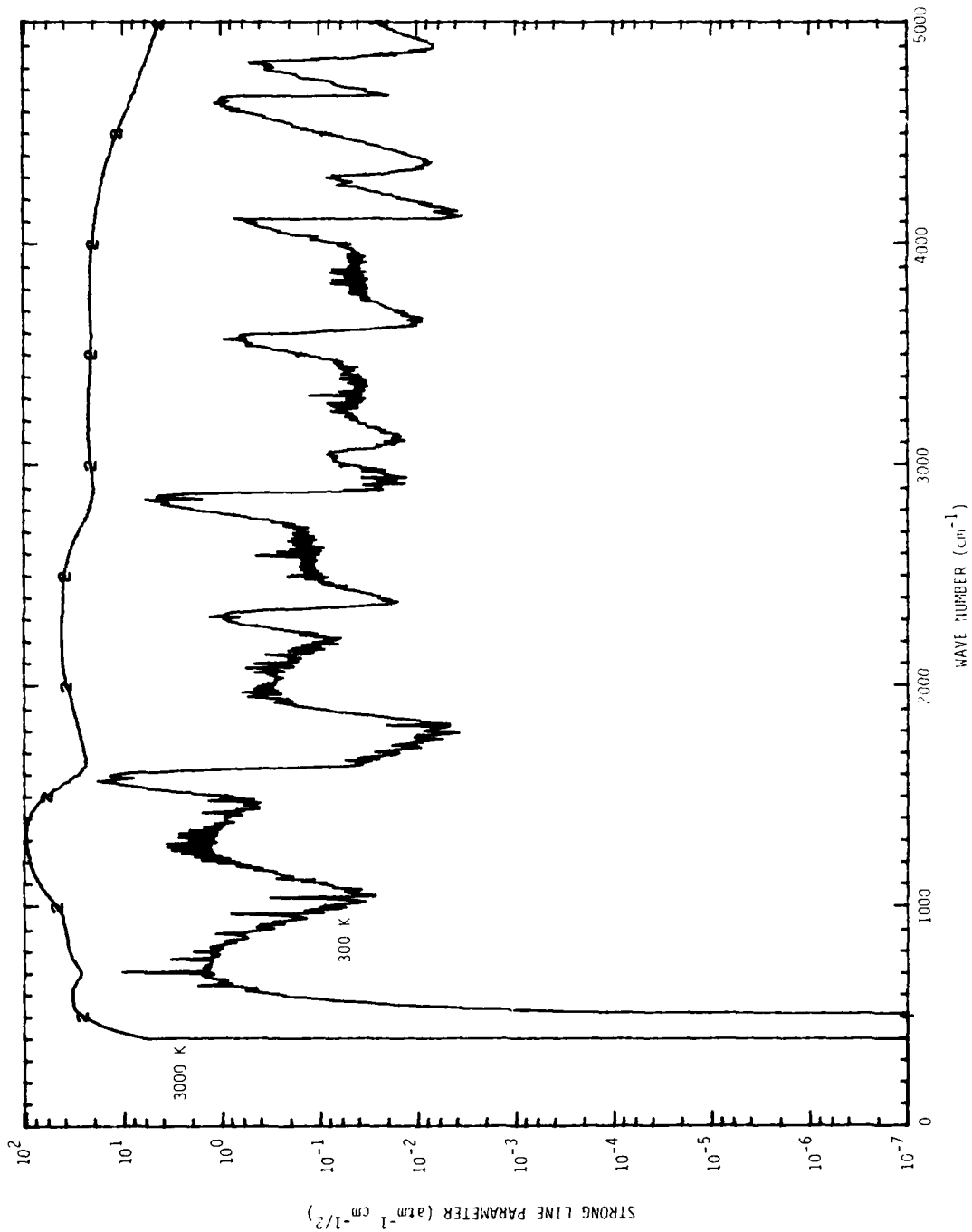


Figure 2-28. Strong line parameters for NO<sub>2</sub>.

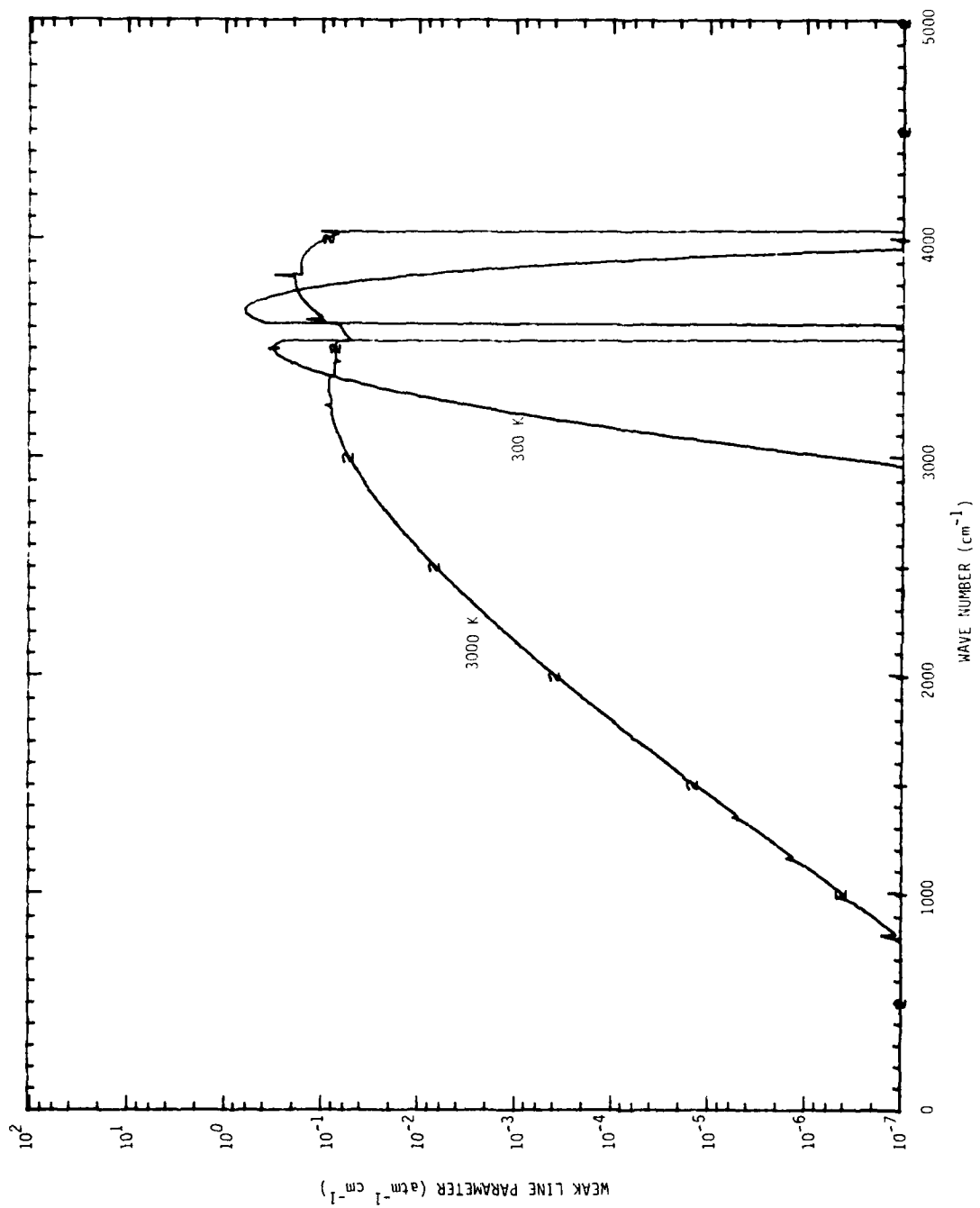


Figure 2-29. Weak line parameters for OH.

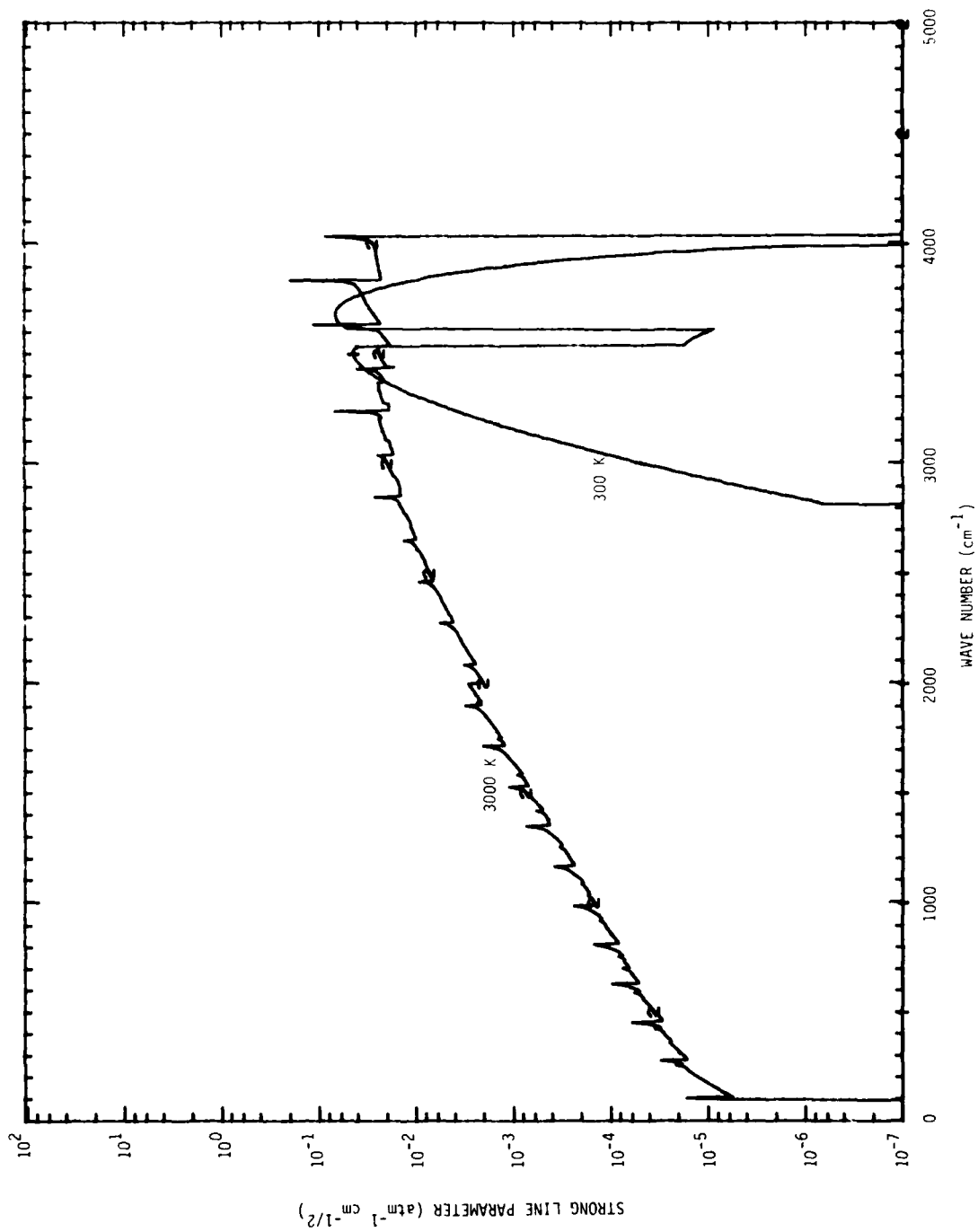


Figure 2-30. Strong line parameters for OH.

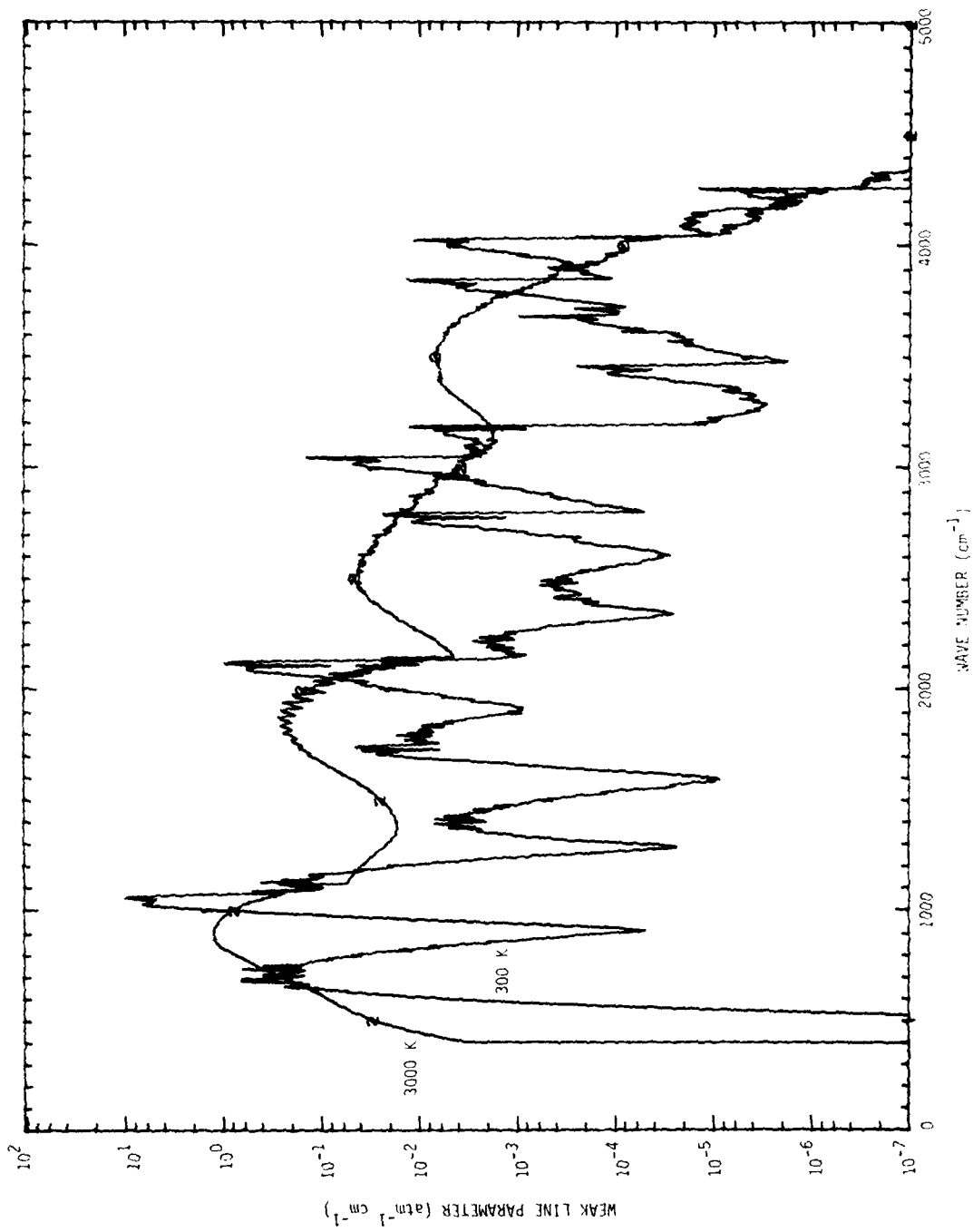


Figure 2-31. Weak line parameters for O<sub>3</sub>.

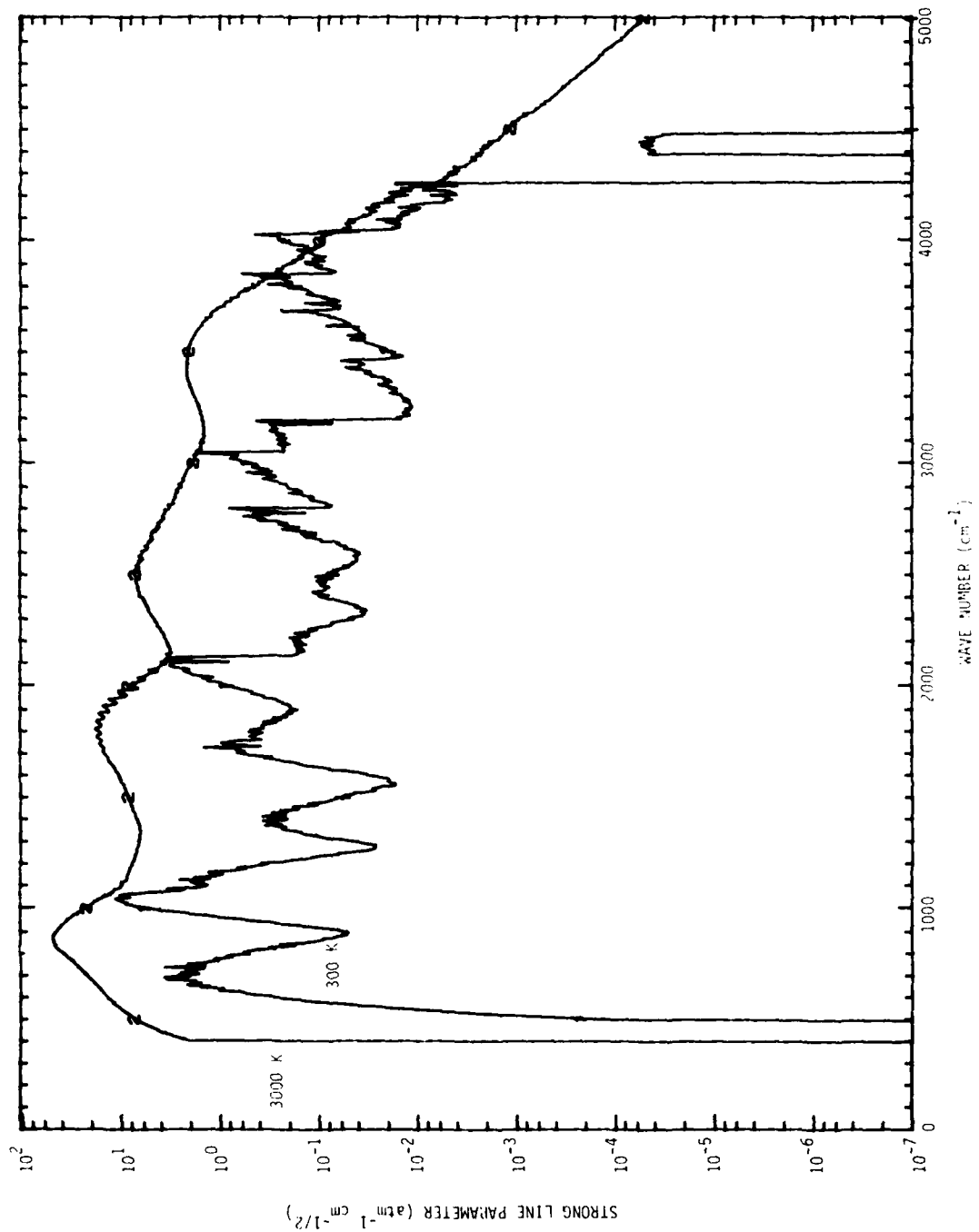


Figure 2-32. Strong line parameters for  $O_3$ .

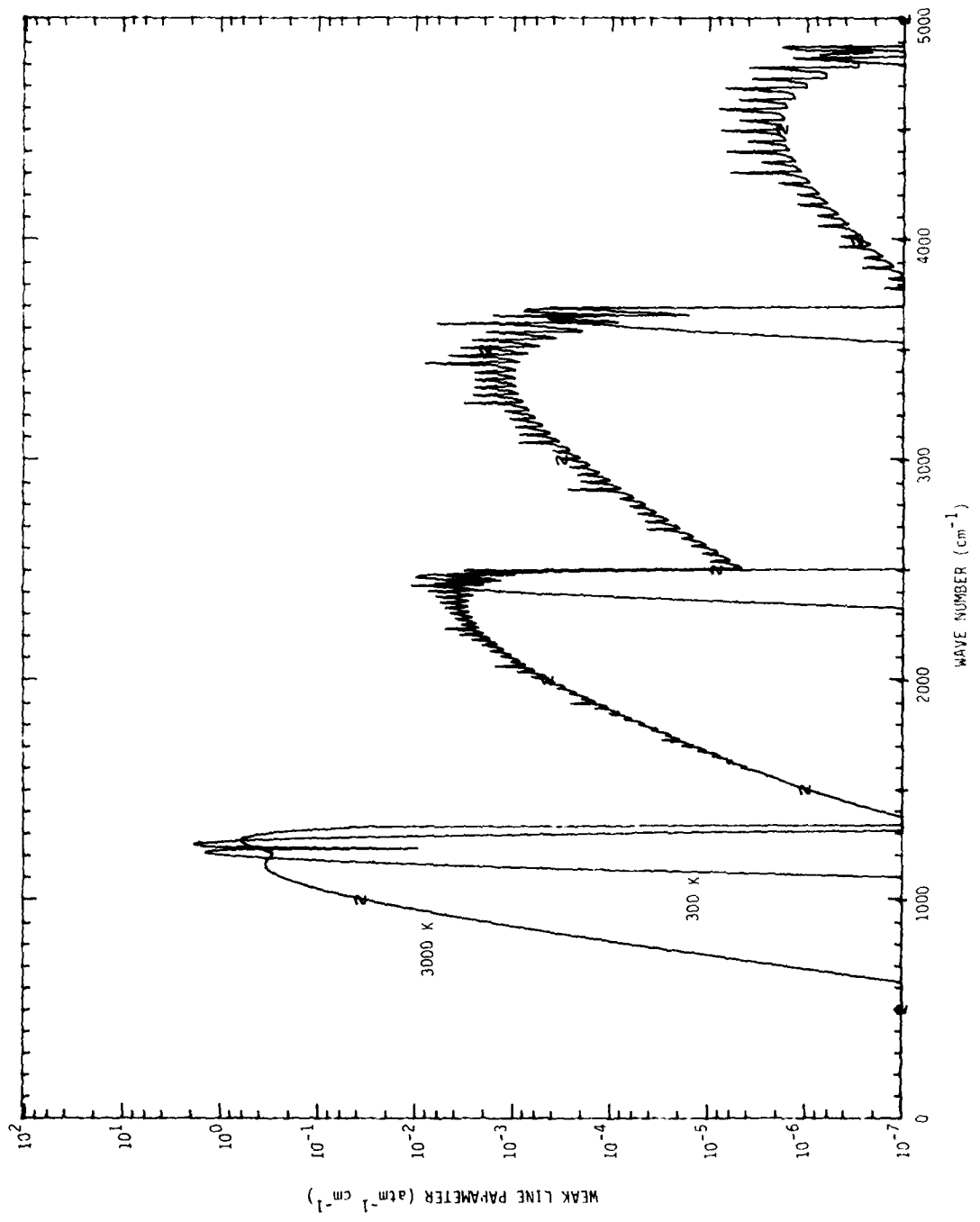


Figure 2-33. Weak line parameters for SiO.

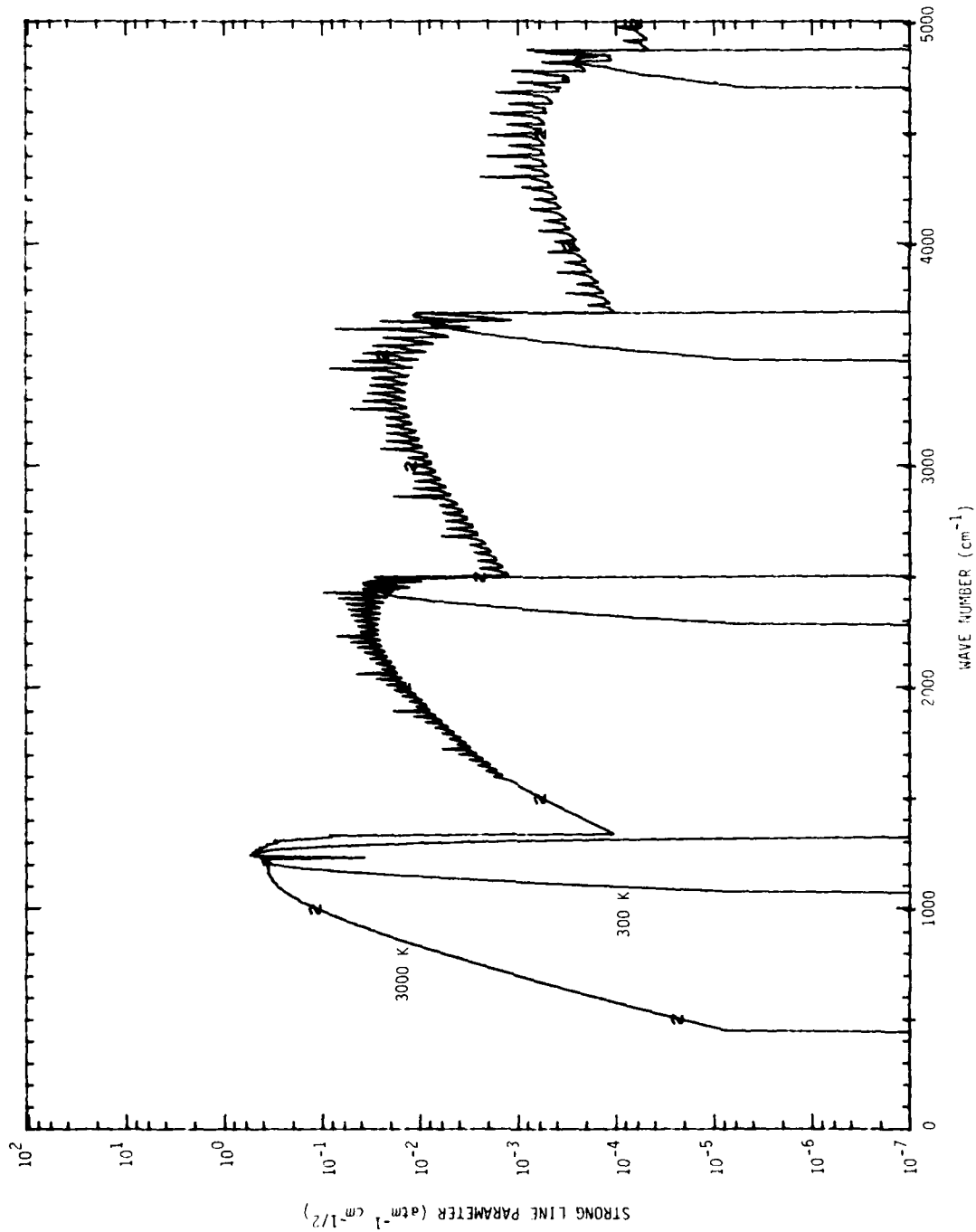


Figure 2-34. Strong line parameters for SiO.

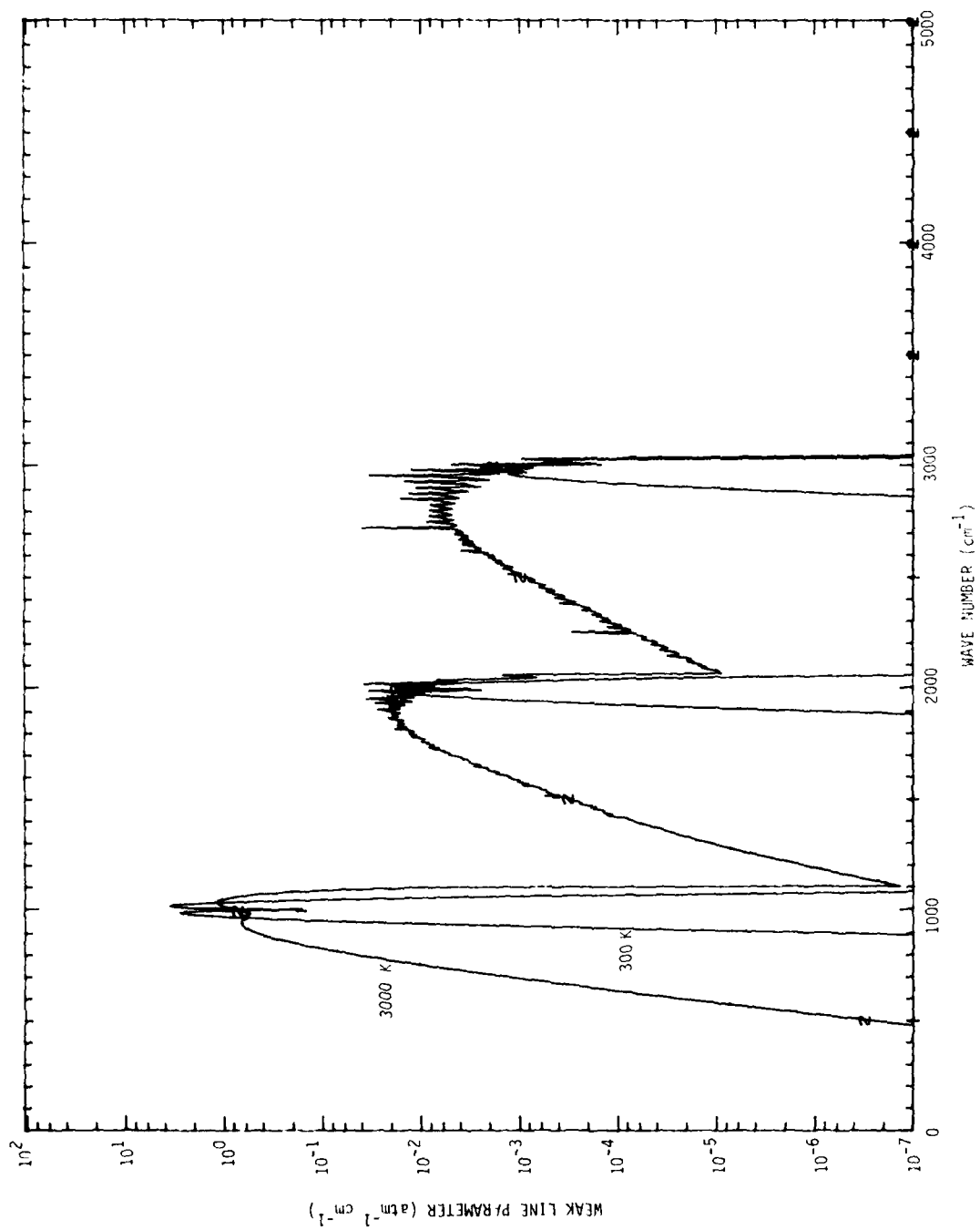


Figure 2-35. Weak line parameters for TiO.



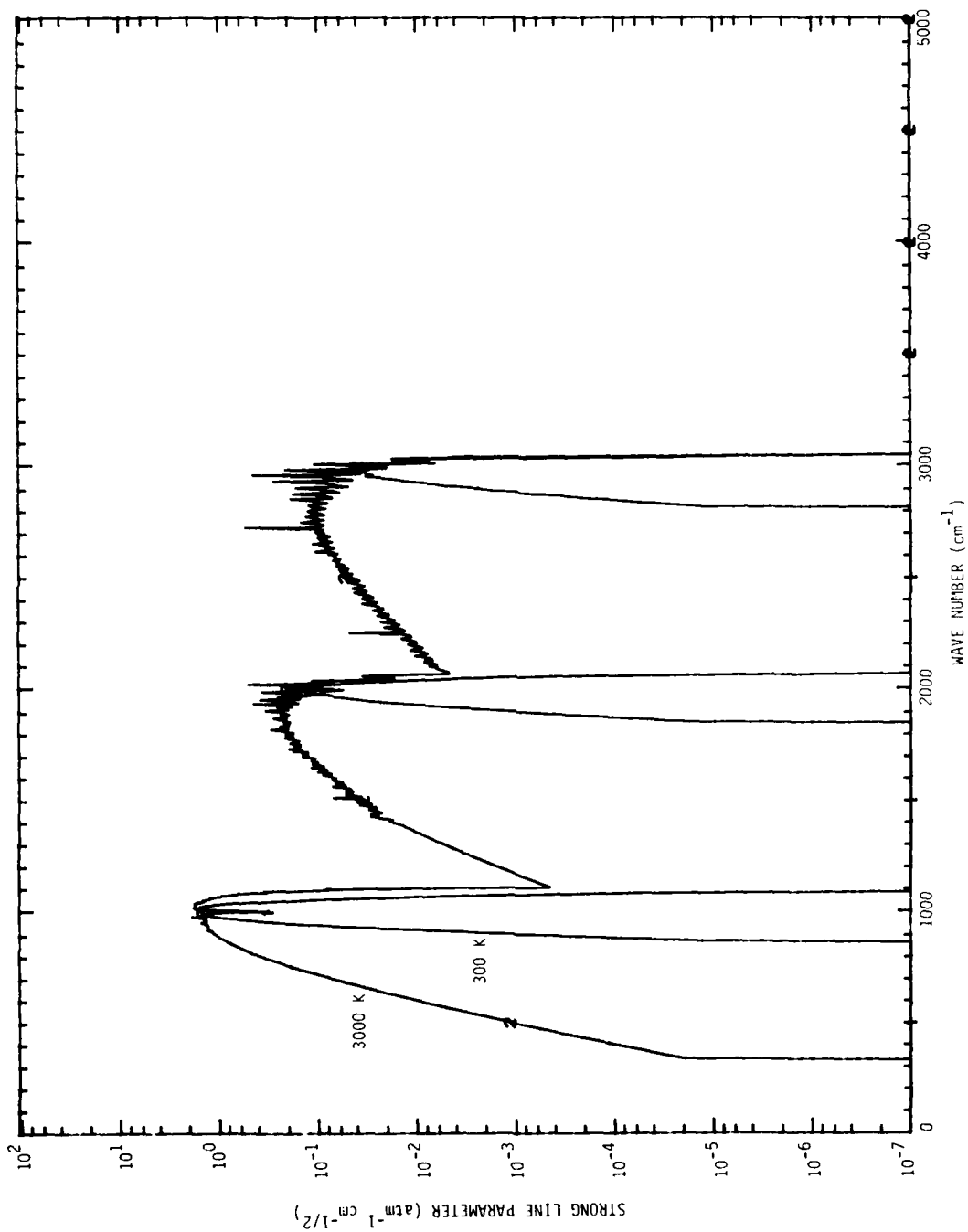


Figure 2-36. Strong line parameters for TiO.

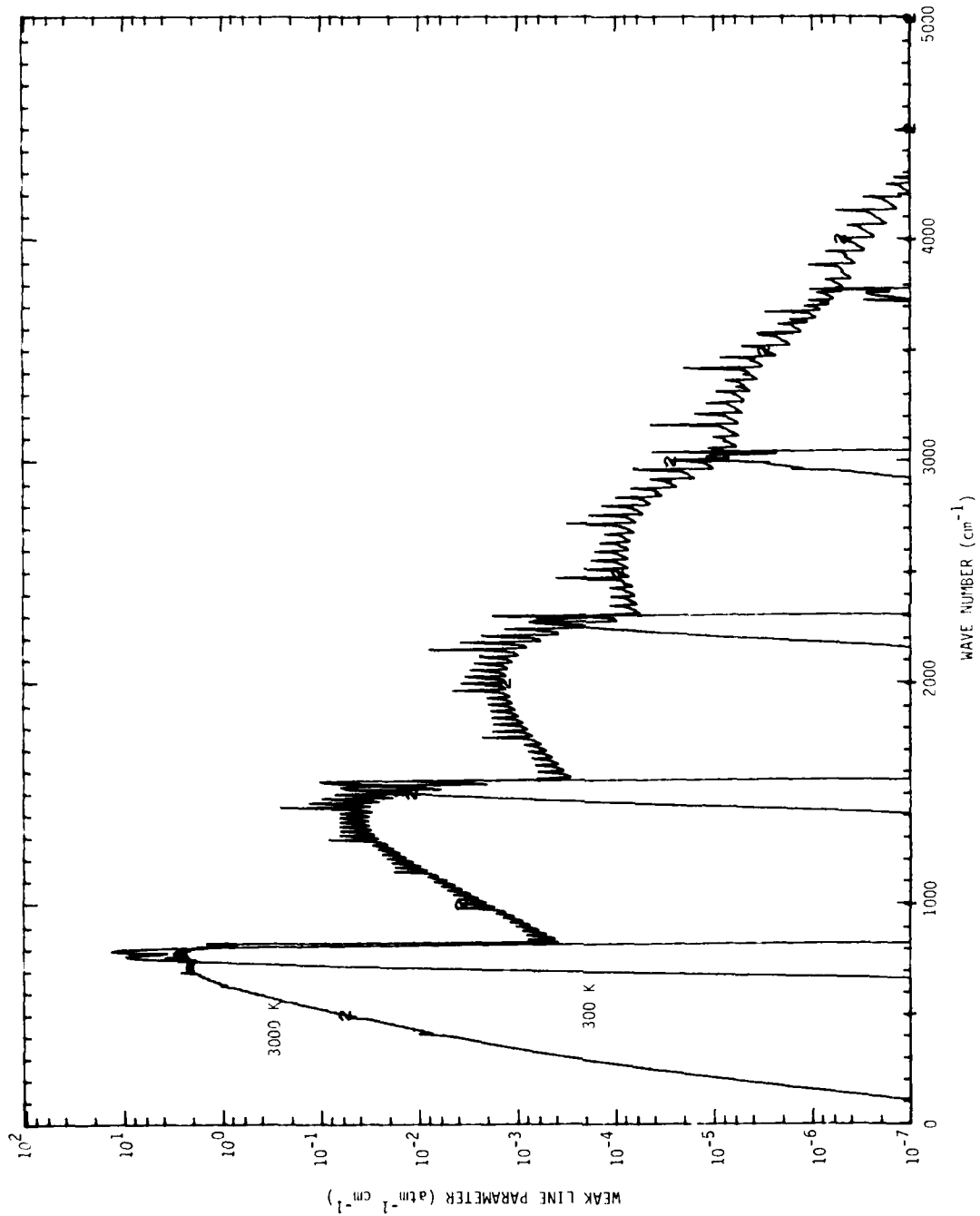


Figure 2-37. Weak line parameters for UO.

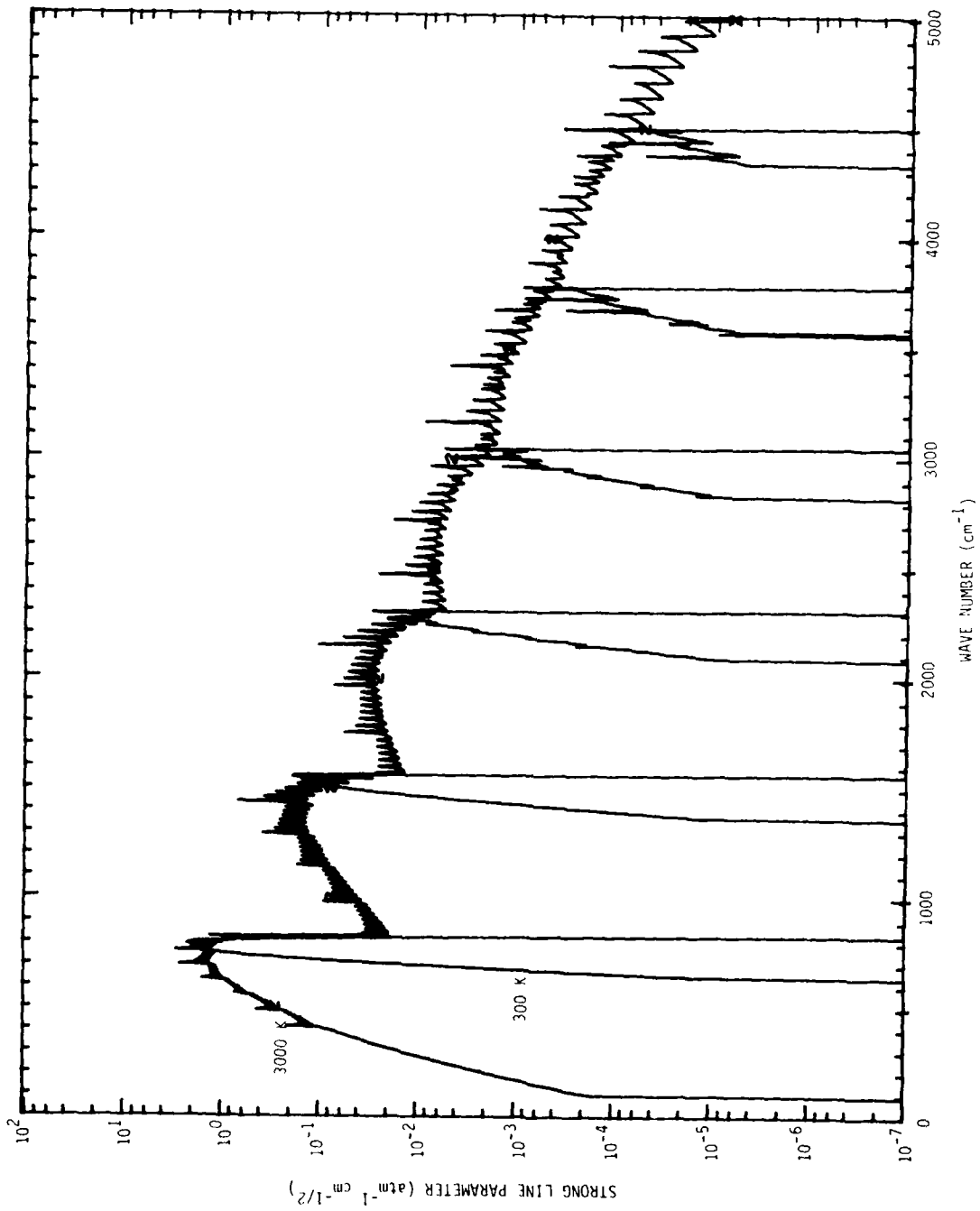


Figure 2-38. Strong line parameters for UO.

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