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RECOMMENDED DATA
ON EXCITATION OF CARBON AND OXYGEN IONS
BY ELECTRON COLLISIONS

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Abstract

Cross sections have been compiled for electron impact excitation of carbon and oxygen ions. A selection has been made to recommend 'best' values for use. The resulting recommended values are fitted to an analytical formula and the fitting coefficients are given in a table. The cross sections (in the form of collision strengths) and the rate coefficients calculated therefrom are shown graphically. The reliability of the recommended data is roughly estimated.

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I. Introduction

Scope

Electron-impact excitation of atomic ions plays a fundamental role in high-temperature plasmas of interest in thermonuclear fusion research and astrophysics.¹⁾ The photon emission caused by the electron-ion collisions, for instance, determines the power balance and provides a useful plasma diagnostics (almost the only one in the case of astrophysics). Cross sections or rates of the electron-impact excitation of ions are the most basic data needed in the relevant research fields.

Although very few detailed (beam type) measurements have been done so far, a large number of data on the excitation cross section are available from theoretical calculations.^{2,3)} Those data, however, are scattered throughout the literature so that it is often difficult to find the appropriate one. Furthermore, the reliability of the theoretical results varies widely depending on the approximate methods used. Thus it is valuable to compile all the data available and assess the reliability of them. The present report is the result of our efforts for all the ions of carbon and oxygen. As a final product, we present here the cross sections (in the form of collision strengths) recommended to be ‘best’ at the present time for various excitation processes. For users’ convenience, the rate coefficients calculated with the Maxwellian distribution of electron velocity are also presented.

The present activity of data compilation and evaluation has been performed as a collaborative program of the U.S. and Japan atomic data centers for fusion research (the Controlled Fusion Atomic Data Center of Oak Ridge National Laboratory and the Research Information Center of Institute of Plasma Physics, Nagoya University). The work is also incorporated in the Coordinated Research Program on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas organized by International Atomic Energy Agency.

Procedure of data compilation and evaluation

In this report, cross sections are expressed in terms of collision strengths. For the excitation of a state i to f , the cross section is given by

$$Q_{if} (\text{in } \pi a_0^2) = \frac{\Omega_{if}}{\omega_i E_e (\text{in Ry})} \quad (1)$$

$$= \frac{1}{\omega_i V_{if} (\text{in Ry})} \frac{\Omega_{if}}{X} , \quad (2)$$

where E_e is the energy of the incident electron, ω_i is the statistical weight of the initial state, V_{if} is the excitation energy, and Ω_{if} is the collision strength. The reduced electron energy is defined by

$$X = E_e / V_{if} . \quad (3)$$

In many cases, Ω_{if} is expressed as a function of X . When the cross section and energy are given in the units of cm^2 and eV, respectively, we have

$$Q_{if} (\text{in } \text{cm}^2) = 11.969 \times 10^{-16} \frac{\Omega_{if}}{\omega_i E_e (\text{in eV})} \quad (4)$$

$$= 11.969 \times 10^{-16} \frac{1}{\omega_i V_{if} (\text{in eV})} \frac{\Omega_{if}}{X} \quad (5)$$

With the Maxwellian distribution of electron velocity for temperature T_e , the rate coefficients are calculated by

$$R_{if} (\text{in } \text{cm}^3 \text{ sec}^{-1}) \\ = \frac{8.010 \times 10^{-8}}{\omega_i \sqrt{T_e (\text{in eV})}} y \int_1^\infty dX \Omega_{if}(X) e^{-yX} \quad (6)$$

with

$$y = V_{if} / T_e . \quad (7)$$

The literature was surveyed extensively through early 1982.^{2,3)} At the final stage of the preparation of the manuscript, some very recent (up to the end of 1982) results have been included. In the present report, all available data, except for 2s-2p excitation of C IV, are theoretical. Based on the critical review of the theoretical methods used, the most reliable data were selected from the literature. In so doing, the following points were taken into account:

- (1) The accuracy of the wave functions employed in the calculation for the target (ion) states.
- (2) The validity of the approximations imposed on the collision dynamics (the degree of the channel couplings, the method of representation of the electron exchange, etc.)
- (3) Whether and how the resonance effects are considered.

In some cases, an inquiry was made to the original authors to get detailed information about their methods of calculations. When the most accurate results are available only in a limited range of electron energies, an extrapolation was made with the help of other calculations. The actual data compilation and evaluation was performed first independently by the U.S. and Japan data centers. Then the results were compared in detail to determine the final set of the recommended data.

Once the recommended cross sections were determined, a fitting was made to analytical formulas, which facilitates their application. Two types of formulas have been used:

Type 1

$$\Omega_{if}(X) = A + \frac{B}{X} + \frac{C}{X^2} + \frac{D}{X^3} + E \ln X \quad (8)$$

Type 2

$$\Omega_{if}(X) = \frac{A}{X^2} + Be^{-FX} + Ce^{-2FX} + De^{-3FX} + Ee^{-4FX} \quad (9)$$

Here A,B,C,D,E, and F are adjustable coefficients. Because of its simplicity the Type 1 is used in most cases. With the use of these formulas, the rate coefficients can be calculated easily in the form

$$R(\text{in cm}^3 \text{ sec}^{-1}) = \frac{8.010 \times 10^{-8}}{\omega_i \sqrt{T_e(\text{eV})}} e^{-y} \gamma$$

with, for Type 1,

$$\gamma = y \left\{ \left(\frac{A}{y} + C \right) + \frac{D}{2} (1 - y) + e^y E_1(y) \left(B - Cy + \frac{D}{2} y^2 + \frac{E}{y} \right) \right\} \quad (10)$$

and, for Type 2,

$$\begin{aligned} \gamma = Ay & \left\{ 1 - e^y E_1(y)y \right\} + \left\{ \frac{B}{F+y} e^{-F} + \frac{C}{2F+y} e^{-2F} \right. \\ & \left. + \frac{D}{3F+y} e^{-3F} + \frac{E}{4F+y} e^{-4F} \right\} y \end{aligned} \quad (11)$$

where $E_1(y) = \int_y^\infty \frac{e^{-t}}{t} dt$.

The fitting error is usually less than 10% and always less than the estimated inaccuracy of the recommended cross sections.

The resonance effect is included as far as it is known to be large and any quantitative information is available. Usually we can divide the collision strength into two parts

$$\Omega = \Omega_{NR}(X) \quad \text{for } X \geq X_1 \quad (12a)$$

$$= \Omega_R(X) \quad \text{for } 1 \leq X < X_1, \quad (12b)$$

where Ω_R and Ω_{NR} are obtained by the calculation with and without resonance effects, respectively. The energy X_1 defines the region where the resonance effect dominates. Since Ω_R has a complicated resonance structure as a function of X , it is almost impossible to fit it to any simple formula. Instead we introduce an effective collision strength in the form

$$\Omega_R^{\text{eff}}(X) = PX + Q \quad , \text{ for } 1 \leq X \leq X_1 . \quad (13)$$

Rate coefficients calculated with Ω_{NR} and Ω_R^{eff} are compared to those presented in the original literature which considered resonance effects. Then the parameters P and Q are determined. To better reproduce the rate coefficients X_1 is adjusted also within the theoretically reasonable values. In the following tables, the fitting coefficients A,B,... for Ω_{NR} and P,Q for Ω_R^{eff} are given. The Ω_R^{eff} , therefore, does not represent the resonance structure of Ω_R but the rate coefficients obtained therefrom give values including the average effect of the resonance.

Explanation of tables and figures

In the next section, the fitting coefficients are given in a tabular form for each excitation process. With these coefficients and the excitation energy (V_{if} , also shown in the table) one can easily obtain numerical values of the cross section or the rate coefficient. In the Appendix, a FORTRAN code is given for the calculation of the rate coefficient. The numerical values of V_{if} have been taken from the NBS tables⁴⁾ (All the original cross sections, on which the present recommended data are based, are stored in the computerized data base (AMDIS) at the Research Information Center, IPP/Nagoya. Those cross sections are available through an on-line terminal or upon request to the Center.)

When using the present recommended data, one should note their validity range and accuracy, both of which are indicated in the table. We have derived the analytical formulas by a fitting procedure over the finite range of electron energies for which the original data exist. It is dangerous to simply extend the formulas outside of their validity range. The accuracy attached to each recommended value should not be considered too rigorous, since it represents only an "educated guess" in most cases.

In Section III, the recommended values of rate coefficients and collision strengths are shown in a graphical form. When the resonance effect is included, the resonance region is indicated by a hatch in the figure of collision strength, instead of showing Ω_R^{eff} there. A brief discussion about the data evaluation and the relevant data sources are given for each isoelectronic stage of the ions. The literature shown is only that selected to provide the recommended data. Other literature is shown in the bibliography.^{2,3)} The data source lists include a notation indicating the excitation process for which the source is used and the theoretical method employed in the calculation.

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References for Introduction

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- 3) Y. Itikawa: Bibliography on electron collisions with atomic positive ions, 1978 through 1982, IPPJ-AM-24 (Inst. Plasma Phys., Nagoya Univ., Nagoya, 1982).
- 4) C.E. Moore: Atomic Energy Levels, vol. I, NSRDS-NBS 35 (1971); Selected Tables of Atomic Spectra, NSRDS-NBS 3, Section 3 (1970), Section 7 (1976), Section 8 (1979).

II. Fitting parameters of the recommended collision strengths and rate coefficients

For each excitation process, the following are presented in the table:

1st line: (initial-final) states

excitation energy, V (in eV)

validity range, $X=X_{\min} - X_{\max}$

type of the fitting formula [see Eqs (8), (9)]

estimated accuracy (A ~ 20%, B ~ 50%, C ~ factor of two)

2nd line: fitting coefficients, A,B,C,D,E,F (only for type 2)

3rd line (when the resonance effect is included):

fitting coefficients, P,Q and the resonance region, X_1 [see Eq (13)]

All the numerical coefficients are expressed in the form

$$2.048 - 1 = 2.048 \times 10^{-1}$$

C VI (H like)

1s - 2s V=367.5eV X ≥ 1.33 Type 1 Accuracy A
 A=2.730-2 B=-3.780-2 C=3.270-2 D=0.0 E=0.0

- 2p V=367.5eV X ≥ 1.33 Type 1 Accuracy A
 A=1.040-2 B=1.720-2 C=4.370-2 D=0.0 E=1.259-1

- 3s V=435.5eV X=1.0-20.0 Type 1 Accuracy B
 A=4.866-3 B=-2.523-3 C=3.158-3 D=-1.765-3 E=0.0

- 3p V=435.5eV X=1.0-20.0 Type 1 Accuracy A
 A=5.264-3 B=7.181-4 C=1.064-2 D=0.0 E=2.136-2

- 3d V=435.6eV X=1.0-20.0 Type 1 Accuracy B
 A=3.877-3 B=-6.120-3 C=4.175-3 D=1.502-3 E=0.0

- 4s V=459.4eV X=1.0-20.0 Type 1 Accuracy B
 A=1.810-3 B=-9.661-4 C=1.295-3 D=-7.331-4 E=0.0

- 4p V=459.4eV X=1.0-20.0 Type 1 Accuracy A
 A=2.682-3 B=-9.488-4 C=4.655-3 D=0.0 E=7.416-3

- 5p V=470.4eV X=1.0-20.0 Type 1 Accuracy A
 A=1.573-3 B=-1.033-3 C=2.628-3 D=0.0 E=3.438-3

C V (He like)

$$\frac{1s^2 \ 1S - 1s2s \ 3S}{A=-1.820-5 \quad B=1.093-3 \quad C=1.675-2 \quad D=-8.788-3 \quad E=0.0} \quad V=298.95\text{eV} \quad X=1.05-42.0 \quad \text{Type 1} \quad \text{Accuracy A}$$

[P=-3.417-1 \quad Q=3.796-1 \quad X1=1.06]

$$\frac{-1s2s \ 1S}{A=2.830-2 \quad B=-3.159-2 \quad C=2.694-2 \quad D=-1.063-2 \quad E=0.0} \quad V=304.4\text{eV} \quad X=1.03-100 \quad \text{Type 1} \quad \text{Accuracy A}$$

$$\frac{-1s2p \ 3P}{A=1.850-5 \quad B=-1.77-3 \quad C=6.155-2 \quad D=-1.570-2 \quad E=0.0} \quad V=304.4\text{eV} \quad X=1.05-42.0 \quad \text{Type 1} \quad \text{Accuracy A}$$

[P=1.786-2 \quad Q=2.710-2 \quad X1=1.28]

$$\frac{-1s2p \ 1P}{A=-6.756-3 \quad B=2.554-2 \quad C=1.448-2 \quad D=0.0 \quad E=1.313-1} \quad V=307.9\text{eV} \quad X=1.02-56.0 \quad \text{Type 1} \quad \text{Accuracy A}$$

$$\frac{-1s3d \ 3D}{A=5.061-5 \quad B=-5.619-4 \quad C=2.116-3 \quad D=7.610-4 \quad E=0.0} \quad V=354.3\text{eV} \quad X=1.0-5.0 \quad \text{Type 1} \quad \text{Accuracy C}$$

$$\frac{-1s3p \ 1P}{A=1.286-2 \quad B=-2.133-2 \quad C=1.656-2 \quad D=0.0 \quad E=2.107-2} \quad V=354.5\text{eV} \quad X=1.0-56.4 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{1s2s \ 3S - 1s2s \ 1S}{A=8.467-3 \quad B=5.722-1 \quad C=-1.475 \quad D=1.498 \quad E=0.0} \quad V=5.43\text{eV} \quad X=1.96-119.3 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-1s2p \ 3P}{A=4.806 \quad B=2.003+1 \quad C=-8.582 \quad D=0.0 \quad E=5.148} \quad V=5.45\text{eV} \quad X=1.89-1000 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-1s2p \ 1P}{A=-5.935-3 \quad B=6.629-1 \quad C=-7.395-1 \quad D=2.695-1 \quad E=0.0} \quad V=8.94\text{eV} \quad X=1.17-70 \quad \text{Type 1} \quad \text{Accuracy B}$$

C V (continued)

$$\frac{1s2s \ ^3S - 1s3p \ ^3P}{A=-7.449-1 \quad B=1.335 \quad C=-3.423-1 \quad D=0.0 \quad E=1.011} \quad V=54.57\text{eV} \quad X=1.0-36.7 \quad \text{Type 1} \quad \text{Accuracy C}$$

$$\frac{1s2s \ ^1S - 1s2p \ ^3P}{A=1.187-2 \quad B=4.767-2 \quad C=-3.971-2 \quad D=3.753-2 \quad E=1.534-1 \quad F=6.0-4} \quad V=0.022\text{eV} \quad X=23.7-7762 \quad \text{Type 2} \quad \text{Accuracy C}$$

$$\frac{- 1s2p \ ^1P}{A=2.073 \quad B=3.990 \quad C=-1.214 \quad D=0.0 \quad E=1.720} \quad V=3.51\text{eV} \quad X=1.43-1000 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{1s2p \ ^3P - 1s2p \ ^1P}{A=2.487-2 \quad B=1.042 \quad C=-3.304 \quad D=6.244 \quad E=-3.249 \quad F=2.0-2} \quad V=3.49\text{eV} \quad X=1.46-80.0 \quad \text{Type 2} \quad \text{Accuracy B}$$

$$\frac{- 1s3s \ ^3S}{A=-1.091-1 \quad B=2.359-1 \quad C=-5.644-2 \quad D=0.0 \quad E=1.758-1} \quad V=47.65\text{eV} \quad X=1.0-42.0 \quad \text{Type 1} \quad \text{Accuracy C}$$

C IV (Li like)

$2s\ ^2S - 2p\ ^2P$ V=8.00eV X=1.01–99.07 Type 1 Accuracy A
A=4.103 B=6.410 C=−1.677 D=0.0 E=4.688

$- 3s\ ^2S$ V=37.55eV X=1.45–100.0 Type 1 Accuracy A
A=4.846−1 B=−2.743−1 C=4.768−1 D=−3.971−1 E=0.0
[P=7.390−1 Q=2.460−1 X1=1.072]

$- 3p\ ^2P$ V=39.68eV X=1.375–100 Type 1 Accuracy A
A=−5.731−1 B=9.548−1 C=−8.931−2 D=0.0 E=5.638−1
[P=0.0 Q=7.500−1 X1=1.013]

$- 3d\ ^2D$ V=40.28eV X=1.355–100 Type 1 Accuracy A
A=1.252 B=−1.243 C=4.930−1 D=1.326−1 E=0.0

C III (Be like)

$2s^2 \ 1S - 2s2p \ ^3P$ V=6.50eV X=3.14–39.9 Type 1 Accuracy B
 A=-4.024–2 B=2.914 C=-4.344 D=2.121 E=0.0
 [P=5.434–1 Q=3.453–1 X1=2.0]

$- 2s2p \ ^1P$ V=12.69eV X=1.05–100 Type 1 Accuracy A
 A=-1.294 B=7.447 C=-2.301 D=0.0 E=4.853

$- 2p^2 \ ^3P$ V=17.04eV X=1.04–11.0 Type 1 Accuracy B
 A=-1.941–3 B=3.086–2 C=-1.387–2 D=-4.363–3 E=0.0
 [P=5.389–3 Q=7.167–3 X1=2.0]

$- 2p^2 \ ^1D$ V=18.09eV X=1.04–17.78 Type 1 Accuracy B
 A=2.785–1 B=7.730–2 C=1.894–1 D=-1.614–1 E=0.0

$- 2p^2 \ ^1S$ V=22.63eV X=1.0–1.5 Type 1 Accuracy B
 A=1.481–1 B=-3.128–1 C=3.116–1 D=-1.114–1 E=0.0

$- 2s3s \ ^3S$ V=29.53eV X=1.01–150 Type 1 Accuracy C
 A=2.709–8 B=1.256–3 C=1.260–1 D=4.108–2 E=0.0

$- 2s3s \ ^1S$ V=30.64eV X=1.01–150 Type 1 Accuracy C
 A=6.082–1 B=-1.927–1 C=-3.615–2 D=3.487–2 E=0.0

$- 2s3p \ ^1P$ V=32.10eV X=1.01–150 Type 1 Accuracy C
 A=-4.225–1 B=4.879–1 C=-3.487–2 D=0.0 E=4.107–1

$- 2s3p \ ^3P$ V=32.20eV X=1.01–150 Type 1 Accuracy C
 A=4.886–4 B=-3.914–3 C=1.885–1 D=-5.672–2 E=0.0

C III (continued)

$2s^2 \underline{1S} - 2s3d \underline{3D}$ V=33.48eV X=1.01–150 Type 1 Accuracy C
 A=2.612–6 B=–7.936–3 C=3.669–1 D=1.441–1 E=0.0

$\underline{- 2s3d} \underline{1D}$ V=34.28eV X=1.01–150 Type 1 Accuracy C
 A=9.396–1 B=–1.105 C=9.915–2 D=2.186–1 E=0.0

$2s2p \underline{3P} - 2s2p \underline{1P}$ V=6.19eV X=1.0–4.16 Type 1 Accuracy B
 A=8.343–2 B=1.645 C=8.765–1 D=–1.605 E=0.0
 [P=–1.154 Q=4.749 X1=3.4]

$\underline{- 2p^2} \underline{3P}$ V=10.54eV X=1.44–100 Type 1 Accuracy B
 A=9.842 B=–8.660 C=2.184+1 D=0.0 E=1.631+1

$\underline{- 2p^2} \underline{1D}$ V=11.59eV X=1.05–2.24 Type 1 Accuracy B
 A=4.974–1 B=3.363–1 C=2.336 D=–1.868 E=0.0

$\underline{- 2p^2} \underline{1S}$ V=16.13eV X=1.01–1.59 Type 1 Accuracy B
 A=7.322–2 B=5.703–2 C=–3.981–2 D=5.783–2 E=0.0

$2s2p \underline{1P} - 2p^2 \underline{3P}$ V=4.35eV X=1.0–33.7 Type 1 Accuracy B
 A=–8.624–3 B=4.141 C=–7.089 D=3.824 E=0.0
 [P=7.072–1 Q=2.889–1 X1=1.85]

$\underline{- 2p^2} \underline{1D}$ V=5.40eV X=1.12–27.3 Type 1 Accuracy B
 A=3.762 B=9.351 C=–3.004 D=0.0 E=7.320

$\underline{- 2p^2} \underline{1S}$ V=9.94eV X=1.02–50.0 Type 1 Accuracy B
 A=3.032 B=–2.375 C=2.675 D=0.0 E=2.991

C III (continued)

$2p^2\ 3P - 2p^2\ 1D$ V=1.04eV X=1.62-15.3 Type 1 Accuracy B
A=1.925 B=1.440+1 C=-3.560+1 D=2.727+1 E=0.0

$- 2p^2\ 1S$ V=5.59eV X=1.03-2.67 Type 1 Accuracy B
A=4.319-2 B=1.004 C=-1.037 D=3.630-1 E=0.0

$2p^2\ 1D - 2p^2\ 1S$ V=4.54eV X=1.04-2.46 Type 1 Accuracy B
A=8.948-1 B=-8.607-1 C=1.007 D=-4.136-1 E=0.0

C II (B like)

$$\frac{2s^2 2p \ ^2P - 2s2p^2 \ ^4P}{A=4.360-1 \ B=1.627 \ C=-2.923 \ D=1.094+1 \ E=-6.580 \ F=5.769-2} \quad V=5.33\text{eV} \quad X=1.01-28.84 \quad \text{Type 2} \quad \text{Accuracy B}$$

$$\frac{-2s2p^2 \ ^2D}{A=-2.155 \ B=1.374+1 \ C=-6.562 \ D=0.0 \ E=1.018+1} \quad V=9.29\text{eV} \quad X=1.62-100 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2s2p^2 \ ^2S}{A=8.572-1 \ B=2.079-1 \ C=7.058-1 \ D=0.0 \ E=4.136} \quad V=11.96\text{eV} \quad X=1.26-100 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2s2p^2 \ ^2P}{A=-6.883-1 \ B=4.106 \ C=3.435-1 \ D=0.0 \ E=1.631+1} \quad V=13.71\text{eV} \quad X=1.08-100 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2s^2 3s \ ^2S}{A=-9.843-1 \ B=2.983 \ C=-9.975-1 \ D=0.0 \ E=8.910-1} \quad V=14.45\text{eV} \quad X=1.0-100 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2s^2 3p \ ^2P}{A=1.678 \ B=-2.238 \ C=4.829 \ D=0.0 \ E=0.0} \quad V=16.33\text{eV} \quad X=1.0-100 \quad \text{Type 1} \quad \text{Accuracy C}$$

$$\frac{-2s^2 3d \ ^2D}{A=-1.703 \ B=2.675 \ C=1.165 \ D=0.0 \ E=5.791} \quad V=18.05\text{eV} \quad X=1.0-100 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{2s2p^2 \ ^4P - 2s2p^2 \ ^2D}{A=-2.799 \ B=-3.349 \ C=2.420+1 \ D=-5.326+1 \ E=4.093+1 \ F=2.2-2} \quad V=3.96\text{eV} \quad X=2.11-50.03 \quad \text{Type 2} \quad \text{Accuracy B}$$

$$\frac{-2s2p^2 \ ^2S}{A=-7.513-1 \ B=-6.903-3 \ C=5.230-1 \ D=-1.767 \ E=2.847 \ F=6.0-2} \quad V=6.629\text{eV} \quad X=1.39-32.77 \quad \text{Type 2} \quad \text{Accuracy B}$$

$$\frac{-2s2p^2 \ ^2P}{A=-4.959-1 \ B=3.437-1 \ C=-8.580-1 \ D=2.802 \ E=3.654-1 \ F=1.2-1} \quad V=8.38\text{eV} \quad X=1.09-25.70 \quad \text{Type 2} \quad \text{Accuracy B}$$

C II (continued)

$2s2p^2 \ 2D - 2s2p^2 \ 2S$ V=2.67eV X=2.12–93.15 Type 1 Accuracy B
A=6.241–1 B=2.283 C=–1.415 D=0.0 E=5.071–1

$- 2s2p^2 \ 2P$ V=4.43eV X=1.18–51.78 Type 1 Accuracy B
A=–1.645–1 B=1.918+1 C=–3.479+1 D=1.897+1 E=0.0

$2s2p^2 \ 2S - 2s2p^2 \ 2P$ V=1.75eV X=1.40–115 Type 2 Accuracy B
A=–1.273–1 B=1.126 C=–4.665 D=8.542 E=–4.666 F=2.3–2

O VIII (H like)

1s - 2s V=653.5eV X≥ 1.33 Type 1 Accuracy A
A=1.520-2 B=-1.810-2 C=1.450-2 D=0.0 E=0.0

- 2p V=653.6eV X≥ 1.33 Type 1 Accuracy A
A=3.980-3 B=-5.660-4 C=4.460-2 D=0.0 E=7.3-2

O VII (He like)

$1s^2 1S - 1s2s 3S$ V=561.0eV X=1.0–30.0 Type 1 Accuracy A
 A=−2.330−5 B=1.029−3 C=5.973−3 D=−2.860−3 E=0.0
 [P=−5.220−2 Q=6.500−2 X1=1.18]

$- 1s2p 3P$ V=568.6eV X=1.0–30.0 Type 1 Accuracy A
 A=5.740−5 B=−8.057−4 C=3.323−2 D=−9.383−3 E=0.0
 [P=1.815−2 Q=7.020−3 X1=1.2]

$- 1s2s 1S$ V=568.7eV X=1.0–30.0 Type 1 Accuracy A
 A=1.605−2 B=−2.413−2 C=2.721−2 D=−1.269−2 E=0.0

$- 1s2p 1P$ V=573.9eV X=1.0–30.0 Type 1 Accuracy A
 A=−2.381−2 B=4.686−2 C=−2.781−3 D=0.0 E=8.117−2

$- 1s3s 3S$ V=661.9eV X=1.01–300 Type 1 Accuracy B
 A=−2.095−6 B=9.692−5 C=2.286−3 D=−1.469−3 E=0.0

$- 1s3p 3P$ V=664.0eV X=1.01–21.4 Type 1 Accuracy B
 A=1.646−5 B=−3.129−4 C=8.096−3 D=−1.389−3 E=0.0

$- 1s3s 1S$ V=664.1eV X=1.01–30.0 Type 1 Accuracy B
 A=2.962−3 B=−1.324−3 C=−5.756−5 D=1.415−4 E=0.0

$- 1s3d 3D$ V=665.1eV X=1.01–30.0 Type 1 Accuracy B
 A=2.406−5 B=−5.986−5 C=5.180−4 D=9.704−4 E=0.0

$- 1s3d 1D$ V=665.2eV X=1.01–30.0 Type 1 Accuracy B
 A=1.797−3 B=−2.615−3 C=8.263−4 D=2.189−4 E=0.0

O VII (continued)

$$\frac{1s^2 \ ^1S - 1s3p \ ^1P}{A=4.432-3 \quad B=-2.303-3 \quad C=2.118-3 \quad D=0.0 \quad E=1.233-2} \quad V=665.6\text{eV} \quad X=1.01-30.0 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{1s2s \ ^3S - 1s2p \ ^3P}{A=3.345 \quad B=3.438 \quad C=6.003 \quad D=0.0 \quad E=2.655} \quad V=7.58\text{eV} \quad X=1.85-316.6 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-1s2s \ ^1S}{A=8.573-3 \quad B=2.091-1 \quad C=-3.500-1 \quad D=1.878-1 \quad E=0.0} \quad V=7.77\text{eV} \quad X=1.85-60.5 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-1s2p \ ^1P}{A=-2.606-3 \quad B=4.078-1 \quad C=-6.281-1 \quad D=3.170-1 \quad E=0.0} \quad V=12.96\text{eV} \quad X=1.09-90.71 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-1s3p \ ^3P}{A=-1.000 \quad B=1.927 \quad C=-8.014-1 \quad D=0.0 \quad E=7.928-1} \quad V=103.0\text{eV} \quad X=1.0-14.0 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{1s2p \ ^3P - 1s2s \ ^1S}{A=4.214-3 \quad B=4.741-2 \quad C=1.919-1 \quad D=-4.080-1 \quad E=2.326-1 \quad F=2.0-3} \quad V=0.186\text{eV} \quad X=23.7-597 \quad \text{Type 2} \quad \text{Accuracy C}$$

$$\frac{-1s2p \ ^1P}{A=-1.564-3 \quad B=5.805-1 \quad C=-1.586 \quad D=2.947 \quad E=-1.570 \quad F=2.2-2} \quad V=5.38\text{eV} \quad X=1.23-81.2 \quad \text{Type 2} \quad \text{Accuracy B}$$

$$\frac{-1s3s \ ^3S}{A=-4.914-2 \quad B=1.152-1 \quad C=-2.967-2 \quad D=0.0 \quad E=8.232-2} \quad V=93.35\text{eV} \quad X=1.0-21.4 \quad \text{Type 1} \quad \text{Accuracy C}$$

$$\frac{1s2s \ ^1S - 1s2p \ ^1P}{A=9.145-1 \quad B=3.313 \quad C=-1.739 \quad D=0.0 \quad E=9.779-1} \quad V=5.19\text{eV} \quad X=1.31-219.9 \quad \text{Type 1} \quad \text{Accuracy B}$$

O VI (Li like)

$2s\ ^2S - 2p\ ^2P$ V=11.98eV X=1.01–89.7 Type 1 Accuracy A
A=2.458 B=4.108 C=-1.364 D=0.0 E=2.155

$-3s\ ^2S$ V=79.35eV X=1.01–100 Type 1 Accuracy A
A=2.376–1 B=−8.963–2 C=5.050–2 D=2.557–2 E=0.0
[P=1.010–1 Q=1.930–1 X1=1.072]

$-3p\ ^2P$ V=82.60eV X=1.01–100 Type 1 Accuracy A
A=−5.263–1 B=9.758–1 C=−3.297–1 D=0.0 E=4.039–1
[P=0.0 Q=3.400–1 X1=1.012]

$-3d\ ^2D$ V=83.64eV X=1.01–100 Type 1 Accuracy A
A=6.552–1 B=−6.557–1 C=3.349–1 D=−3.643–3 E=0.0

O V (Be like)

$2s^2 1S - 2s2p\ 3P$ $V=10.20\text{eV}$ $X=1.2-31.7$ Type 1 Accuracy B

$A=-2.210-2 \quad B=1.800 \quad C=-4.590 \quad D=4.150 \quad E=0.0$

$[P=-1.001-1 \quad Q=6.774-1 \quad X1=4.5]$

$- 2s2p\ 1P$ $V=19.68\text{eV}$ $X=1.03-100$ Type 1 Accuracy A

$A=9.739-1 \quad B=2.167 \quad C=-6.987-1 \quad D=0.0 \quad E=1.791$

$- 2p^2 3P$ $V=26.50\text{eV}$ $X=1.0-2.18$ Type 1 Accuracy B

$A=2.298-3 \quad B=1.502-3 \quad C=1.469-2 \quad D=-1.356-2 \quad E=0.0$

$[P=7.921-3 \quad Q=7.421-4 \quad X1=1.40]$

$- 2p^2 1D$ $V=28.50\text{eV}$ $X=1.02-1.89$ Type 1 Accuracy B

$A=1.080-1 \quad B=-9.765-2 \quad C=2.089-1 \quad D=1.077-1 \quad E=0.0$

$- 2p^2 1S$ $V=35.69\text{eV}$ $X=1.04-1.60$ Type 1 Accuracy B

$A=-1.925-2 \quad B=4.741-2 \quad C=-1.064-2 \quad D=0.0 \quad E=2.589-2$

$- 2s3s\ 3S$ $V=67.82\text{eV}$ $X=1.01-100$ Type 1 Accuracy A

$A=-5.520-6 \quad B=7.562-4 \quad C=5.532-2 \quad D=-3.634-2 \quad E=0.0$

$[P=-4.745-1 \quad Q=6.157-1 \quad X1=1.07]$

$- 2s3s\ 1S$ $V=69.57\text{eV}$ $X=1.01-100$ Type 1 Accuracy B

$A=2.909-1 \quad B=3.083-2 \quad C=-1.596-1 \quad D=8.767-2 \quad E=0.0$

$- 2s3p\ 1P$ $V=71.99\text{eV}$ $X=1.01-100$ Type 1 Accuracy B

$A=-2.736-1 \quad B=3.828-1 \quad C=-8.139-2 \quad D=0.0 \quad E=3.068-1$

$- 2s3p\ 3P$ $V=72.27\text{eV}$ $X=1.01-100$ Type 1 Accuracy A

$A=1.215-4 \quad B=-1.079-3 \quad C=9.940-2 \quad D=-6.484-2 \quad E=0.0$

$[P=-1.768-1 \quad Q=2.745-1 \quad X1=1.30]$

O V (continued)

$$\frac{2s^2 \ 1S - 2s3d \ 3D}{A=6.414-6 \ B=-8.291-4 \ C=2.429-1 \ D=-1.071-1 \ E=0.0} \quad V=74.49\text{eV} \quad X=1.01-100 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2s3d \ 1D}{A=5.936-1 \ B=-6.319-1 \ C=7.450-2 \ D=1.170-1 \ E=0.0} \quad V=75.93\text{eV} \quad X=1.01-100 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{2s2p \ 3P - 2s2p \ 1P}{A=3.689-2 \ B=1.151 \ C=-1.343 \ D=5.549-1 \ E=0.0} \quad V=9.48\text{eV} \quad X=1.0-4.94 \quad \text{Type 1} \quad \text{Accuracy B}$$

[P=-2.588-1 Q=1.530 X1=3.46]

$$\frac{-2p^2 \ 3P}{A=4.910 \ B=5.510 \ C=1.654 \ D=0.0 \ E=7.761} \quad V=16.30\text{eV} \quad X=1.87-100 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2p^2 \ 1D}{A=7.408-2 \ B=8.592-1 \ C=-5.639-1 \ D=7.353-2 \ E=0.0} \quad V=18.52\text{eV} \quad X=1.03-2.56 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2p^2 \ 1S}{A=-2.759-3 \ B=1.189-1 \ C=-9.594-2 \ D=3.108-2 \ E=0.0} \quad V=25.48\text{eV} \quad X=1.06-1.85 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{2s2p \ 1P - 2p^2 \ 3P}{A=1.465-1 \ B=4.035-1 \ C=-5.441-2 \ D=-1.255-1 \ E=0.0} \quad V=6.82\text{eV} \quad X=1.0-5.66 \quad \text{Type 1} \quad \text{Accuracy B}$$

[P=-3.015-1 Q=9.326-1 X1=1.80]

$$\frac{-2p^2 \ 1D}{A=3.086 \ B=7.441 \ C=-3.595 \ D=0.0 \ E=3.406} \quad V=9.04\text{eV} \quad X=1.07-42.4 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2p^2 \ 1S}{A=1.375 \ B=5.958-1 \ C=3.957-1 \ D=0.0 \ E=1.385} \quad V=16.0\text{eV} \quad X=1.09-31.0 \quad \text{Type 1} \quad \text{Accuracy B}$$

O V (continued)

$$\frac{2p^2 \ 3P - 2p^2 \ 1D}{A=9.002-1 \quad B=4.163 \quad C=-7.000 \quad D=3.615 \quad E=0.0} \quad V=2.22\text{eV} \quad X=1.0-14.0 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2p^2 \ 1S}{A=2.242-2 \quad B=5.103-1 \quad C=-5.846-1 \quad D=2.452-1 \quad E=0.0} \quad V=9.18\text{eV} \quad X=1.14-32.9 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{2p^2 \ 1D - 2p^2 \ 1S}{A=3.465-1 \quad B=-1.604-1 \quad C=1.969-1 \quad D=-9.603-2 \quad E=0.0} \quad V=6.96\text{eV} \quad X=1.19-3.99 \quad \text{Type 1} \quad \text{Accuracy B}$$

O IV (B like)

$2s^2 2p\ ^2P - 2s2p\ ^24P$ V=8.817eV X=3.01–100 Type 2 Accuracy B
 A=-1.022–1 B=1.140–1 C=2.543–1 D=-9.621–1 E=1.737 F=2.0–2
 [P=3.006 Q=-2.029 X1=1.66]

$- 2s2p\ ^2D$ V=15.71eV X=1.0–50 Type 1 Accuracy B
 A=2.162 B=4.458 C=-1.030 D=0.0 E=3.218

$- 2s2p\ ^2S$ V=20.35eV X=1.0–100 Type 1 Accuracy B
 A=1.054 B=1.252 C=-2.153–1 D=0.0 E=1.333

$- 2s2p\ ^2P$ V=22.36eV X=1.0–100 Type 1 Accuracy B
 A=1.241 B=6.902 C=-1.398 D=0.0 E=6.723

$- 2s^2 3s\ ^2S$ V=44.34eV X=1.0–100 Type 1 Accuracy C
 A=-2.530–1 B=4.230–1 C=6.706–2 D=0.0 E=3.171–1

$- 2s^2 3d\ ^2D$ V=52.02eV X=1.0–100 Type 1 Accuracy C
 A=-1.202 B=3.442 C=3.830–1 D=0.0 E=3.182

$2s2p\ ^24P - 2s2p\ ^22D$ V=6.89eV X=1.96–96.88 Type 2 Accuracy B
 A=2.990–1 B=4.261–1 C=-1.923–1 D=-2.971–1 E=3.472 F=2.794–2

$- 2s2p\ ^22S$ V=11.53eV X=1.26–62.28 Type 2 Accuracy B
 A=4.727–3 B=2.812–2 C=1.875–3 D=-5.547–3 E=4.784–1 F=5.129–2

$- 2s2p\ ^22P$ V=13.54eV X=1.04–51.29 Type 2 Accuracy B
 A=7.622–2 B=7.117–2 C=-5.254–2 D=-9.925–2 E=6.900–1 F=5.625–2

O IV (continued)

$2s2p^2 \ ^2D - 2s2p^2 \ ^2S$ V=4.64eV X=1.73–172.59 Type 1 Accuracy B
A=2.619–1 B=7.945–1 C=–4.561–1 D=0.0 E=1.790–1

$- 2s2p^2 \ ^2P$ V=6.65eV X=1.08–107.86 Type 2 Accuracy B
A=–4.831–2 B=–1.468–1 C=2.635 D=–6.246 E=5.529 F=2.0–2

$2s2p^2 \ ^2S - 2s2p^2 \ ^2P$ V=2.01eV X=1.21–285.94 Type 2 Accuracy B
A=–3.310–3 B=3.223–1 C=–8.822–1 D=1.611 E=–7.981–1 F=2.0–2

O III (C like)

$2s^2 2p^2 3P - 2s^2 2p^2 1D$ $V=2.49\text{eV}$ $X=10-54.2$ Type 1 Accuracy A
 A=2.048-1 B=2.267+1 C=-5.568+1 D=3.534+1 E=0.0
 [P=2.329-1 Q=1.905 X1=8.0]

$- 2s^2 2p^2 1S$ $V=5.33\text{eV}$ $X=5.0-54.2$ Type 1 Accuracy A
 A=-2.830-2 B=2.333 C=-4.292 D=2.362 E=0.0
 [P=2.033-1 Q=3.971-2 X1=2.2]

$- 2s2p^3 5S$ $V=7.45\text{eV}$ $X=1.01-50.0$ Type 1 Accuracy A
 A=-4.209-2 B=4.366 C=-7.508 D=4.093 E=0.0
 [P=1.908 Q=-9.649-1 X1=1.6]

$- 2s2p^3 3D$ $V=14.86\text{eV}$ $X=1.0-6.7$ Type 1 Accuracy A
 A=2.792 B=7.147 C=-3.044 D=0.0 E=3.305

$- 2s2p^3 3P$ $V=17.63\text{eV}$ $X=1.0-5.7$ Type 1 Accuracy A
 A=2.790 B=3.733 C=-1.388 D=0.0 E=3.952

$- 2s2p^3 1D$ $V=23.16\text{eV}$ $X=1.01-50.0$ Type 2 Accuracy B
 A=2.175-1 B=3.147-2 C=9.017-2 D=-5.206-1 E=7.260-1 F=4.0-2

$- 2s2p^3 3S$ $V=24.40\text{eV}$ $X=1.0-4.1$ Type 1 Accuracy A
 A=3.773 B=-6.630-1 C=0.0 D=0.0 E=3.517

$- 2s2p^3 1P$ $V=26.06\text{eV}$ $X=1.01-50.0$ Type 1 Accuracy B
 A=-3.712-2 B=3.877-1 C=-1.420-1 D=8.145-3 E=0.0

$2s^2 2p^2 1D - 2s^2 2p^2 1S$ $V=2.84\text{eV}$ $X=1.0-73.6$ Type 1 Accuracy B
 A=7.529-2 B=5.365-1 C=-2.708-1 D=0.0 E=1.154-1
 [P=4.438-1 Q=2.198-2 X1=2.5]

O III (continued)

$$\frac{2s^2 2p^2 1D - 2s2p^3 3D}{A=8.217-2 \quad B=3.273 \quad C=-2.764 \quad D=9.926-1 \quad E=0.0} \quad V=12.37\text{eV} \quad X=1.48-6.58 \quad \text{Type 1} \quad \text{Accuracy B}$$

$$\frac{-2s2p^3 3P}{A=-4.866-2 \quad B=1.117 \quad C=-1.210 \quad D=5.528-1 \quad E=0.0} \quad V=15.14\text{eV} \quad X=1.2-5.4 \quad \text{Type 1} \quad \text{Accuracy B}$$

[P=1.584 Q=-1.270 X1=1.3]

$$\frac{2s^2 2p^2 1S - 2s2p^3 3D}{A=-2.814-3 \quad B=2.446-2 \quad C=1.183-1 \quad D=-1.001-1 \quad E=0.0} \quad V=9.53\text{eV} \quad X=1.93-8.58 \quad \text{Type 1} \quad \text{Accuracy B}$$

[P=-2.629-1 Q=3.412-1 X1=1.4]

$$\frac{-2s2p^3 3P}{A=-2.556-2 \quad B=1.567 \quad C=-2.512 \quad D=1.540 \quad E=0.0} \quad V=12.30\text{eV} \quad X=1.49-6.64 \quad \text{Type 1} \quad \text{Accuracy C}$$

$$\frac{2s2p^3 5S - 2s2p^3 3D}{A=-7.277-2 \quad B=-1.839+2 \quad C=5.719+2 \quad D=-5.911+2 \quad E=2.055+2 \quad F=1.6-2} \quad V=7.40\text{eV} \quad X=2.5-11.1 \quad \text{Type 2} \quad \text{Accuracy B}$$

[P=-3.455-1 Q=2.632 X1=1.24]

$$\frac{-2s2p^3 3P}{A=5.087-2 \quad B=4.700+1 \quad C=-2.392+2 \quad D=3.450+2 \quad E=-1.523+2 \quad F=1.1-2} \quad V=10.18\text{eV} \quad X=1.8-8.0 \quad \text{Type 2} \quad \text{Accuracy B}$$

[P=2.967-1 Q=3.243-1 X1=1.8]

$$\frac{2s2p^3 3D - 2s2p^3 3P}{A=2.948 \quad B=5.846 \quad C=-4.840 \quad D=5.456-1 \quad E=0.0} \quad V=2.78\text{eV} \quad X=6.62-29.4 \quad \text{Type 1} \quad \text{Accuracy C}$$

O II (N like)

$2s^2 2p^3 4S - 2s^2 2p^3 2D$ V=3.32eV X=1.0–4.0 Type 1 Accuracy B
A=2.016 B=−1.650 C=8.640−1 D=7.931−2 E=0.0
[P=9.967−1 Q=−5.161−2 X1=1.8]

$- 2s^2 2p^3 2P$ V=5.02eV X=1.0–3.0 Type 1 Accuracy B
A=2.306−1 B=3.160−1 C=−7.135−2 D=0.0 E=3.133−1

$- 2s^2 2p^4 4P$ V=14.87eV X=1.0–5.3 Type 1 Accuracy A
A=6.673 B=−4.043 C=0.0 D=0.0 E=1.835

$- 2s^2 2p^2 3s^4 P$ V=22.99eV X=1.0–3.5 Type 1 Accuracy A
A=−2.173 B=4.090 C=−1.510 D=0.0 E=1.465

$2s^2 2p^3 2D - 2s^2 2p^3 2P$ V=1.69eV X=1.0–6.9 Type 1 Accuracy B
A=3.072 B=−4.123 C=5.151 D=−2.322 E=0.0

III. Recommended collision strengths and rate coefficients: Graphs and discussions

For each isoelectronic ion of carbon and oxygen, a brief discussion about the data evaluation and a list of data sources are presented first. Then the sets of graphs of the collision strength and the rate coefficient are shown for the excitations of the relevant isoelectronic ions.

The collision strengths are plotted as a function of the reduced energy, X ($=E_e/V_{ij}$). The ordinate scale is indicated by the multiplication factor ' $E - n$ ' ($= 10^{-n}$) at the upper left corner of the graph. The recommended values of the collision strengths are shown only over the validity range given in the table of the last section. The rate coefficients (in cm^3/sec) are plotted against the electron temperature (in eV). It is rather difficult to define the corresponding validity range for the rate coefficients. Here the rate coefficients are shown mostly over the whole temperature range considered. Thus, if the validity range of the collision strength is very narrow, a large error may be included in the rate coefficients presented for the lowest and/or highest region of the temperature.

H-like (C VI, O VIII)

For $1s - 2s$, $2p$, Abu-Salbi and Callaway (1981) made a close-coupling (CC) type calculation with a pseudostate expansion. Based on their results with the basis set of $1s$, $2s$, $2p$ states plus three pseudostates, they obtained the collision strengths for $1s - 2s$ and $1s - 2p$ in the analytical form of Type 1. To extend their formula to higher energy, they supplemented their cross section with the Coulomb-Born-Exchange (CBX) calculation at the high energy. Their fitting coefficients are adopted here. Below the threshold of $n = 3$, they made also a calculation with a larger basis set to estimate resonance effects. They found a 6% resonance enhancement of the rate coefficient for $1s - 2s$ and 3% for $1s - 2p$ at the lowest temperature. The larger-basis calculation, however, gave somewhat lower non-resonant cross sections. Therefore the present analytical formulas for $1s - 2s$ and $1s - 2p$ effectively reproduce the cross sections calculated with the resonance effect taken into account.

For the excitation of the states higher than the $n = 2$ of C VI, Mann's CBX cross sections are employed here. For highly charged ions like C VI, the CBX method gives fairly good values, especially for the optically-allowed transitions.

Data sources

Abu-Salbi, N. and Callaway, J. (1981), Phys. Rev. A **24** 2372

[1s – 2s, 2p, CC]

- Mann, J.B. (1977), quoted in Los Alamos Scientific Laboratory Report, LA-6691-MS,
ed. N.H. Magee, Jr., J.B. Mann, A.L. Merts and W.D. Robb
[1s – 3s, 3p, 3d, 4s, 4p, 5p of C VI, CBX]

Fig. 1

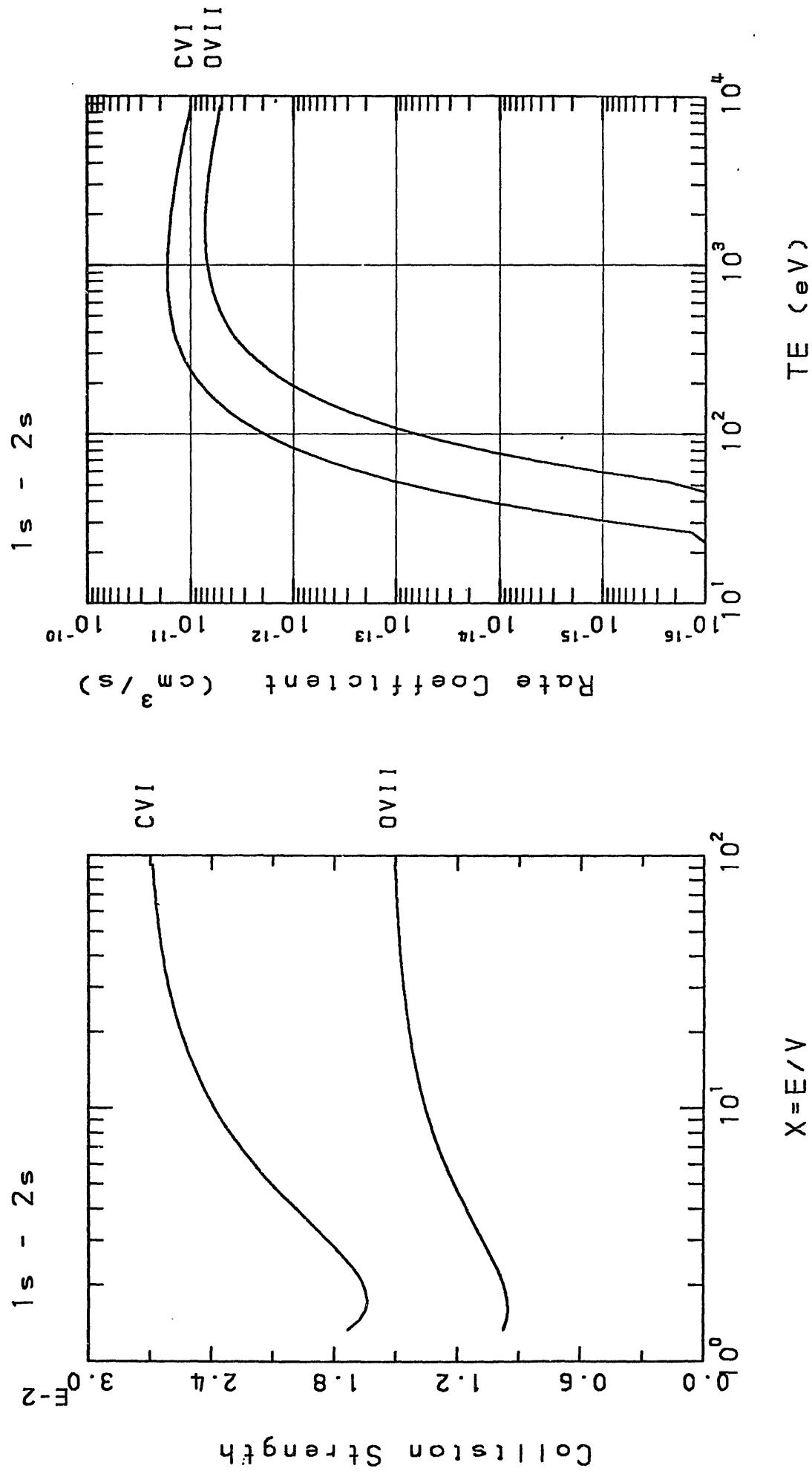


Fig. 2

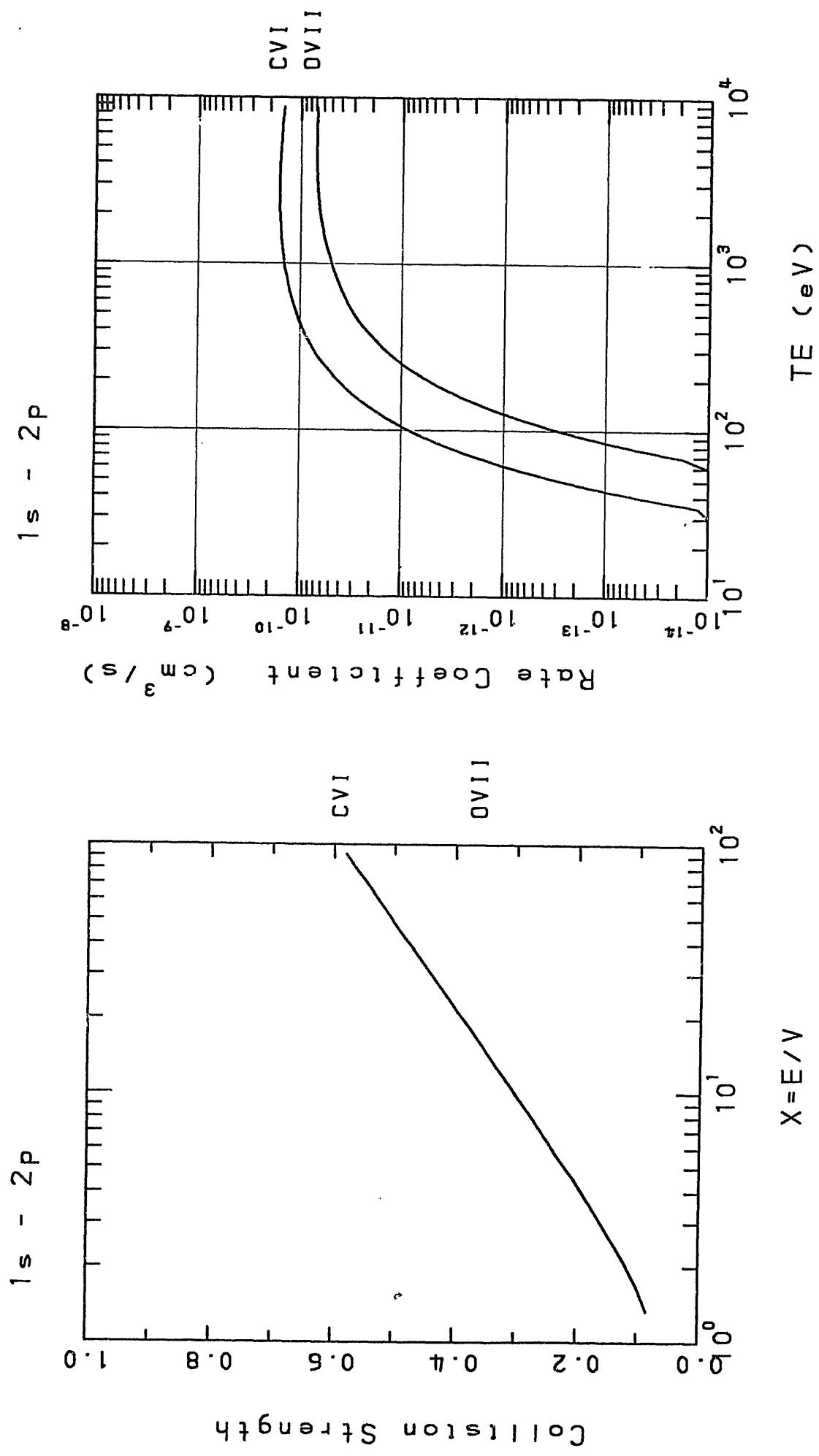


Fig. 3

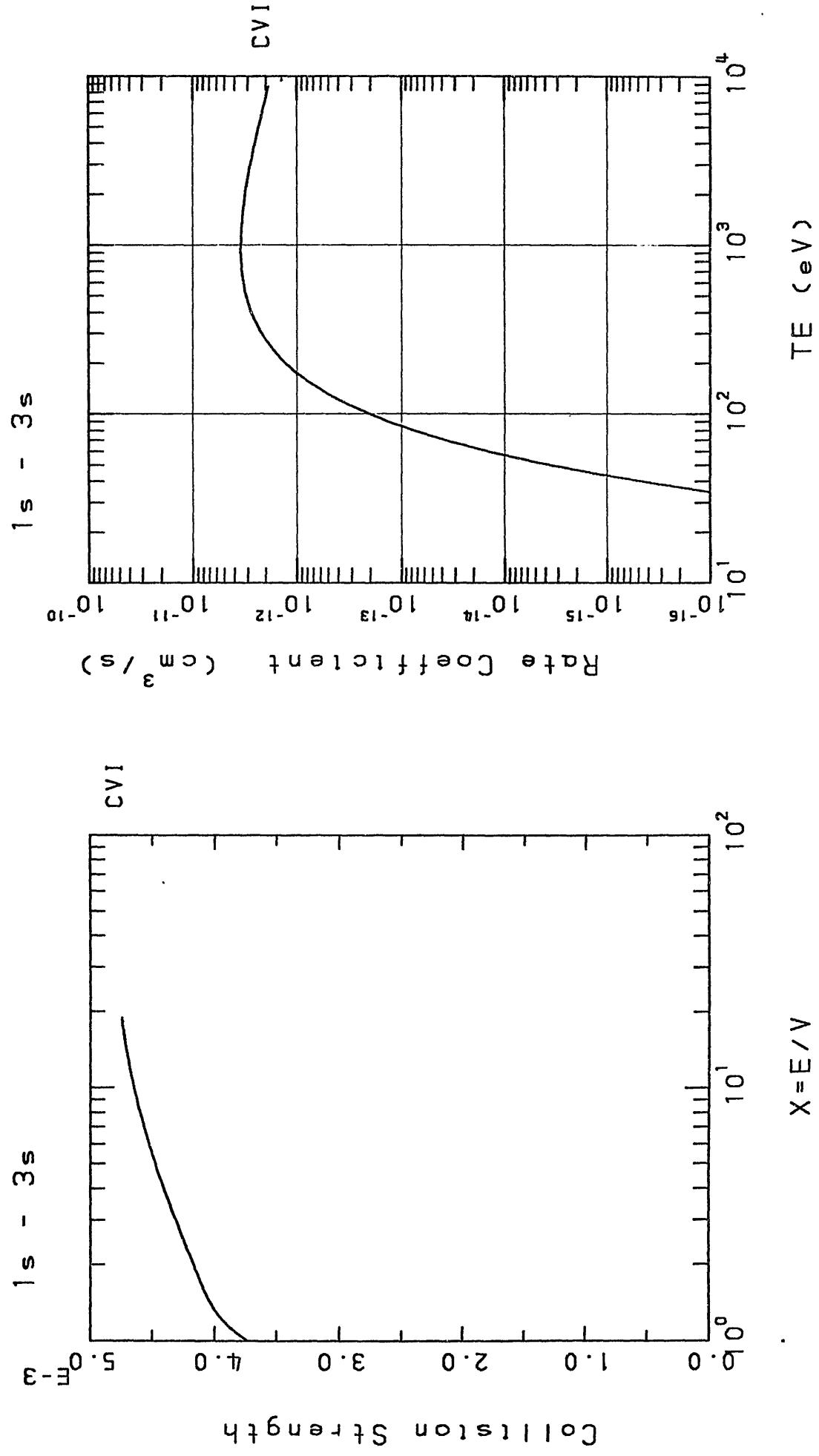


Fig. 4

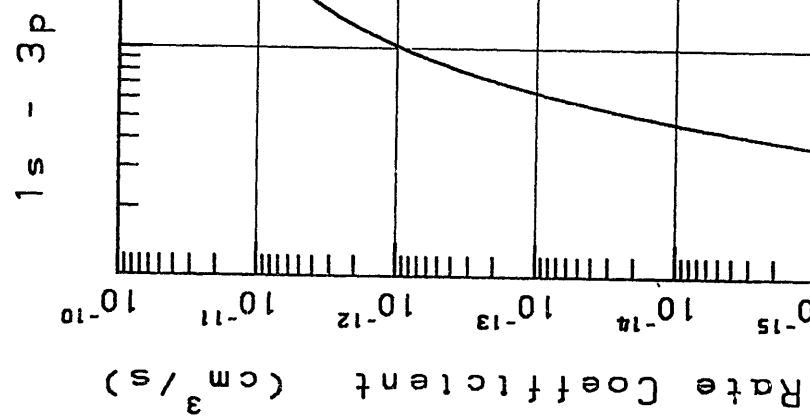
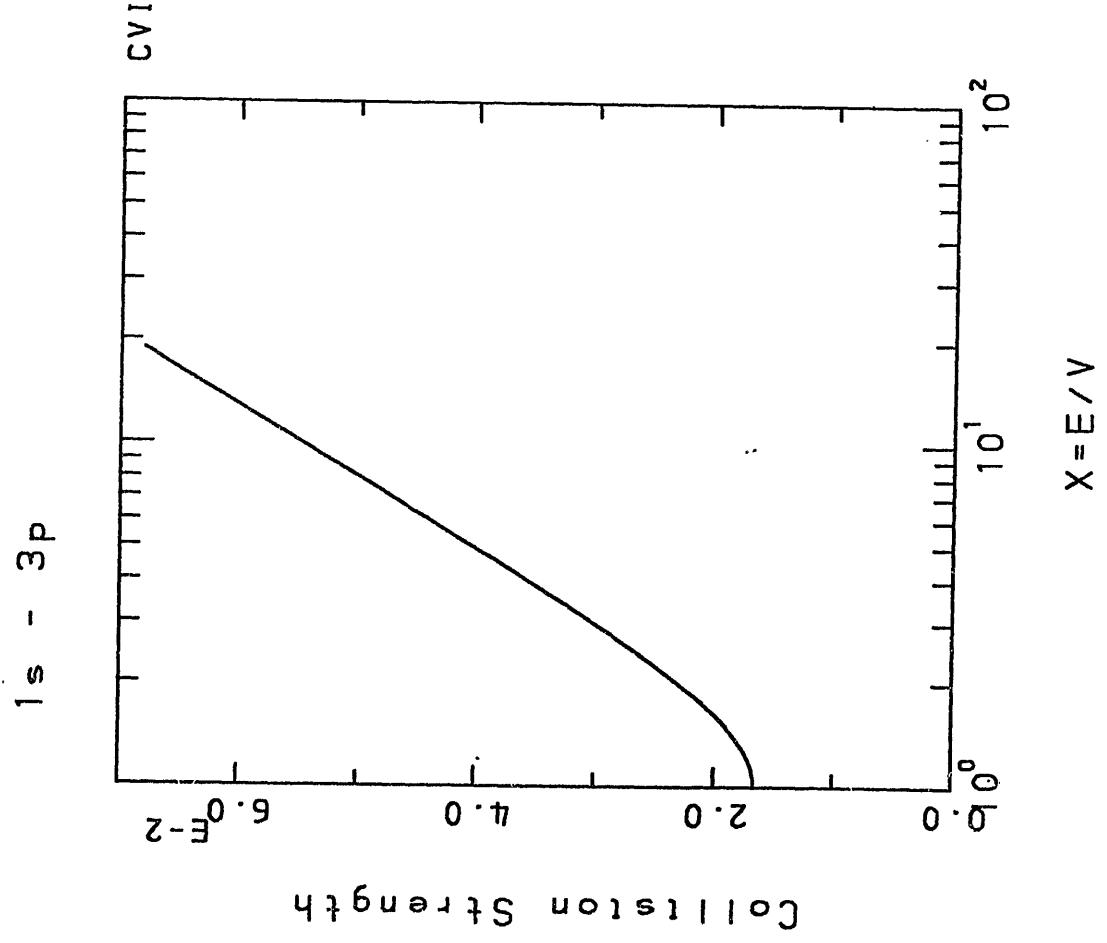


Fig. 5

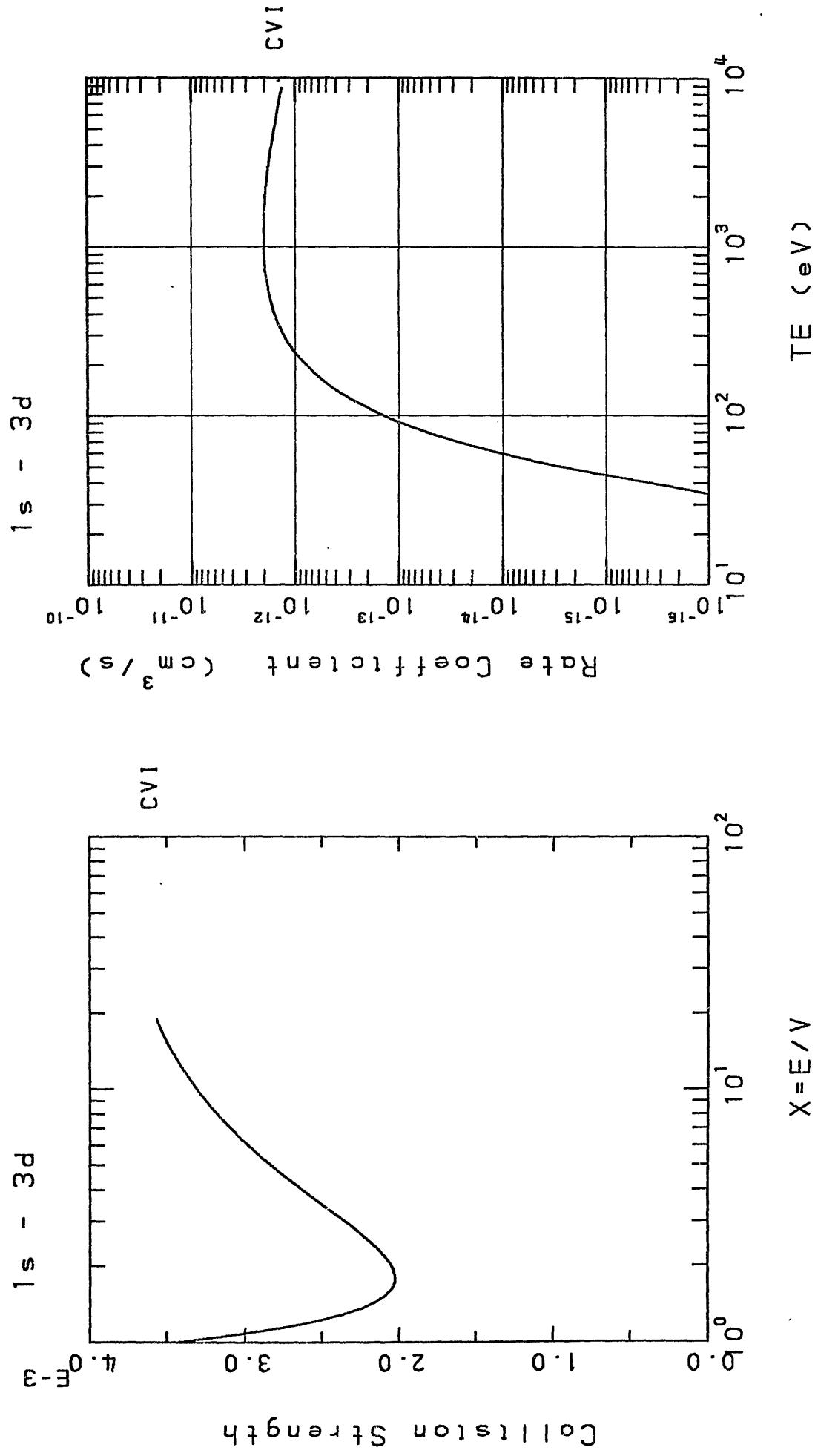


Fig. 6

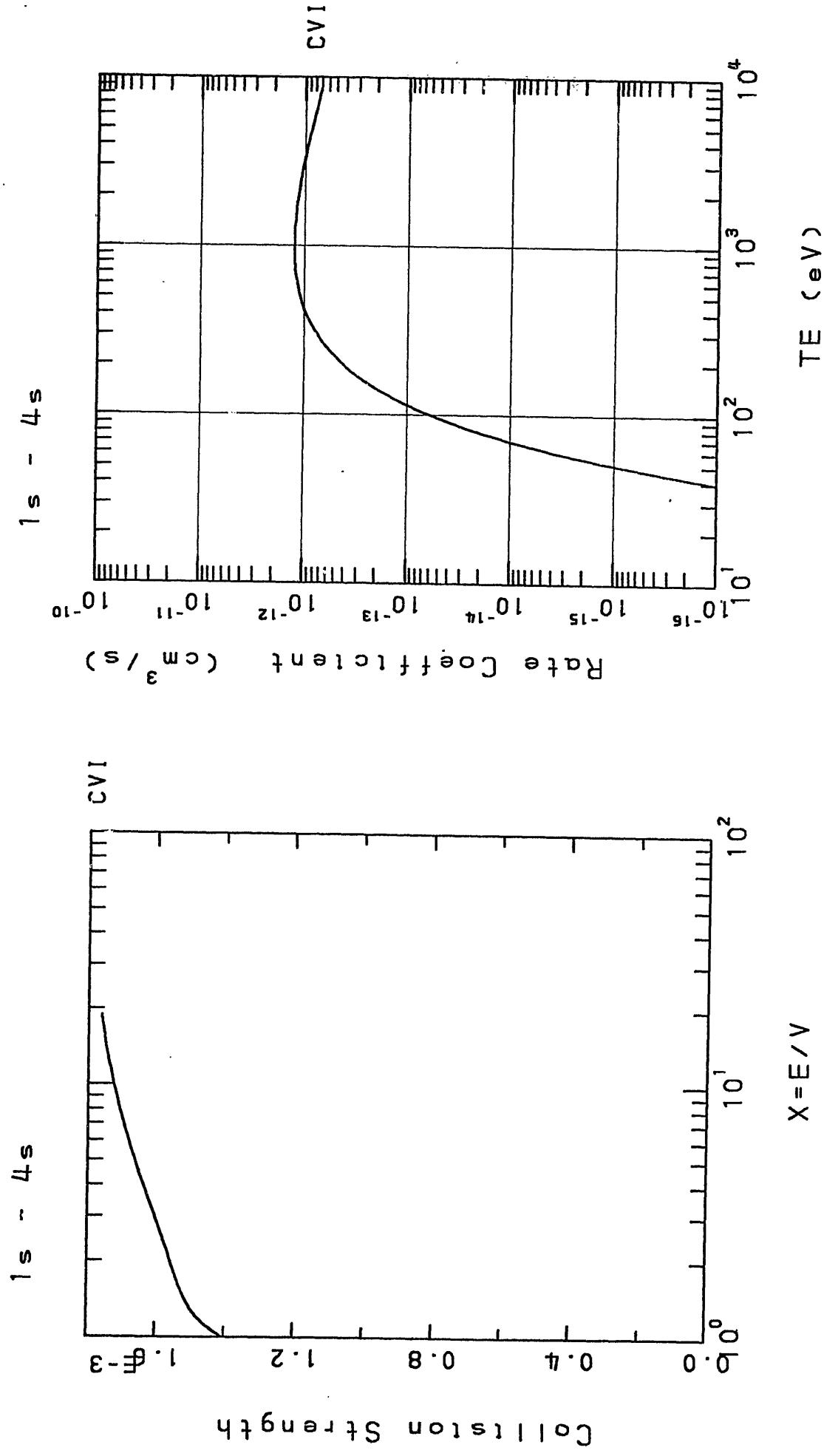


Fig. 7

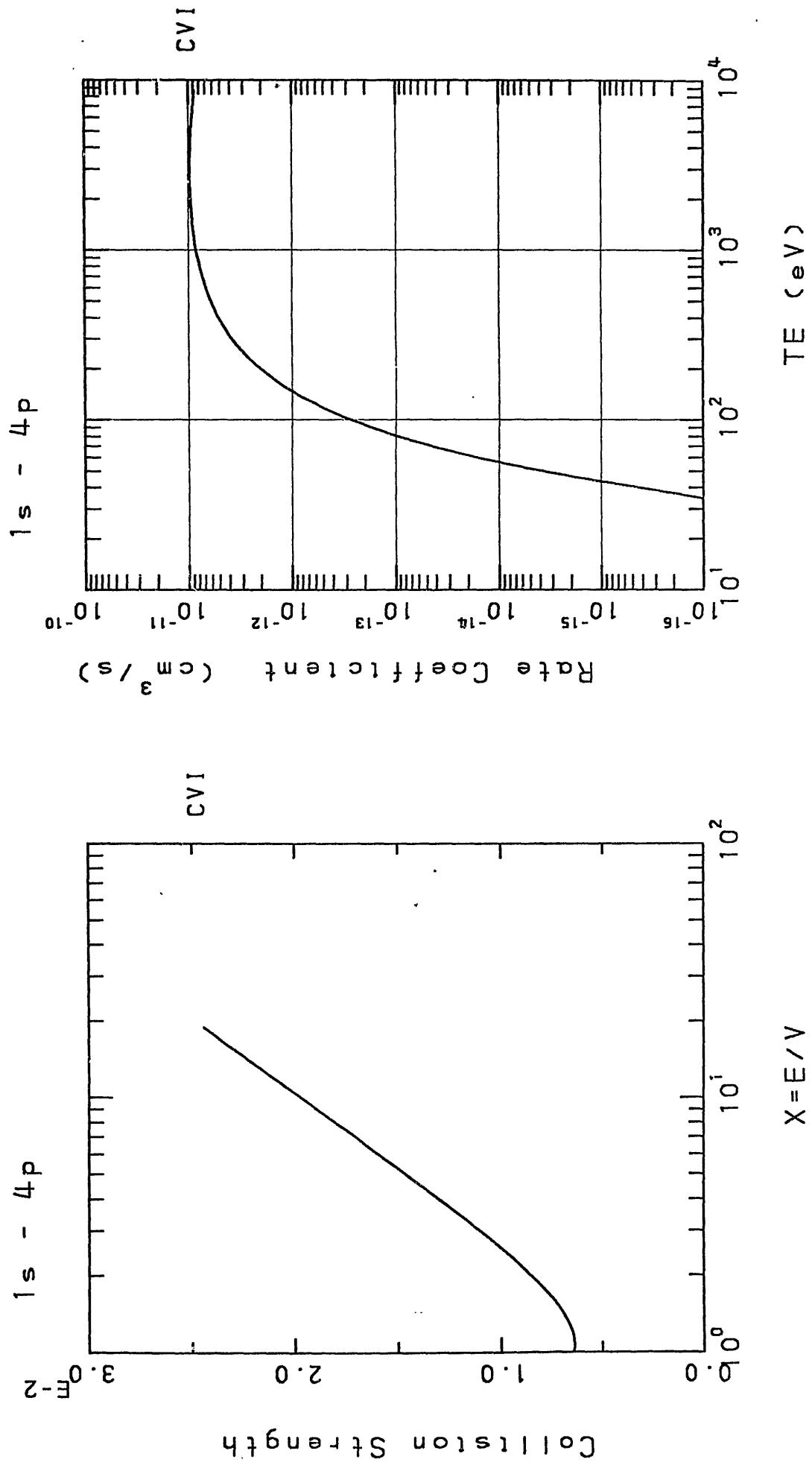
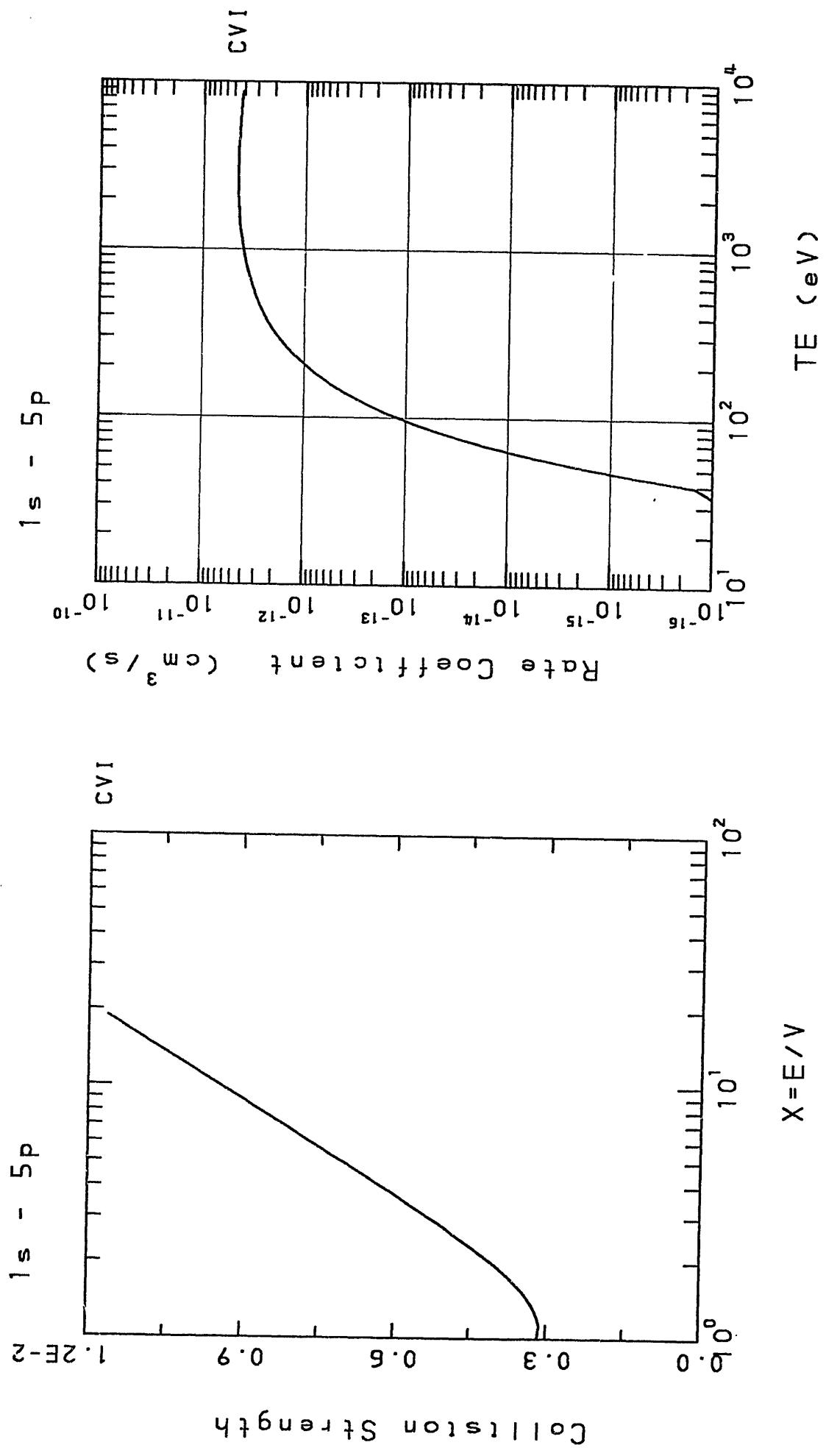


Fig. 8



He-like (C V, O VII)

van Wyngaarden et al. (1979) made a close-coupling (CC) calculation with very accurate wavefunctions for the target ions. They coupled five states (1^1S , 2^1S , 2^3S , 2^1P , 2^3P). Unfortunately they did not take into account the resonance effect. Pradhan et al. (1981a, b) estimated the resonance effect by using the distorted-wave (DW) method. Their target function is not as accurate as that employed by van Wyngaarden et al. Though an extensive calculation was made (for all the transitions among the ground and $n = 2$ excited states), Pradhan et al. gave only rate coefficients for most cases. For the excitation of the $n = 2$ states from the ground one, therefore, we adopt the results of van Wyngaarden et al. When the resonance effect is large, the contribution was estimated from the rate coefficient given by Pradhan et al. (1981b) according to the procedure described in the Introduction. For higher energies, we use the distorted wave (DW) calculation by Peek (1977) and Mann (1981).

Recently Pradhan pointed out the radiative correction (due to the effect of radiative decay of the resonant state) should be taken into account in the calculation of Ω_R . He estimated the correction in the case of OVII. His calculation, however, was made over a very limited range of electron energy, so that it is difficult to quantitatively correct the rates given here. The present recommended data do not include the radiative correction. It should be noted therefore that the resonance effect shown in this report might be reduced slightly when the radiative correction is included.

For the transitions among the $n = 2$ states, the DW method is less reliable at least near threshold, because the levels concerned are nearby in energy and the couplings among them cannot be ignored. Thus, for the transitions among the $n = 2$ states, we adopt the results of the five-state CC made by Robb (1977) near threshold. Norcross (1977) calculated the same cross sections by using another type of the DW method. He employed more refined target wavefunctions. To obtain the present recommended values, Robb's cross sections are smoothly connected with Norcross' values at higher electron energies ($X \gtrsim 10$). For the transition between 2^1S and 2^3P , the cross

section depends sensitively on the target wave function because the two states lie very close. The uncertainty of the cross section may be large for the transition.

A very limited number of calculations have been reported so far for the excitation of higher ($n \geq 3$) states. Although it is hard to check the reliability of them, we include here those cross sections. They are the Coulomb-Born (CB) calculations of Nakazaki (1976) and Tully and Serrao (1974) and the DW calculation by Davis et al. (1978) and Mann (1981).

Data sources

- Davis, J., Whitney, K.G. and Apruzese, J.P. (1978), *J. Quant. Spectrosc. Radiat. Transf.* **20** 353
[$1^1S - 3^3D, 3^1P$ of C V, DW]
- Mann, J.B. (1981), private communication by A.L. Merts
[$1^1S - 2^3S, 2^1S, 2^3P, 2^1P, 3^3S, 3^1S, 3^3P, 3^1P, 3^3D, 3^1D$ of O VII, DW]
- Nakazaki, S. (1976), *J. Phys. Soc. Jpn.* **41** 2084
[$1^1S - 3^1P, 2^3P - 3^3P, 2^3P - 3^3S$ of C V; $2^3S - 3^3P$ of O VII, CB]
- Norcross, D.W. (1977), quoted in Los Alamos Scientific Laboratory Report, LA-6691-MS, ed. N.H. Magee, Jr. et al.
[$2^3S - 2^1S, 2^3P, 2^1P, 2^1S - 2^1P, 2^3P - 2^1P$, DW]
- Peek, J.M. (1977), quoted in Los Alamos Scientific Laboratory Report, LA-6691-MS, ed. N.H. Magee, Jr. et al.
[$1^1S - 2^3S, 2^1S, 2^3P, 2^1P$ of C V, DW]
- Pradhan, A.K., Norcross, D.W. and Hummer, D.G. (1981a), *Phys. Rev. A* **23** 619
[$1^1S - 2^3S, 2^3P$, DW]
- Pradhan, A.K., Norcross, D.W. and Hummer, D.G. (1981b), *Astrophys. J.* **246** 1031
[$1^1S - 2^3S, 2^3P$, DW]
- Robb, W.D. (1977), quoted in Los Alamos Scientific Laboratory Report, LA-6691-MS, ed. N.H. Magee, Jr. et al.
[transitions among $n = 2$ states, CC]
- Tully, J.A. and Serrao, J.M.P. (1974), *Astron. Astrophys.* **33** 187
[$2^3S - 3^3P$ of O VII, CB]
- van Wyngaarden, W.L., Bhadra, K. and Henry, R.J.W. (1979), *Phys. Rev. A* **20** 1409
[$1^1S - 2^3S, 2^1S, 2^3P, 2^1P$, CC]

Fig. 9

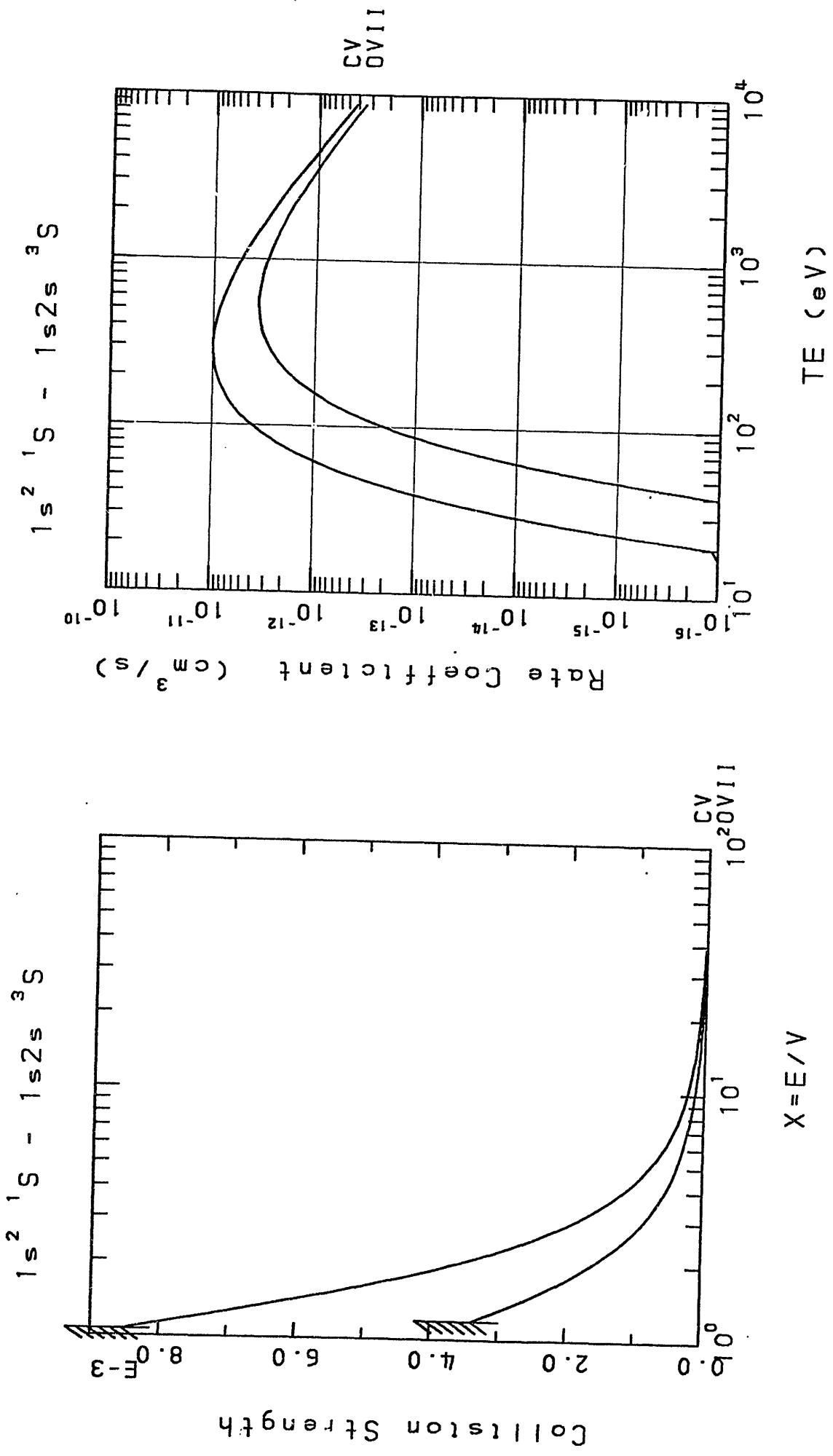


Fig. 10

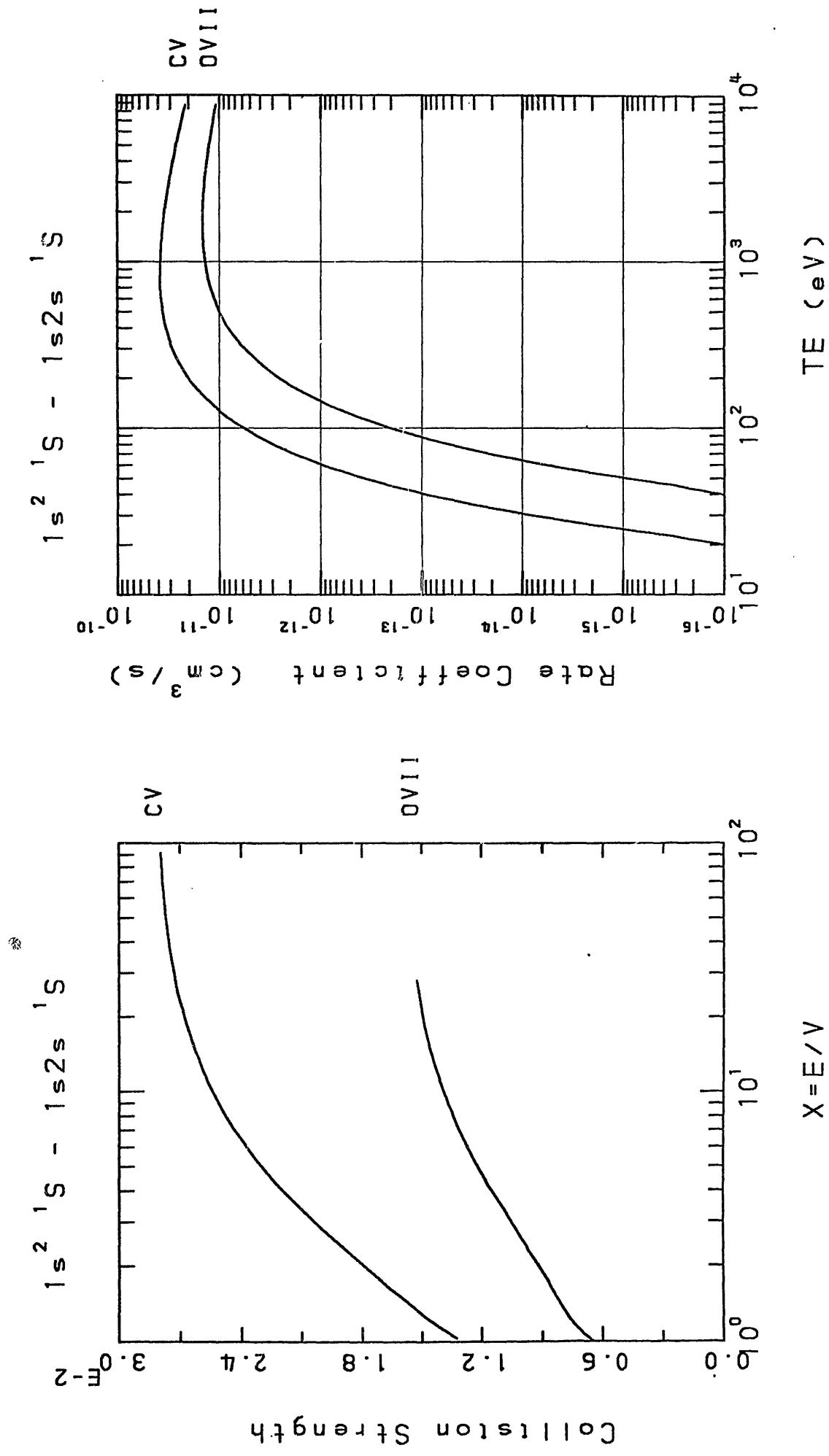


Fig. 11

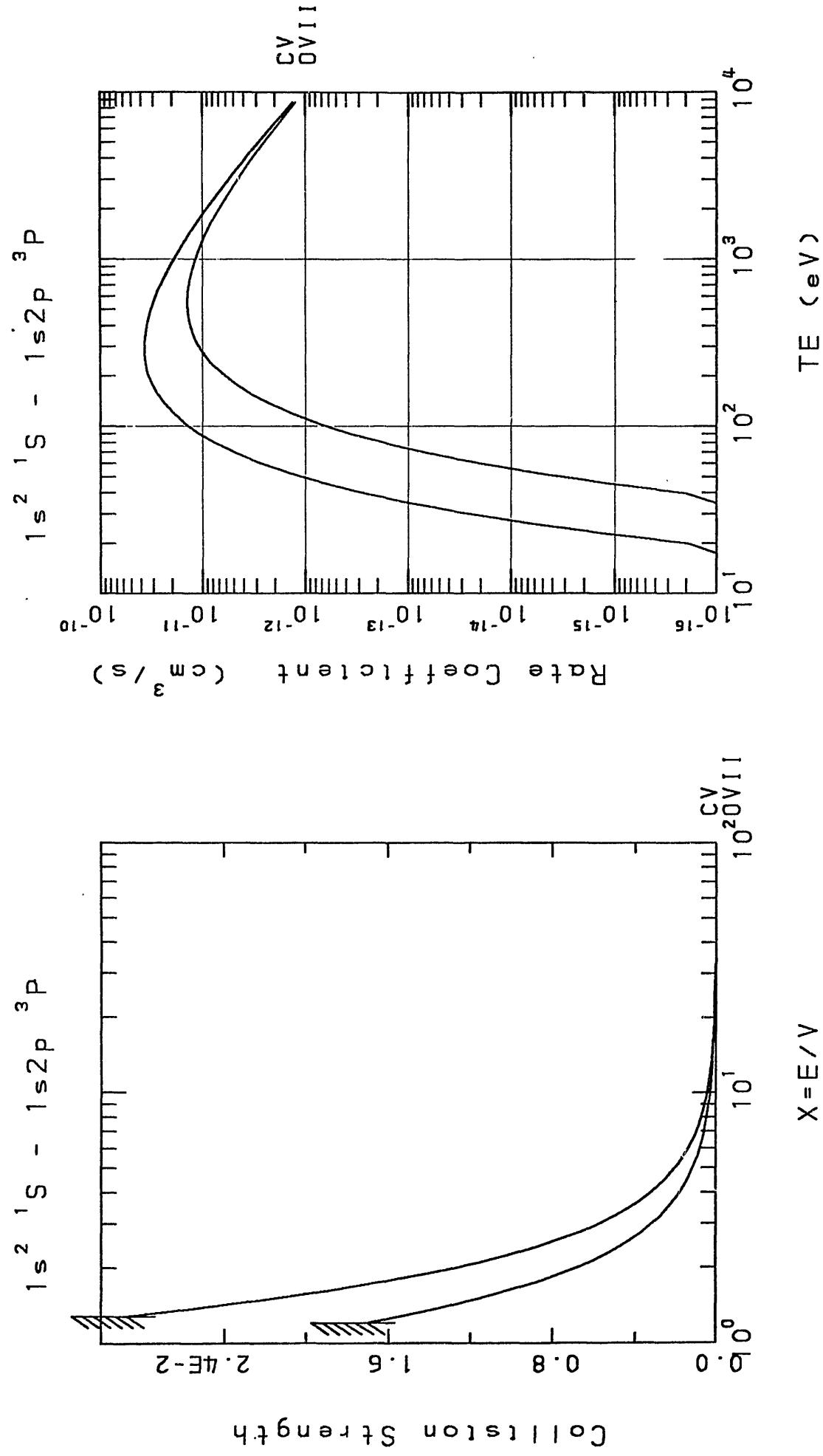


Fig. 12

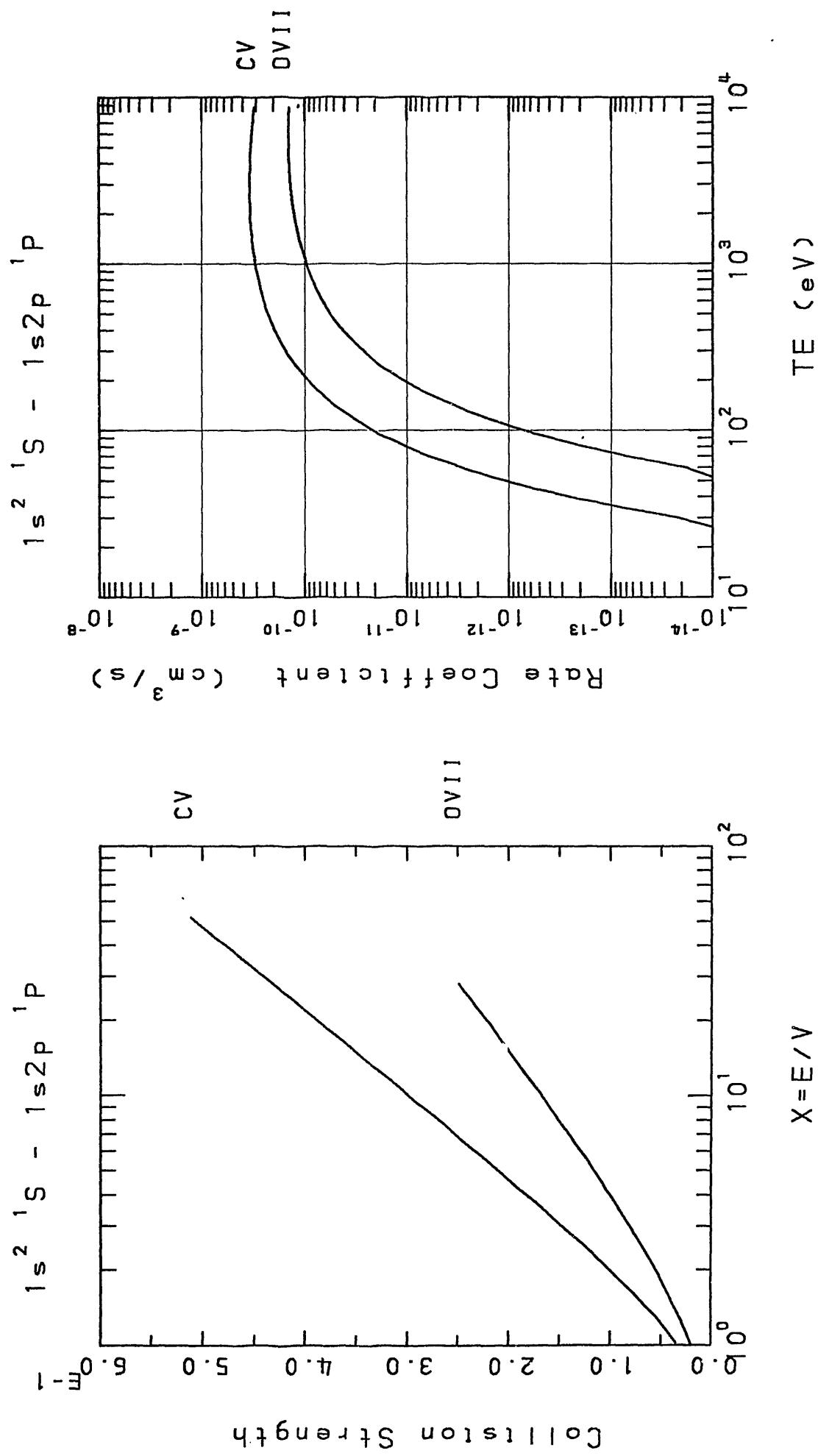


Fig. 13

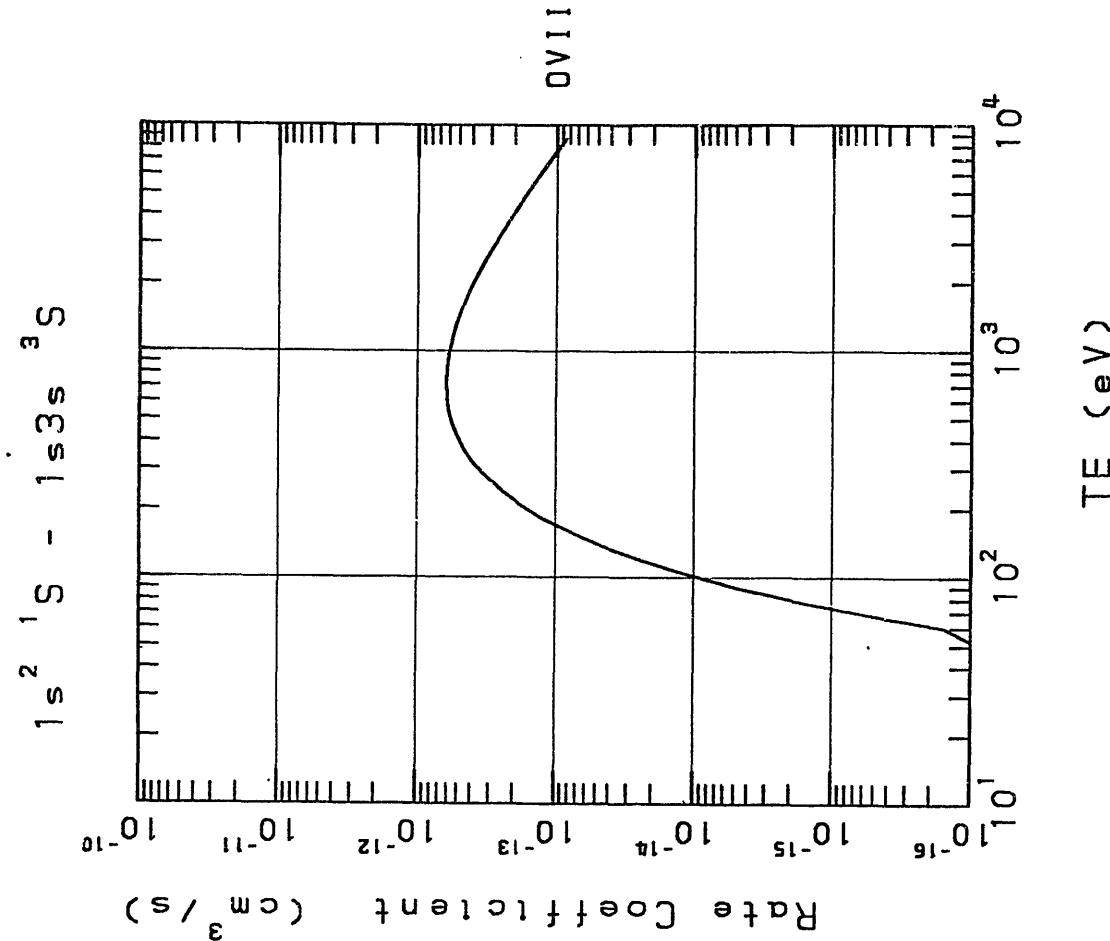
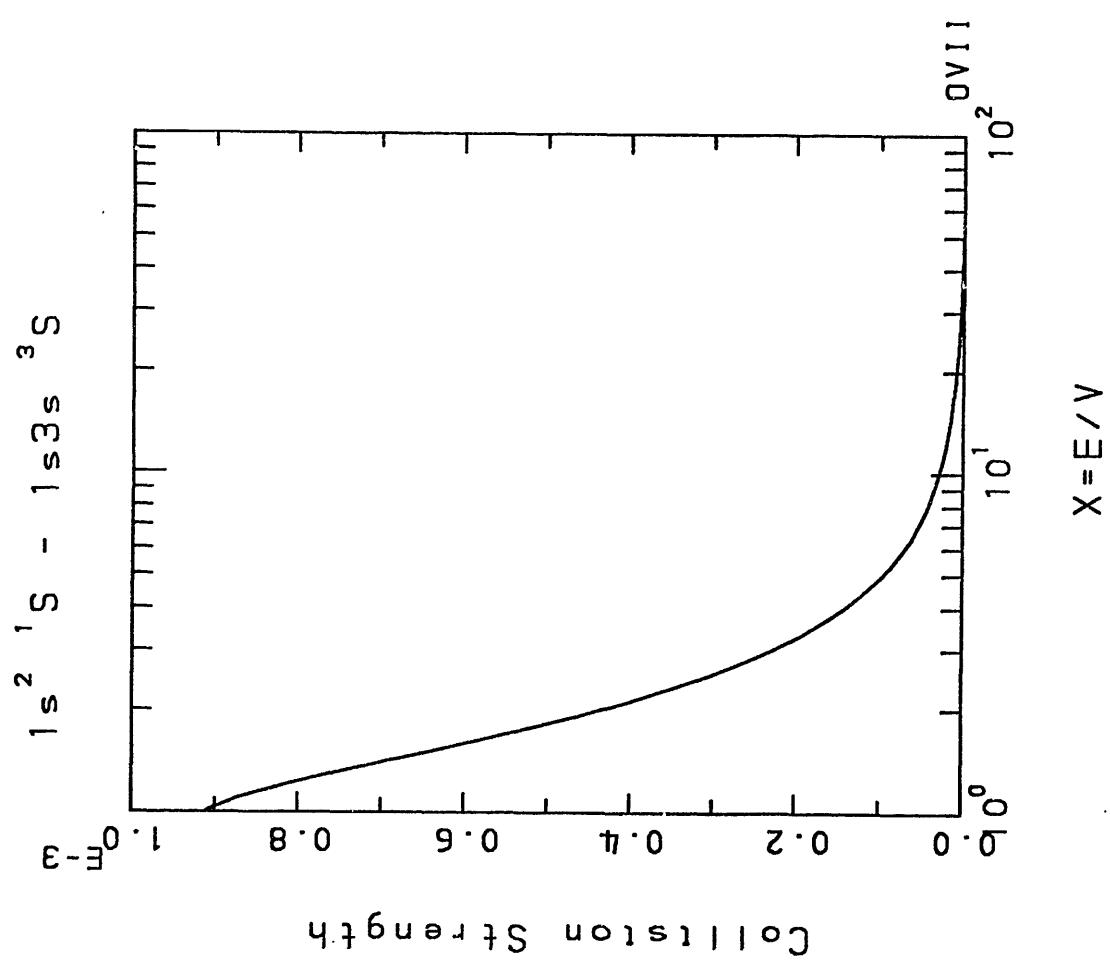


Fig. 14

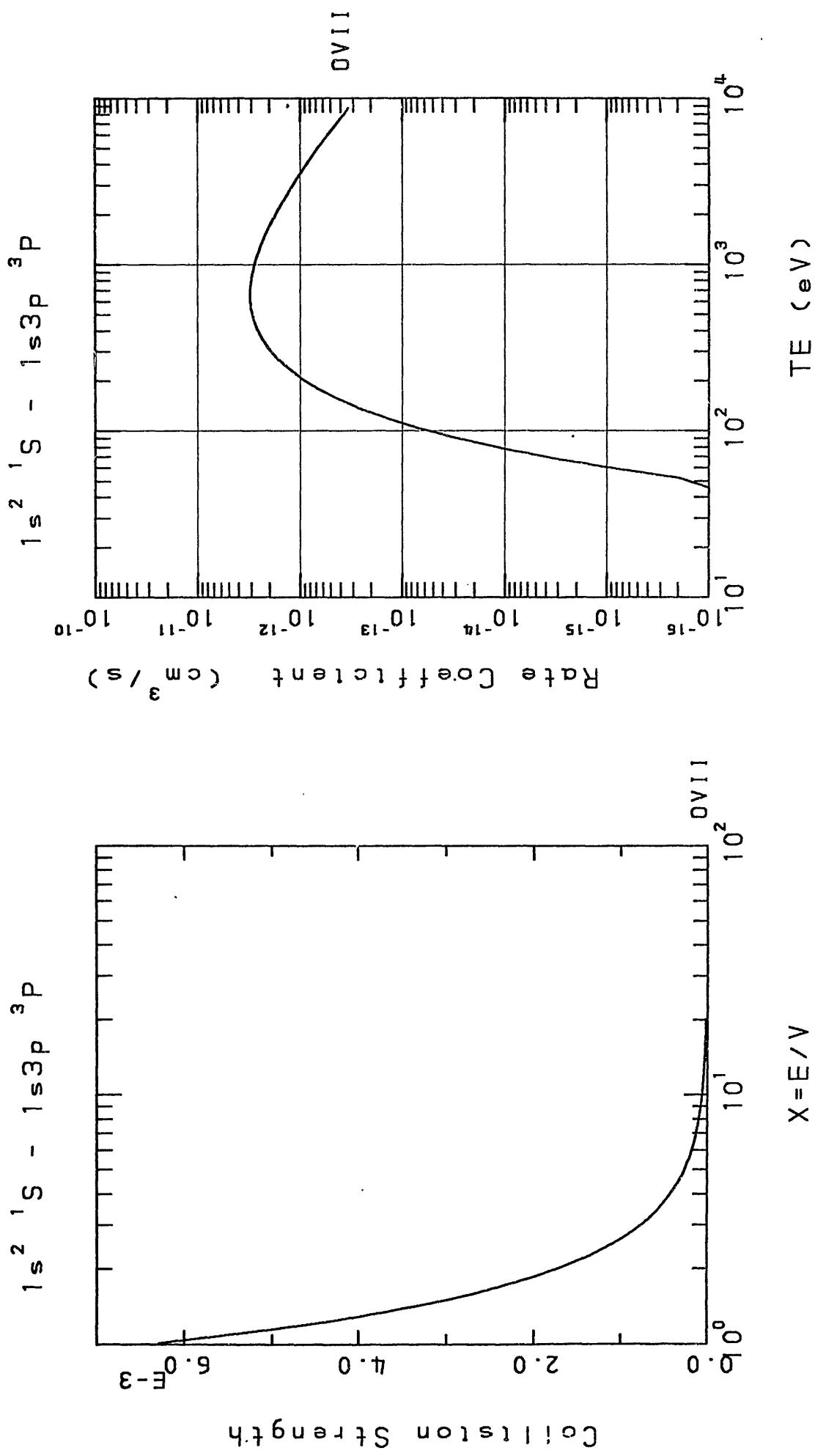


Fig. 15

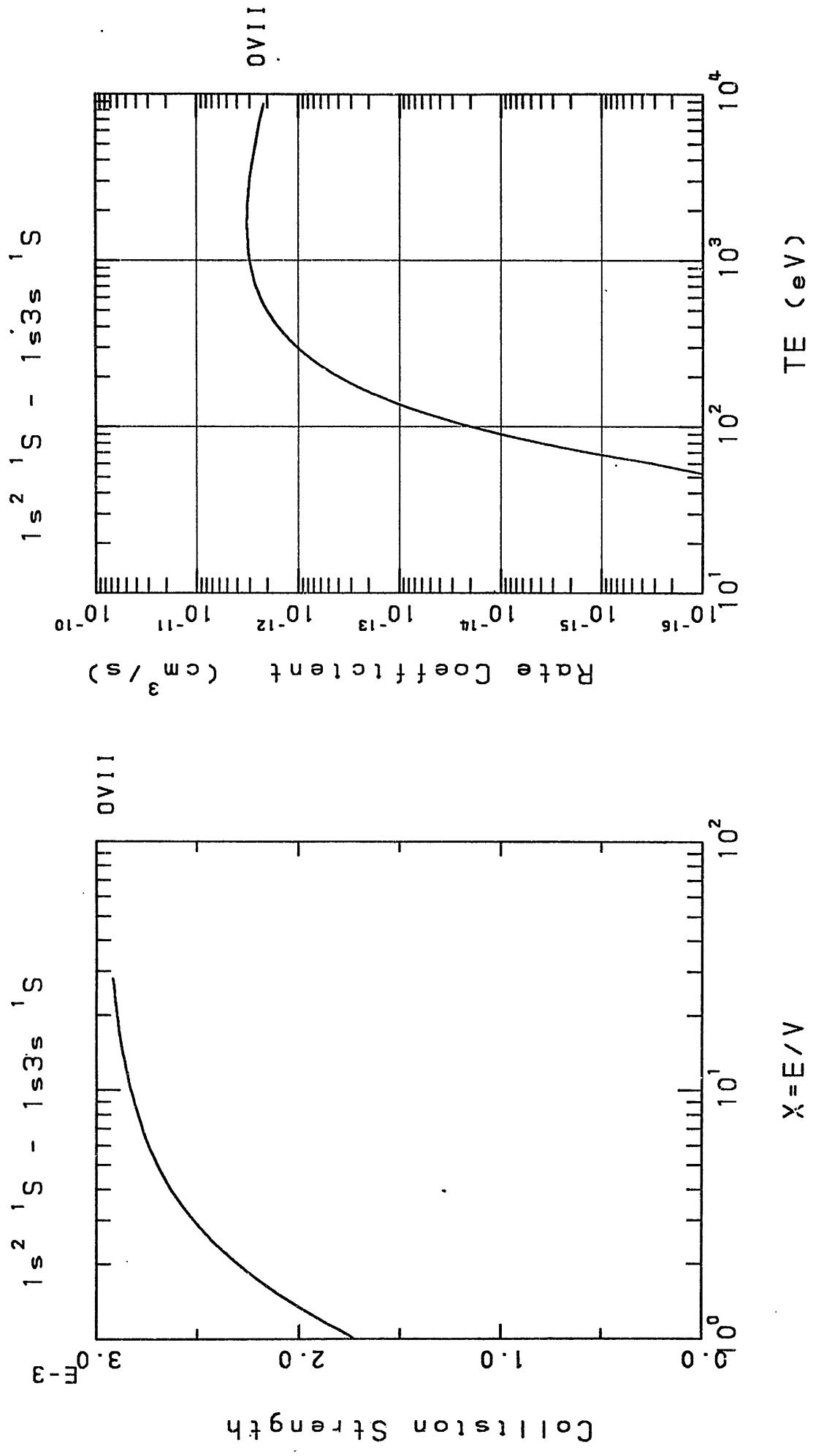


Fig. 16

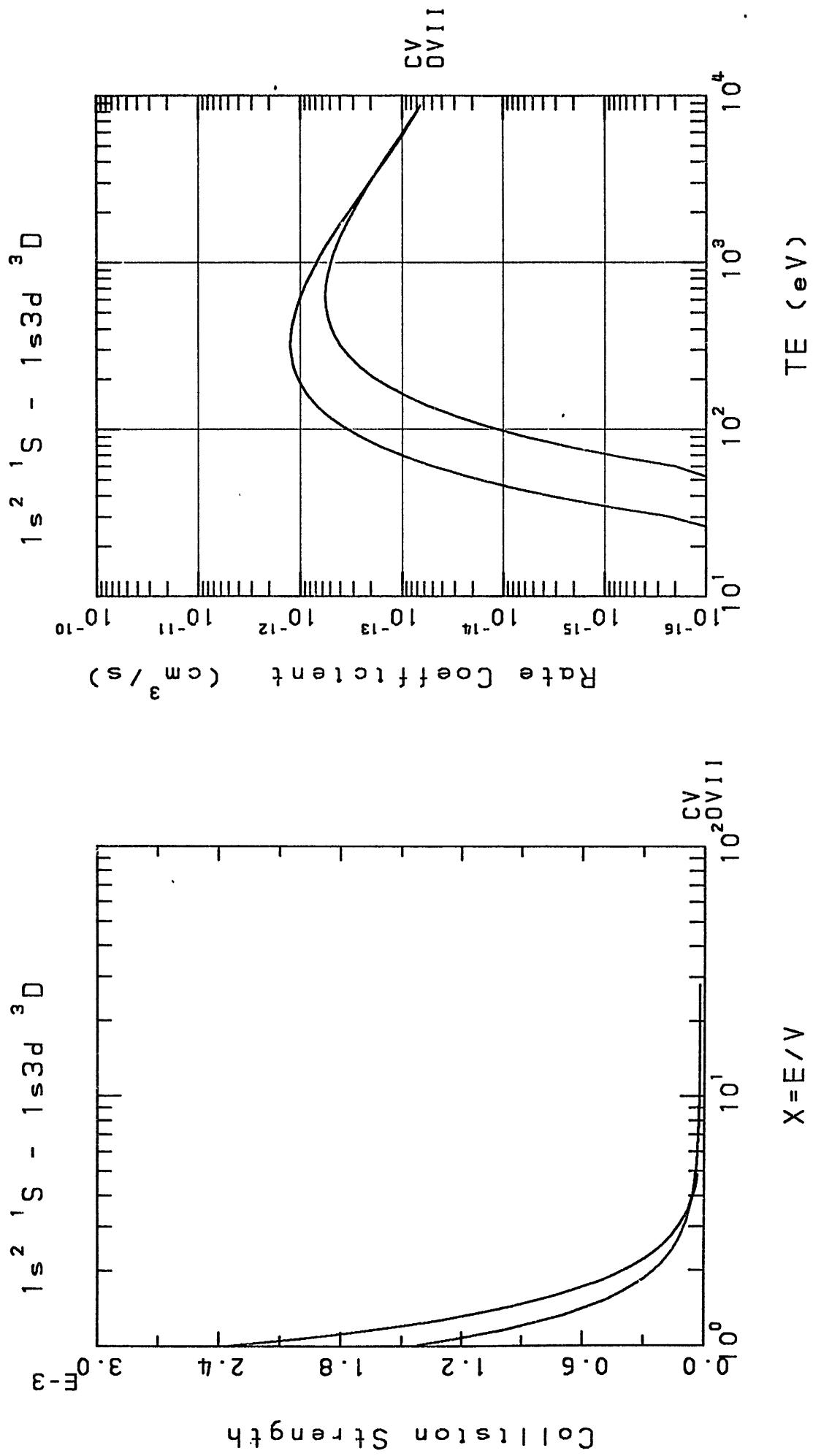


Fig. 17

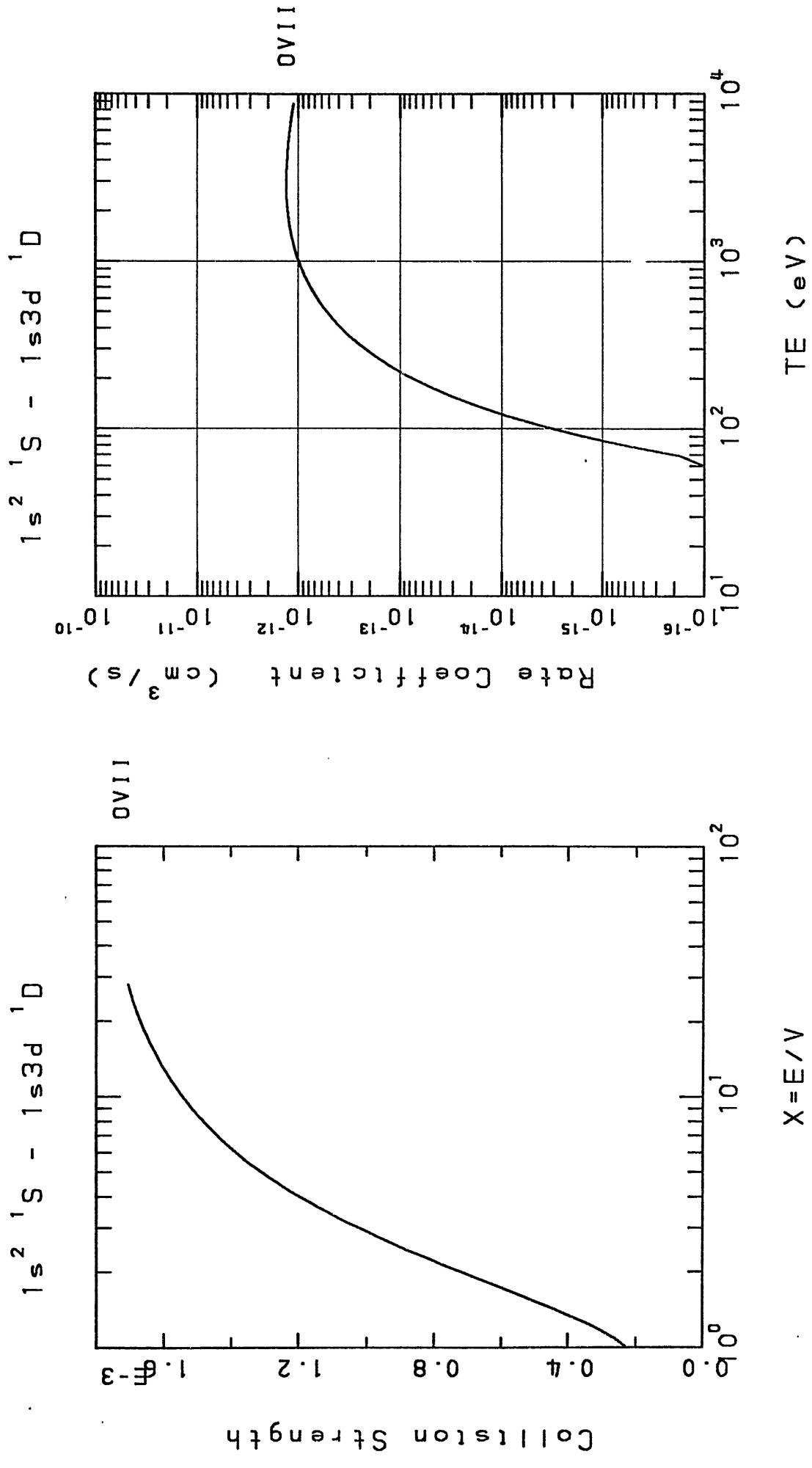


Fig. 18

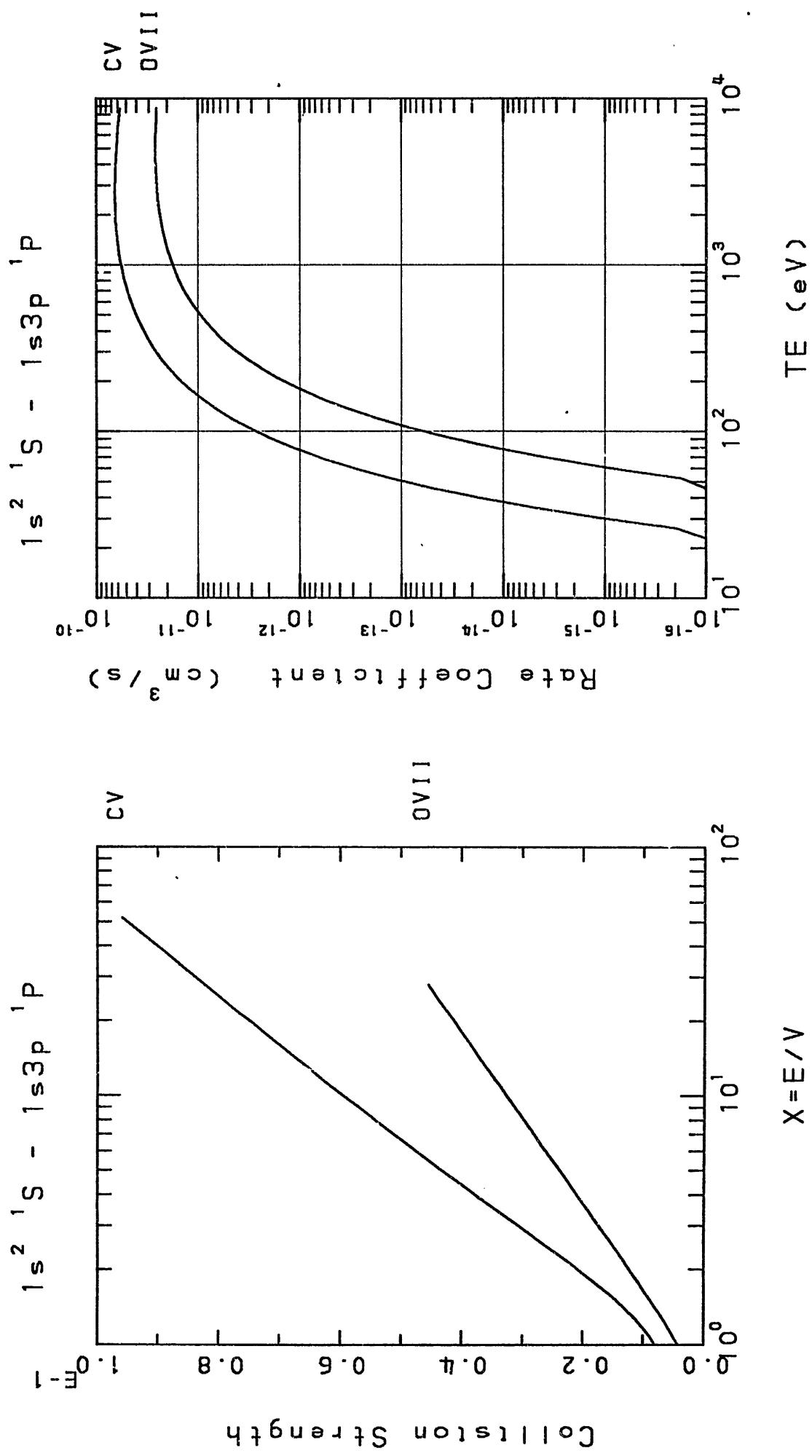


Fig. 19

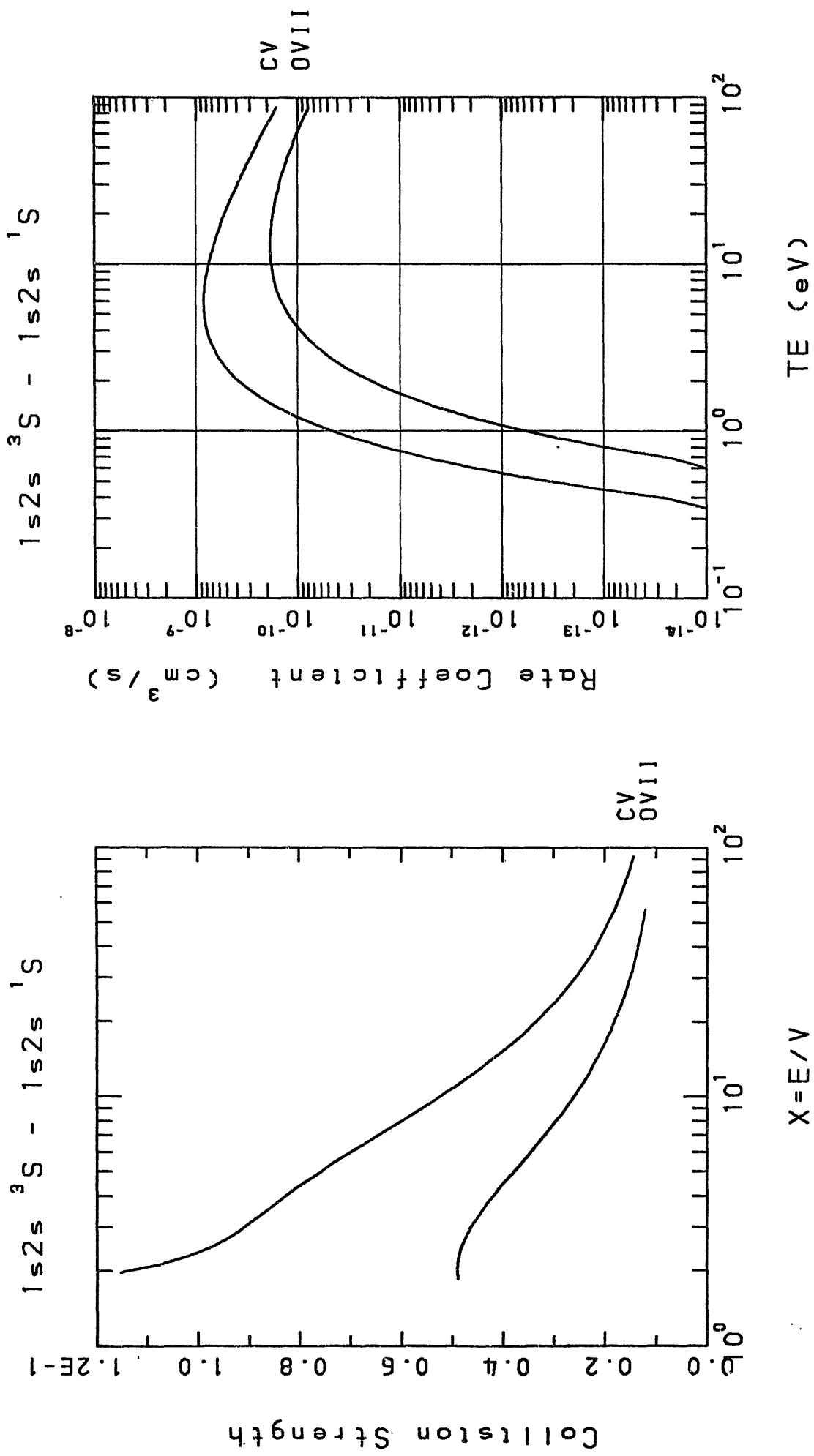


Fig. 20

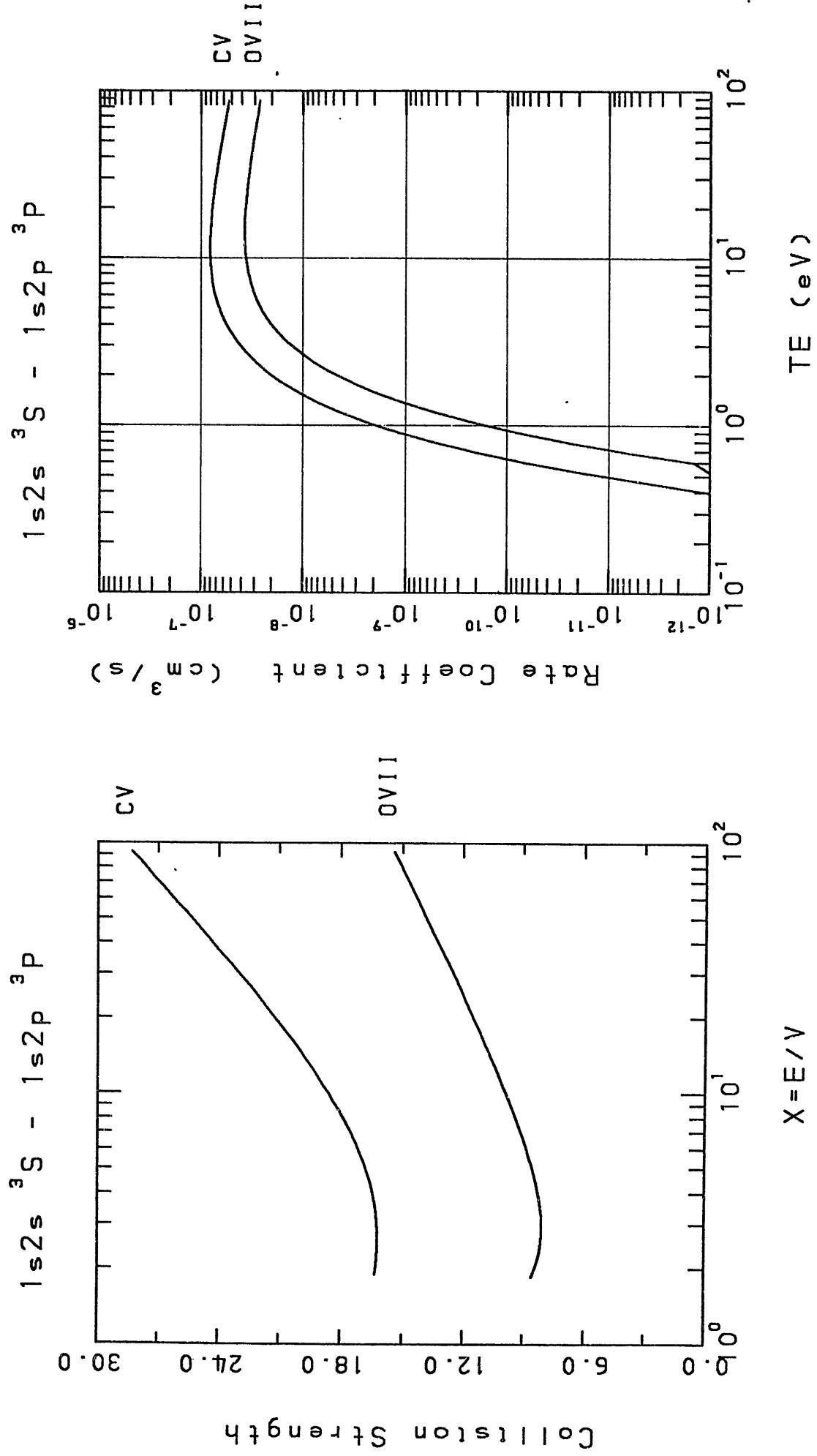
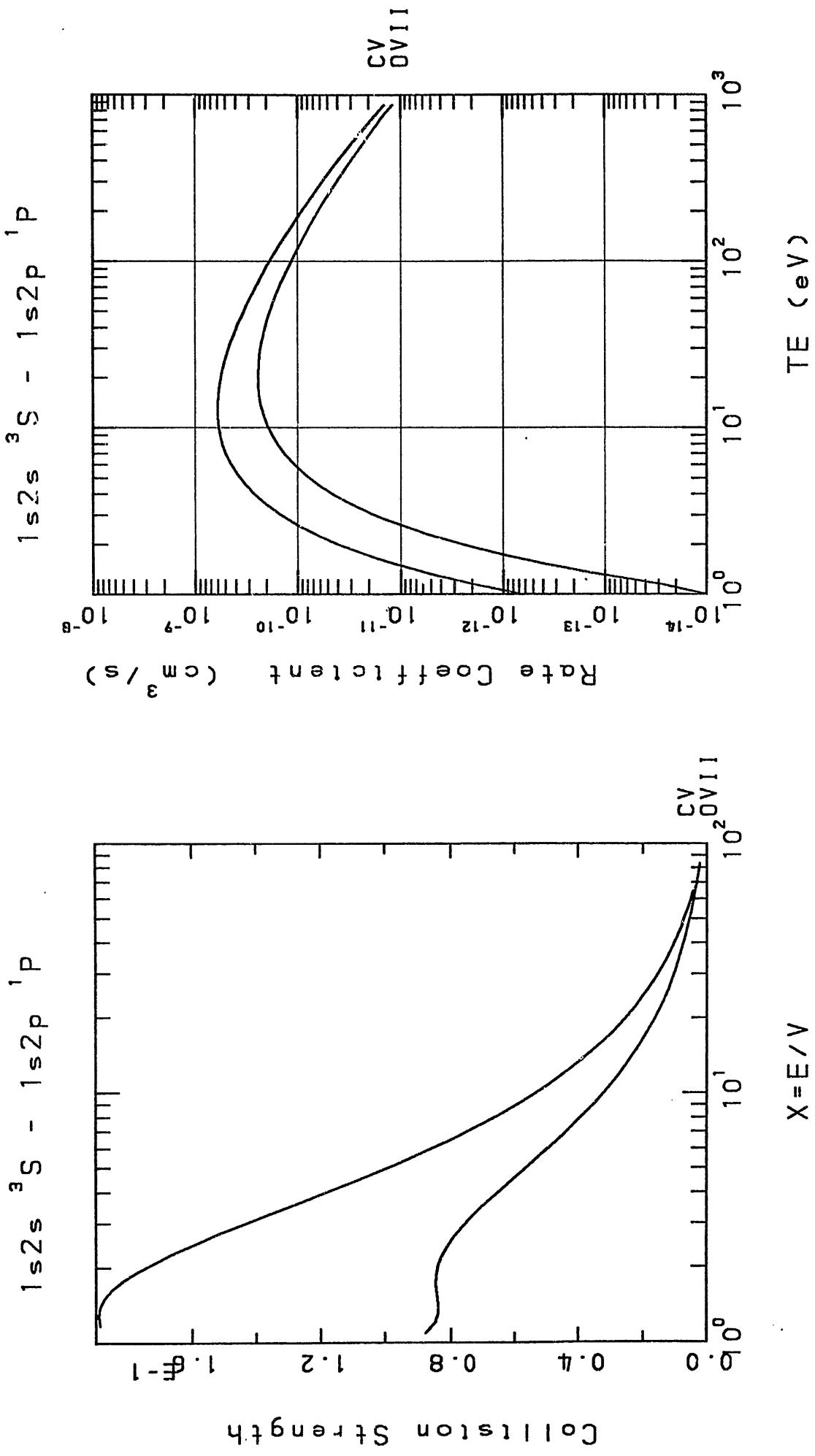


Fig. 21



Collision Strength

Fig. 22

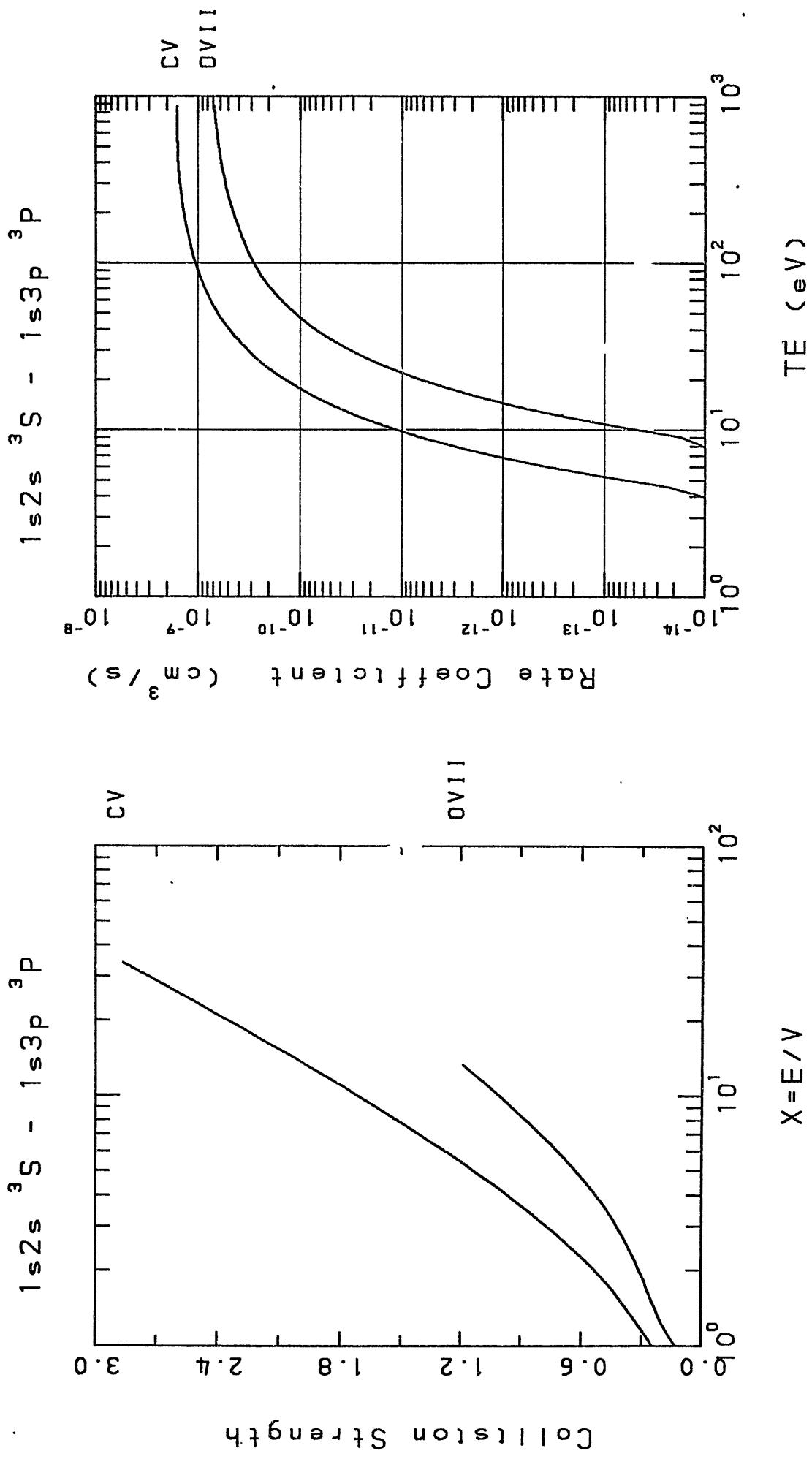
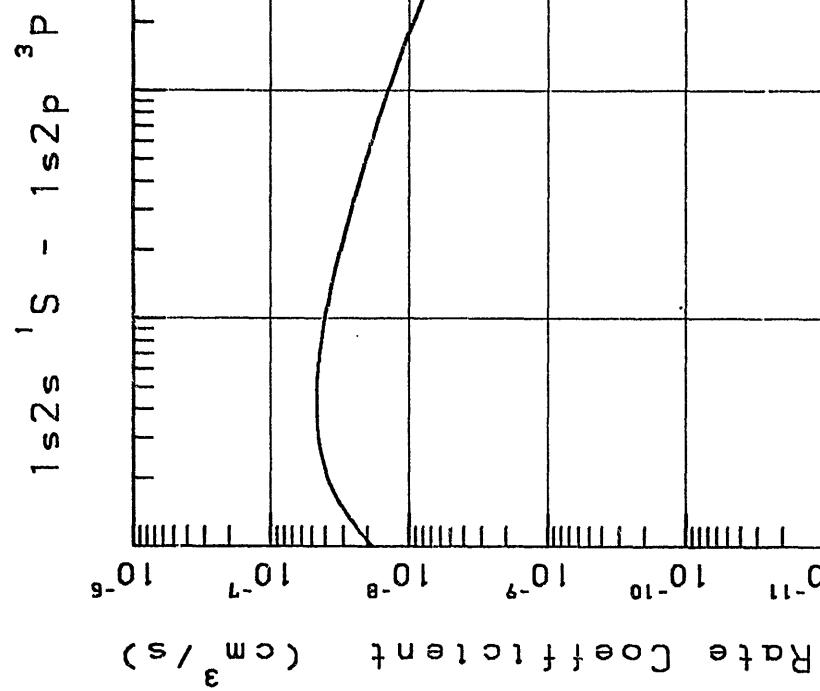
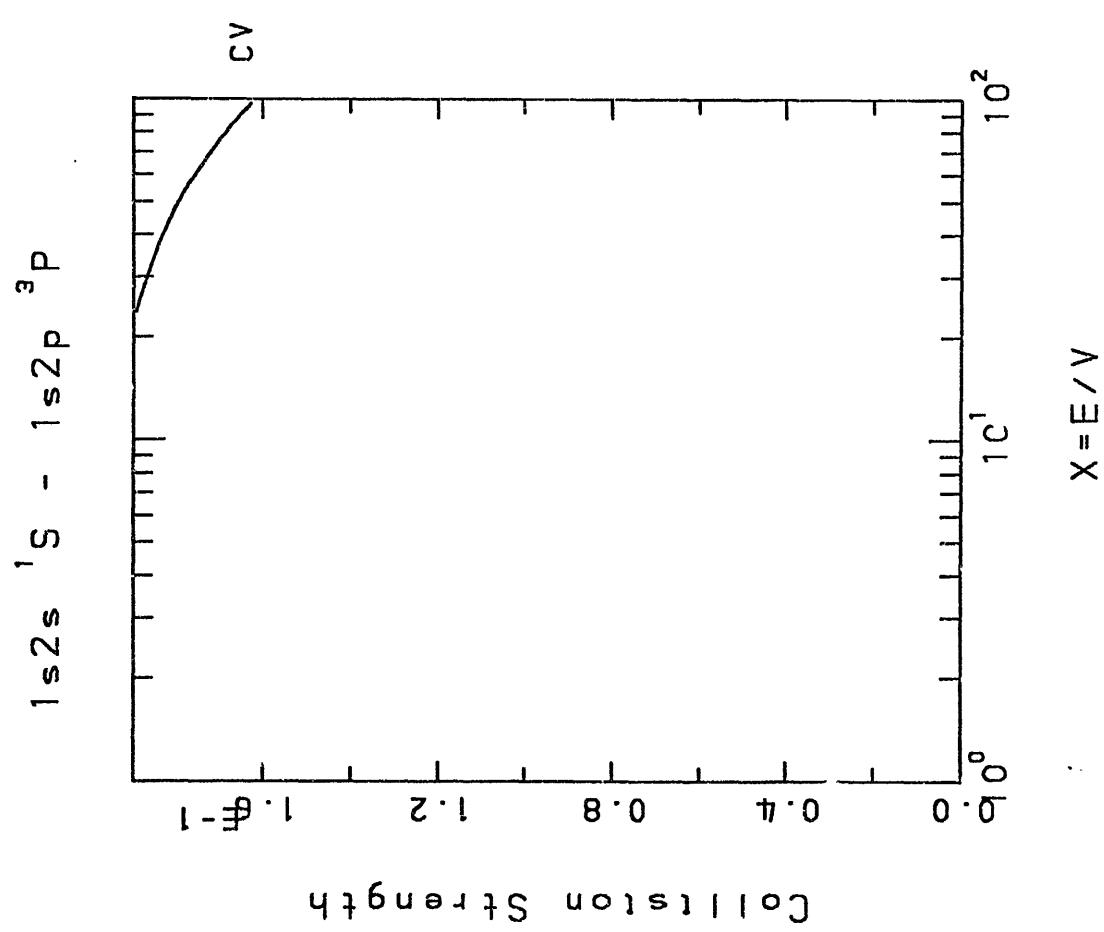


Fig. 23



TE (eV)

E/V

Collision Strength

Fig. 24

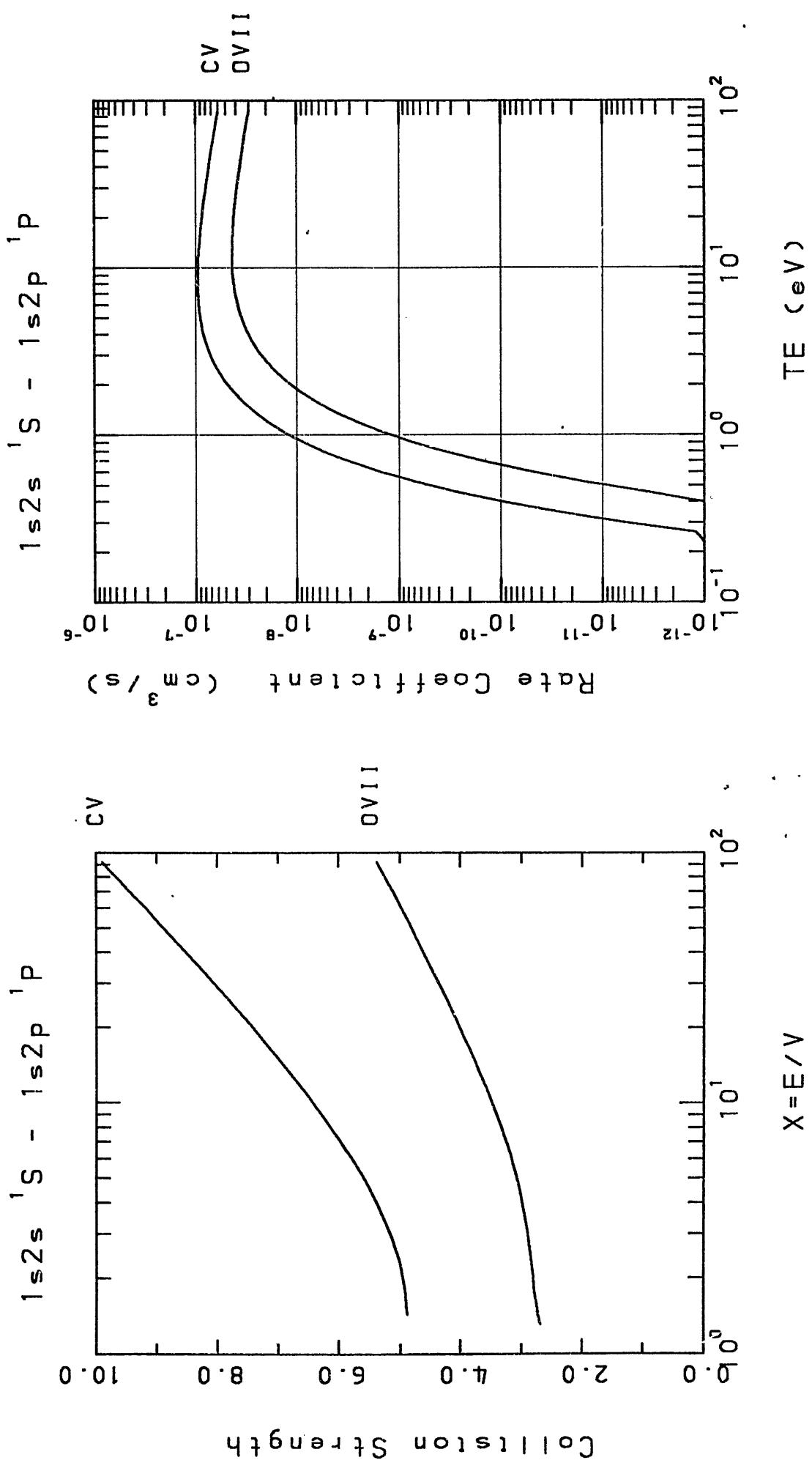


Fig. 25

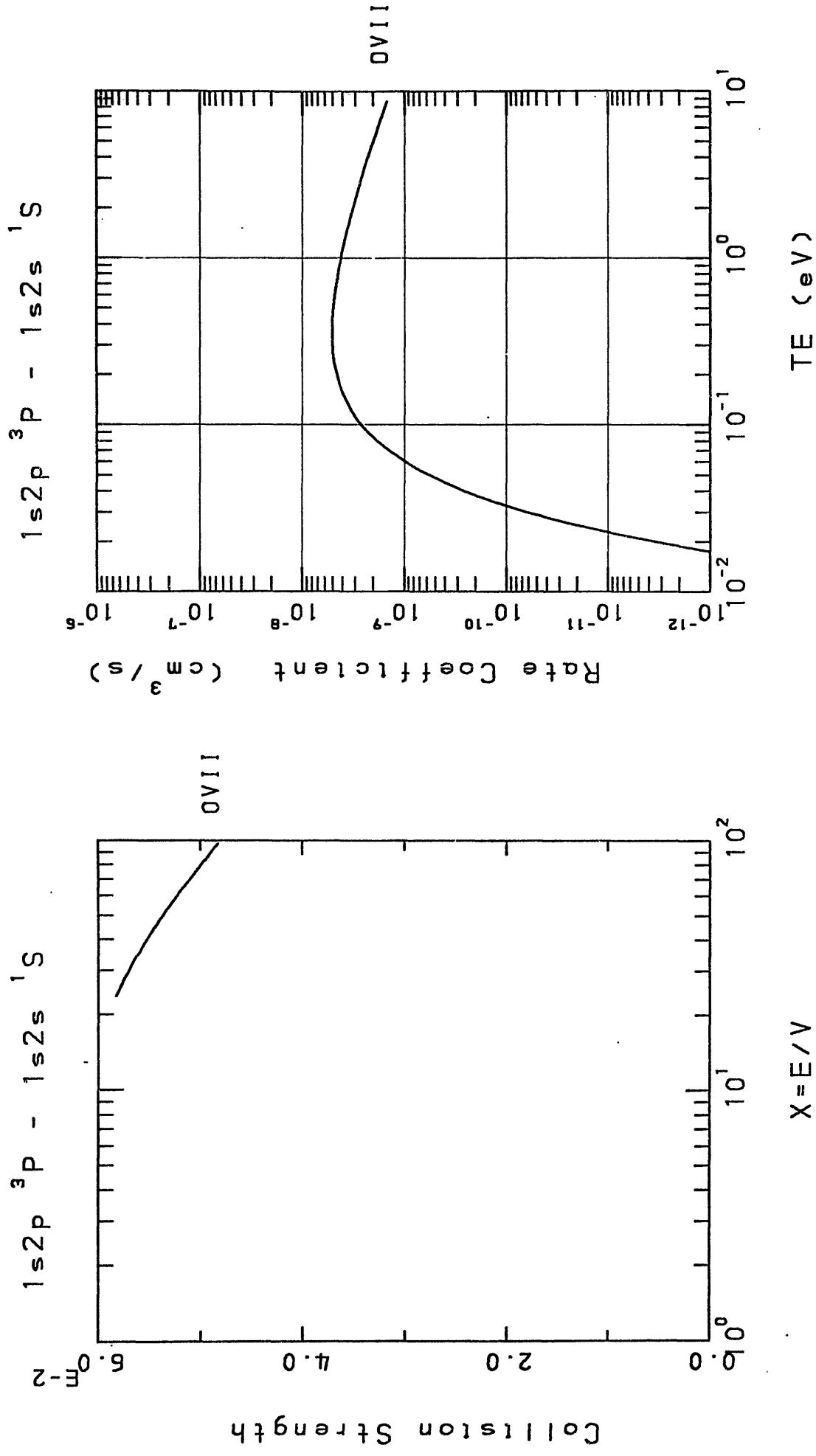


Fig. 26

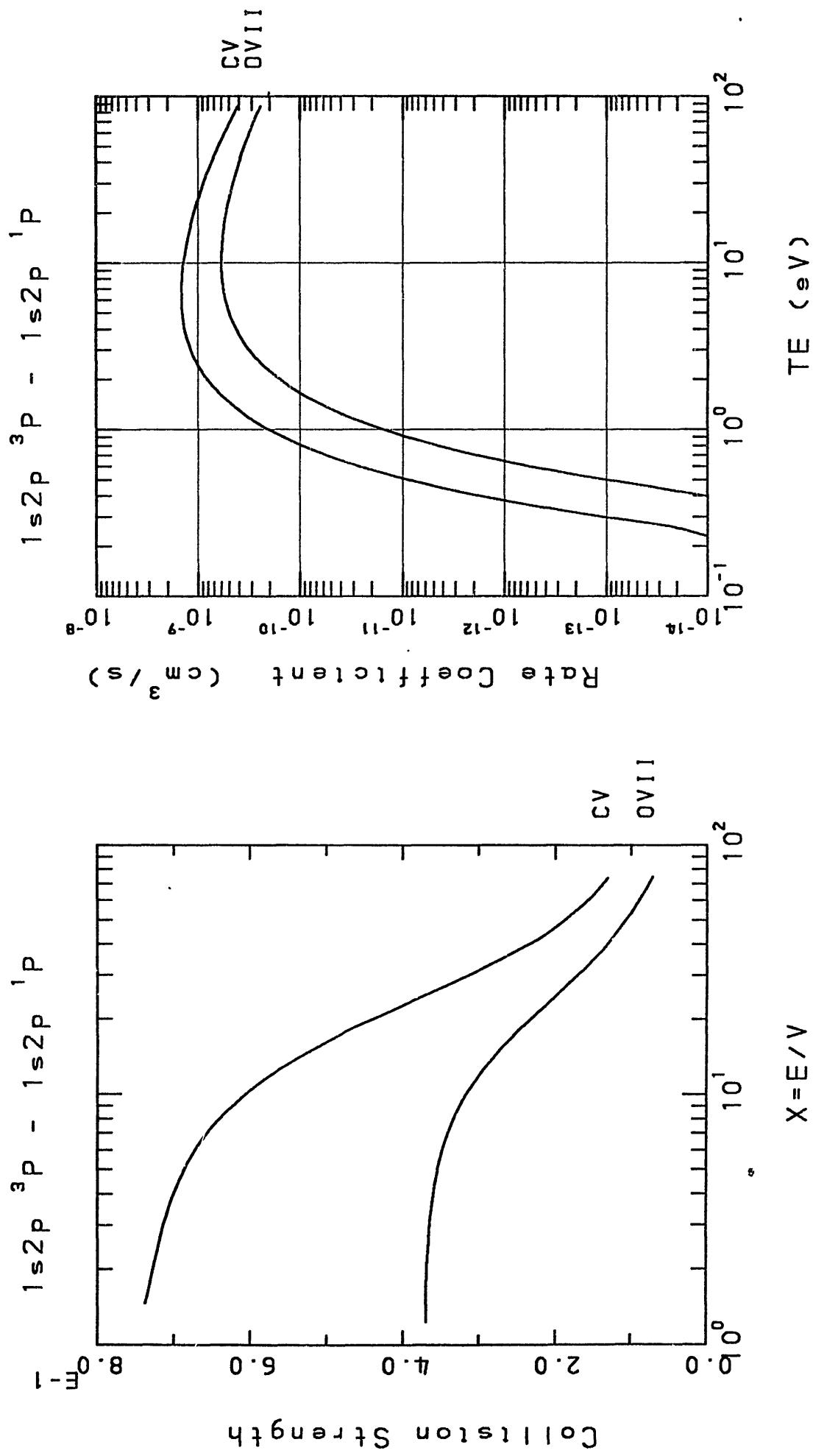
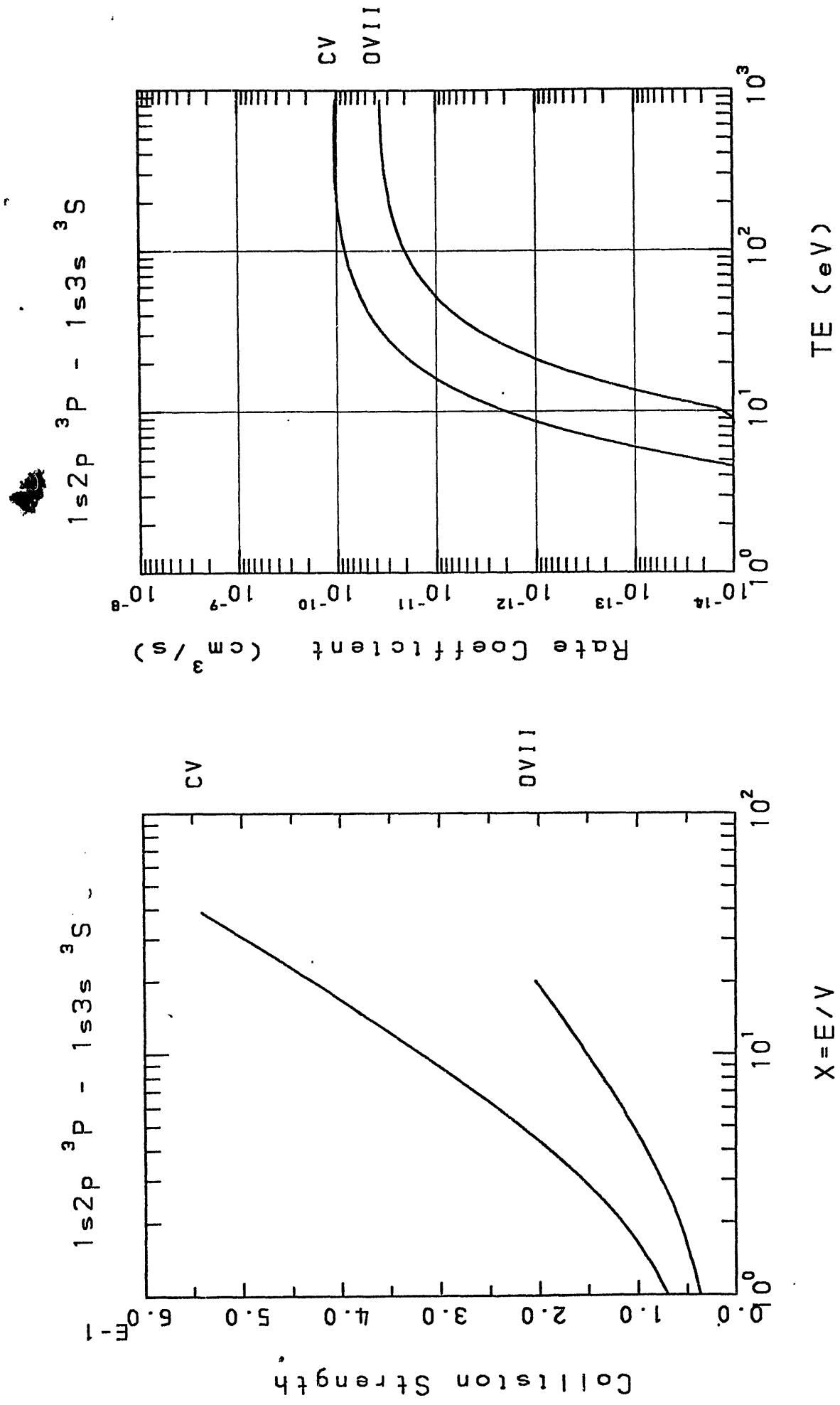


Fig. 27



Li-like (C IV, O VI)

Gau and Henry (1977) made a close-coupling (CC) calculation with five states ($1s^22s$, $1s^22p$, $1s^23s$, $1s^23p$, $1s^23d$). In their calculation, they did not take into account the closed-channel resonance. Later Bhadra and Henry (1982) performed a similar calculation including closed channels. They found that the transition $2s - 2p$ is slightly affected by the resonances, while $2s - 3s$ and $2s - 3p$ are strongly affected. The cross sections presently recommended are taken from the calculation of Gau and Henry corrected with the resonance enhancement factor obtained for $2s - 3s$ and $2s - 3p$ by Bhadra and Henry. For O VI, Gau and Henry did not actually calculate the cross section, but their interpolation formula along the isoelectronic sequence is adopted here.

For the transition $2s - 2p$ of C IV, beam-experiment data were obtained by Taylor et al. (1977). Those data are in quite good agreement with the theoretical values obtained by Gau and Henry. Thus the present cross sections for $2s - 2p$ are believed to be very accurate.

The CC calculation mentioned above was made only up to $X = 5$ for $2s - 3s$, $3p$, $3d$. For higher energies, we use the Coulomb-Born-Exchange (CBX) results of Mann (1977) and the distorted wave (DW) values of Mann (1981). These high-energy cross sections are smoothly connected with the low-energy CC values.

Data sources

Bhadra, K. and Henry, R.J.W. (1982), Phys. Rev. A **26** 1848

[$2s - 3s, 3p$, CC]

Gau, J.N. and Henry, R.J.W. (1977), Phys. Rev. A **16** 986

[$2s - 2p, 3s, 3p, 3d$, CC]

Mann, J.B. (1977), quoted in Los Alamos Scientific Laboratory Report, LA-6691-MS,
ed. N.H. Magee, Jr. et al.

[$2s - 2p, 3s, 3p, 3d$ of C IV, CBX]

Mann, J.B. (1981), private communication

[$2s - 2p, 3s, 3p, 3d$ of O VI, DW]

Taylor, P.O., Gregory, D., Dunn, G.H., Phaneuf, R.A. and Crandall, D.H. (1977), Phys.
Rev. Lett. **39** 1256

[$2s - 2p$ of C IV, beam experiment]

Fig. 28

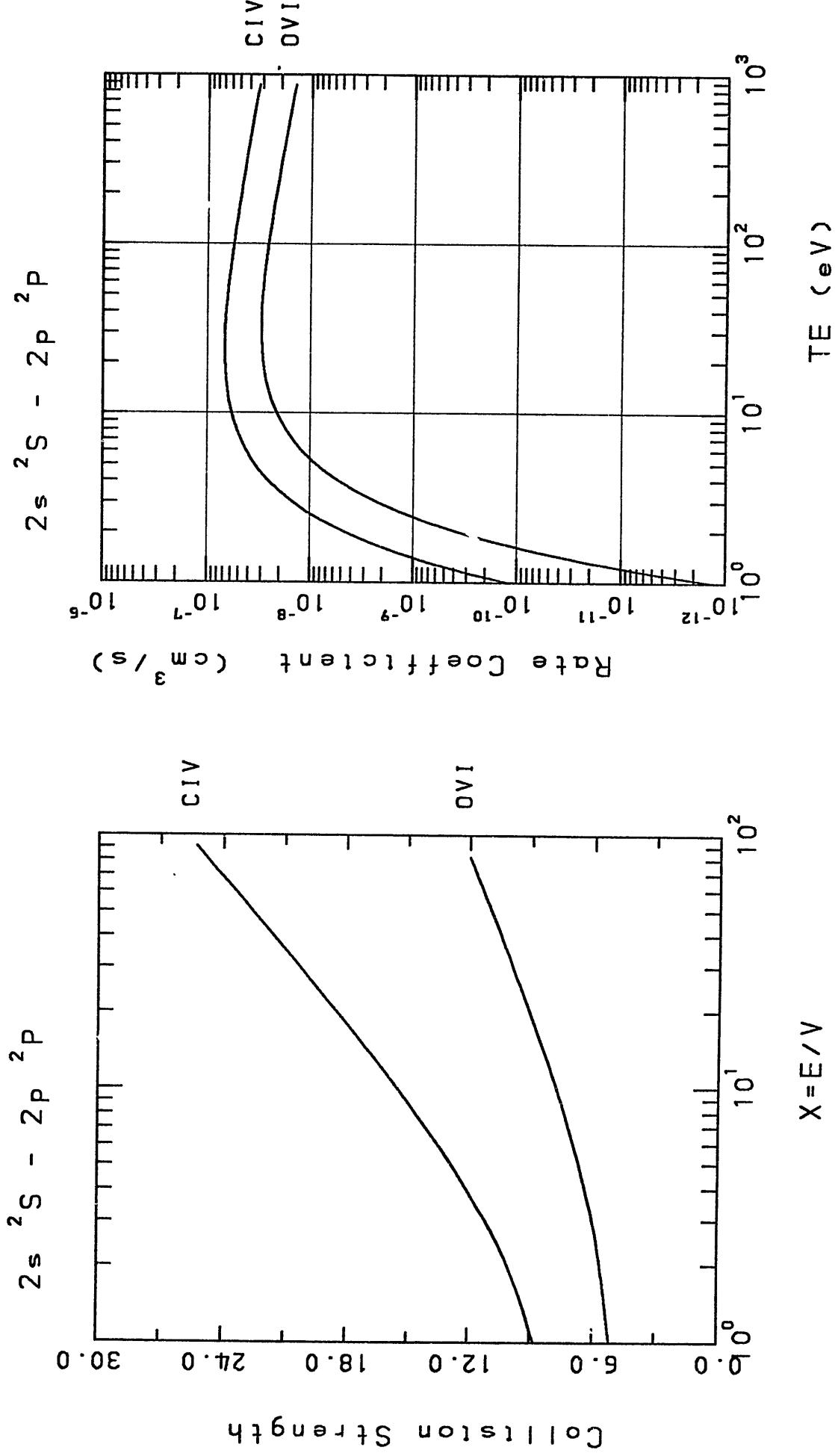


Fig. 29

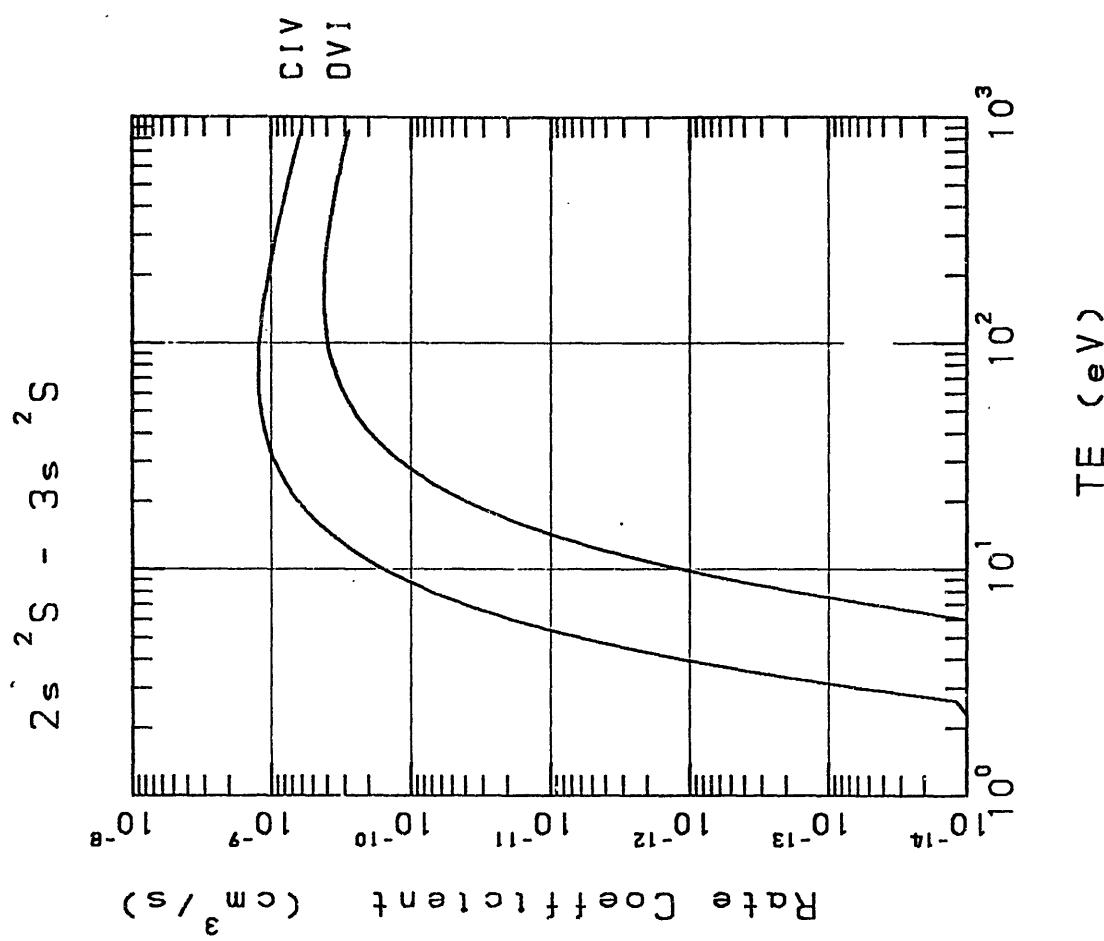
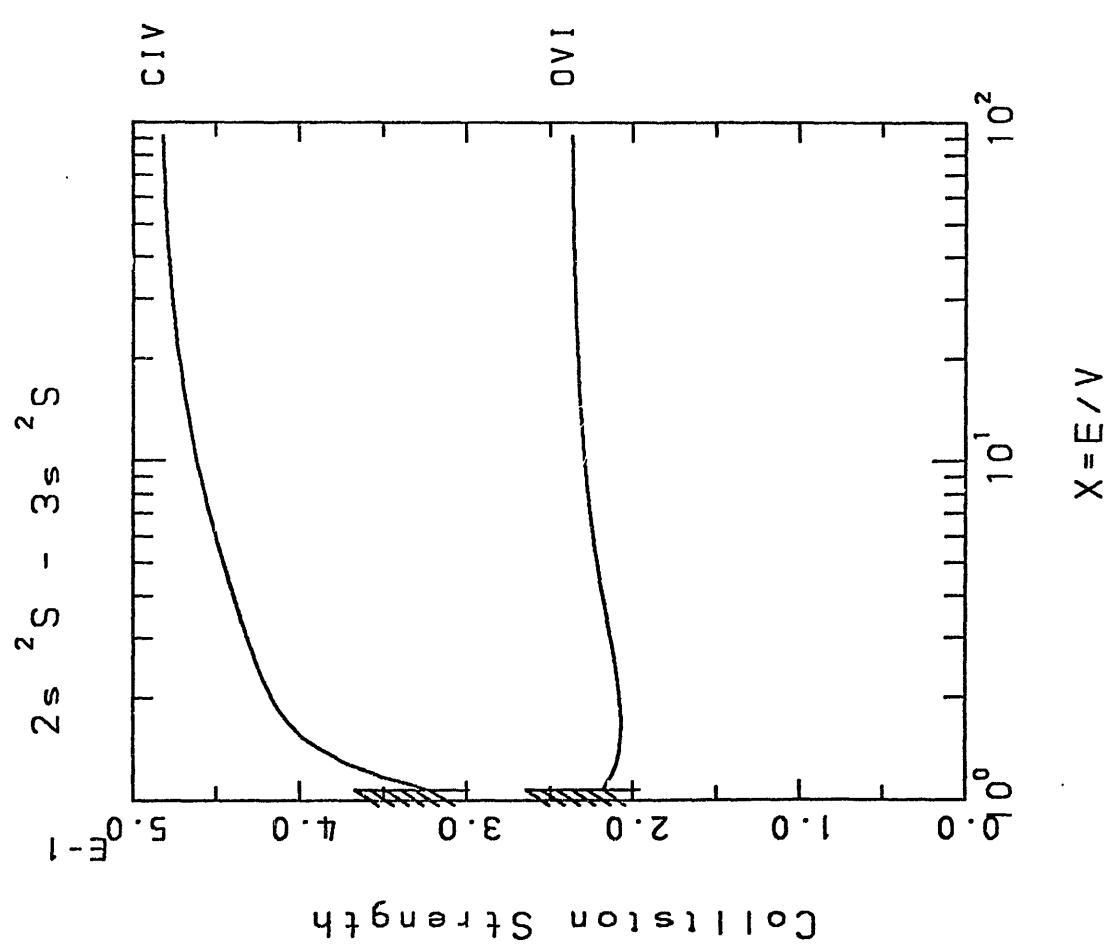


Fig. 30

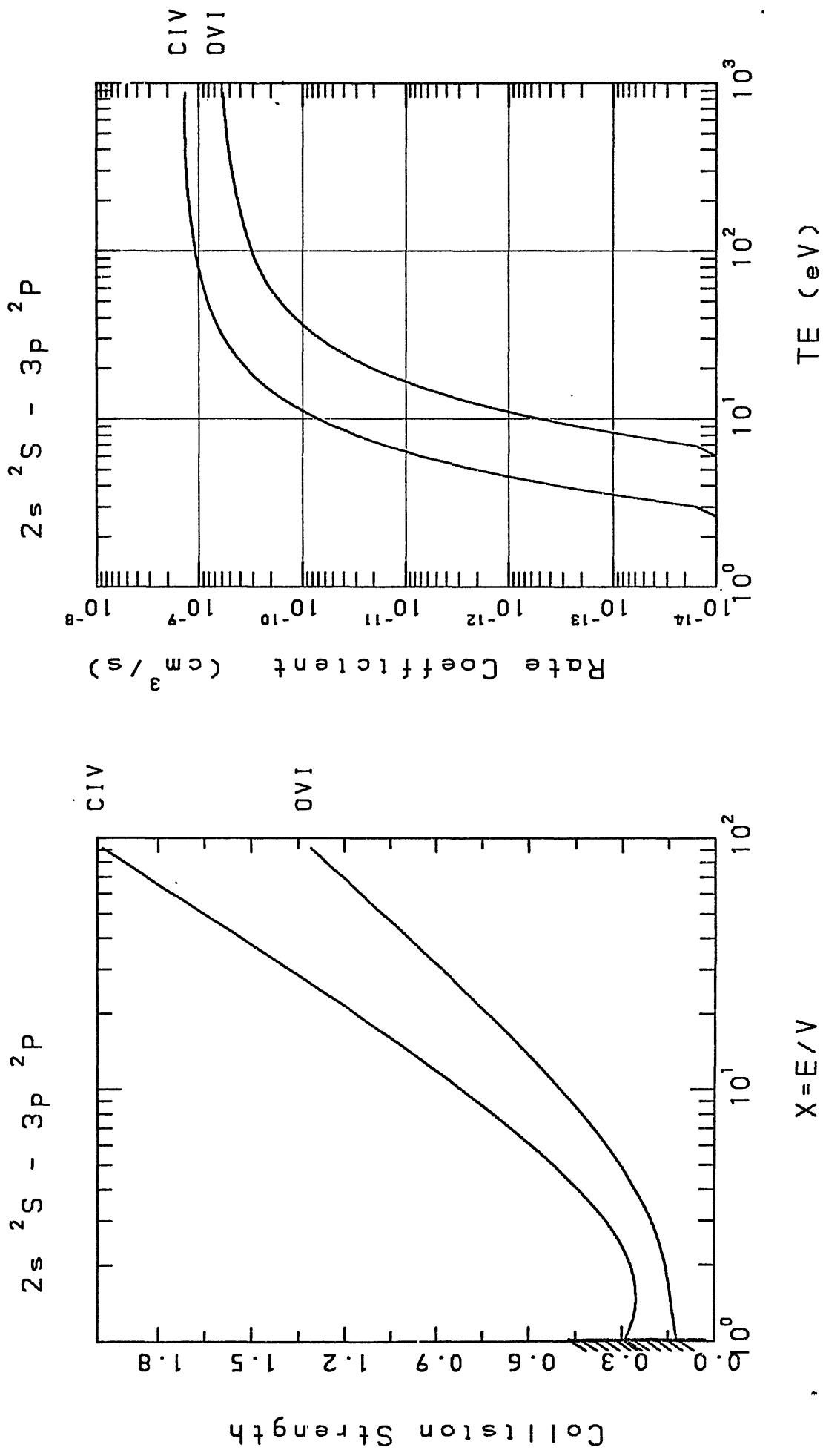
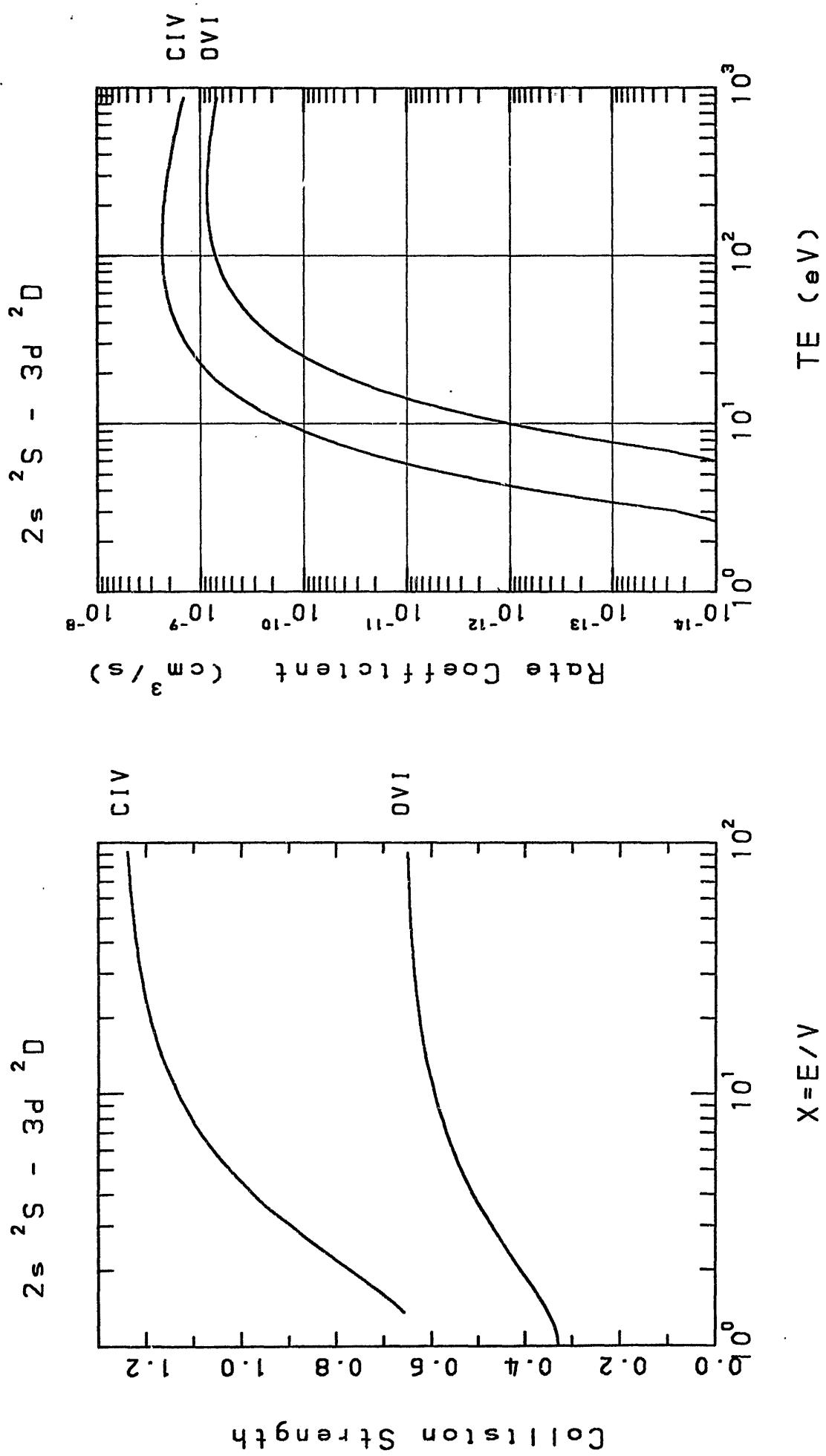


Fig. 31



Be-like (C III, O V)

Berrington et al. (1981) reported their cross sections obtained by the R-matrix method including six ionic states ($2s^2 \ ^1S$, $2s2p \ ^3P$, 1P , $2p^2 \ ^3P$, 1D , 1S). Their results included the effect of the resonances converging to the $n = 2$ thresholds. The rate coefficients based on the cross sections were reported separately by Dufton et al. (1978). These results, though the most elaborate and extensive ones published so far, have two drawbacks. First, they reported the collision strengths only for very limited energy range near threshold. That is, the rate coefficients are given only for very narrow range of electron temperature (over one decade around 10^5 K). Further, the effect of the resonances converging to the $n = 3$ thresholds cannot always be ignored. Berrington et al. (1979) found, in fact, that the resonances increase the $2s^2 \ ^1S - 2s2p \ ^3P$ collision strength of O V by about a factor of two, if $n = 3$ states are included in the calculation. The transition, $2s^2 \ ^1S - 2s2p \ ^1P$, was slightly affected.

The present recommended data are based essentially on the calculation of Berrington et al. (1981) and augmented by some other calculations made over a wider energy region. By using the rate coefficients of Dufton et al., the resonance effects are incorporated into the present data, when the effects are large.

For the excitation of $n = 3$ states, the CBX and the distorted-wave cross sections obtained by Mann (1977, 1981b) are adopted. Recently Widing et al. (1982) published the rate coefficients for $2s^2 \ ^1S - 2s3s \ ^3S$, 1S , $2s3p \ ^3P$, 1P , $2s3d \ ^3D$, 1D of O V. They obtained them from the R-matrix calculation with 12 states. The collision strengths recommended here for $2s^2 \ ^1S - 2s3s \ ^3S$ and $2s^2 \ ^1S - 2s3p \ ^3P$ of O V are adjusted to give those more accurate rate coefficients. For other transitions, the present recommended values are in fair agreement with the Widing calculation when his data are available. Widing et al. (1982) have reported rate coefficients also for $2s2p \ ^3P - 2s3s \ ^3S$, 1S , $2s3p \ ^3P$, 1P , $2s3d \ ^3D$, 1D of O V. Since they show their data for a very limited range of electron temperature ($8 \times 10^4 - 5 \times 10^5$ K), we do not show them here.

Data sources

Berrington, K.A., Burke, P.G., Dufton, P.L., Kingston, A.E. and Sinfailam, A.L. (1979),

J. Phys. B 12 L275

[$2s^2 \text{ } ^1\text{S} - 2s2p \text{ } ^3\text{P}, ^1\text{P}$ of O V, R-matrix]

Berrington, K.A., Burke, P.G., Dufton, P.L. and Kingston, A.E. (1981), Atomic Data Nucl. Data Tables 26 1

[all transitions among the states of $2s^2$, $2s2p$, $2p^2$ configurations, R-matrix]

Dufton, P.L., Berrington, K.A., Burke, P.G. and Kingston, A.E. (1978), Astron. Astrophys. 62 111

[rate coefficients calculated from the collision strengths in Berrington et al. (1981)]

Mann, J.B. (1977), quoted in Los Alamos Scientific Laboratory Report, LA-6691-MS, ed. N.H. Magee, Jr. et al.

[$2s^2 \text{ } ^1\text{S} - 2s3s \text{ } ^3\text{S}, ^1\text{S}$, $2s3p \text{ } ^3\text{P}, ^1\text{P}$, $2s3d \text{ } ^3\text{D}, ^1\text{D}$ of C III, CBX]

Mann, J.B. (1981a), private communication by A.L. Merts

[$2s^2 \text{ } ^1\text{S} - 2s2p \text{ } ^3\text{P}, ^1\text{P}$, $2s2p \text{ } ^3\text{P} - 2p^2 \text{ } ^3\text{P}$, DW]

Mann, J.B. (1981b) private communication

[$2s^2 \text{ } ^1\text{S} - 2s3s \text{ } ^3\text{S}, ^1\text{S}$, $2s3p \text{ } ^3\text{P}, ^1\text{P}$, $2s3d \text{ } ^3\text{D}, ^1\text{D}$ of O V, DW]

Nakazaki, S. and Hashino, T. (1982), J. Phys. B 15 2767

[$2s2p \text{ } ^1\text{P} - 2p^2 \text{ } ^1\text{D}, ^1\text{S}$, Coulomb-Born-Bely]

Robb, W.D. (1977), quoted in Los Alamos Scientific Laboratory Report, LA-6691-MS, ed. N.H. Magee, Jr. et al.

[$2s^2 \text{ } ^1\text{S} - 2p^2 \text{ } ^3\text{P}, ^1\text{D}$, $2s2p \text{ } ^1\text{P} - 2p^2 \text{ } ^3\text{P}$ of C III, CC]

Widing, K.G., Doyle, J.G., Dufton, P.L. and Kingston, A.E. (1982), Astrophys. J. 257 913

[$2s^2 \text{ } ^1\text{S} - 2s3s \text{ } ^3\text{S}$, $2s3p \text{ } ^3\text{P}$ of O V, R-matrix]

Fig. 32

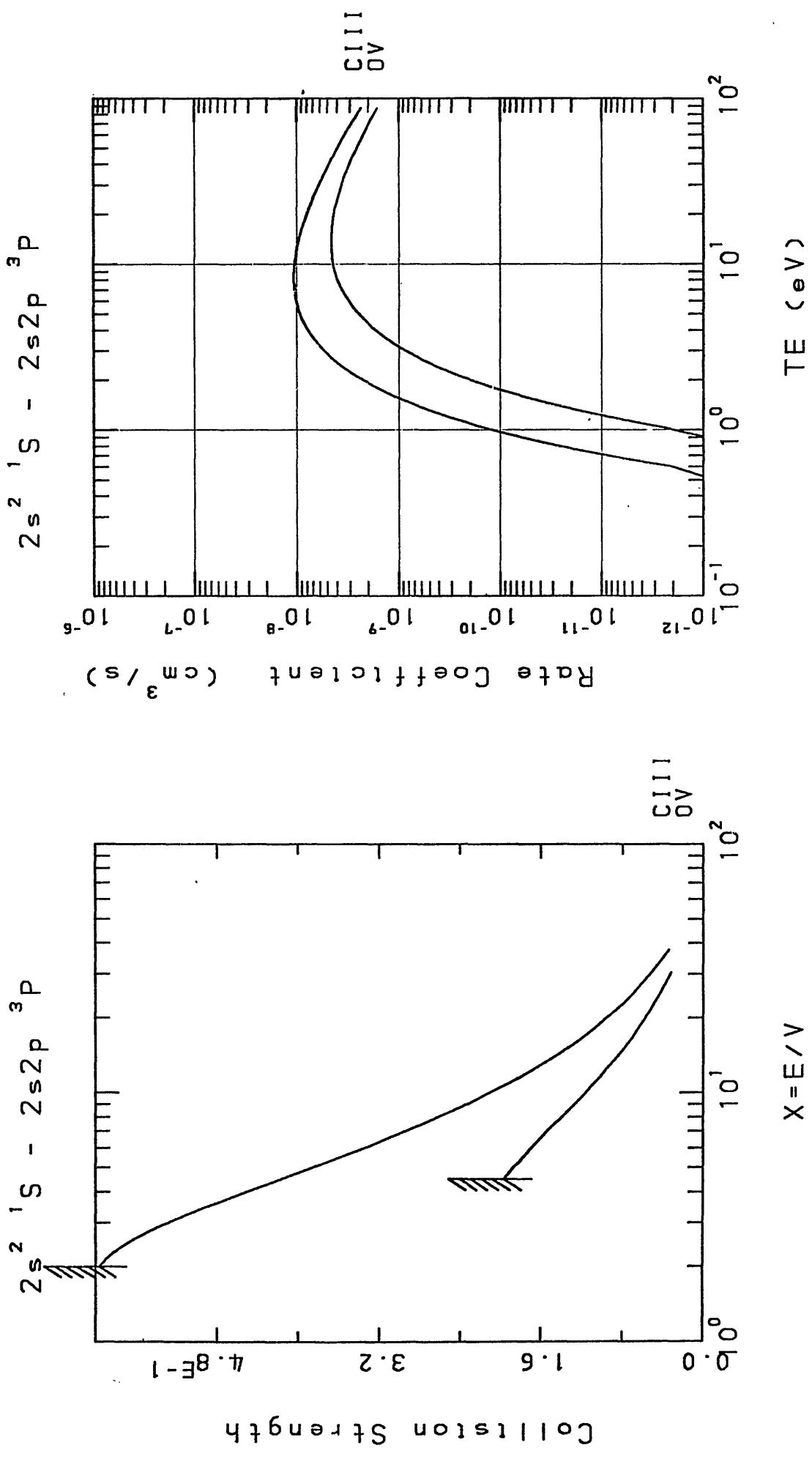
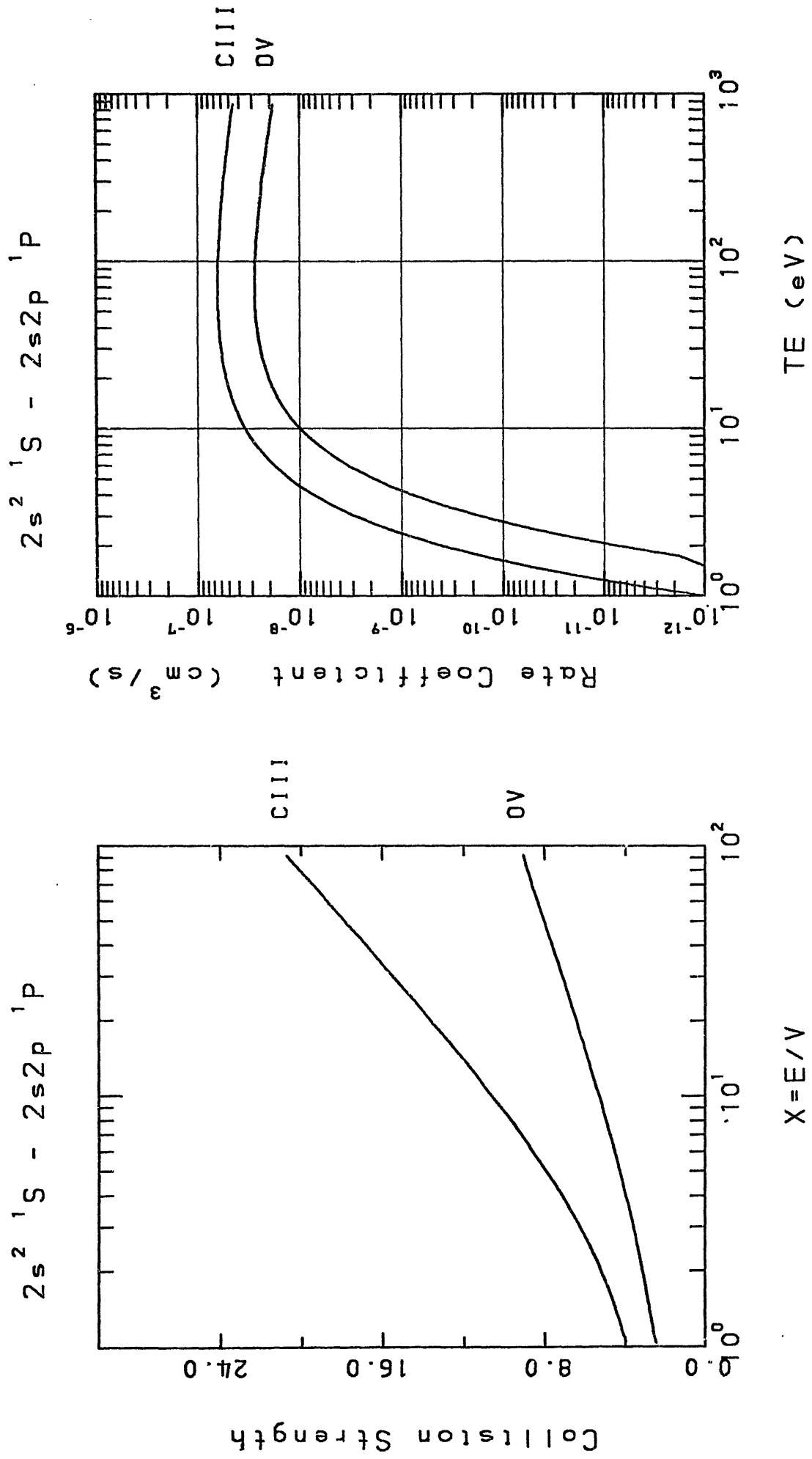


Fig. 33



Collision Strength

Fig. 34

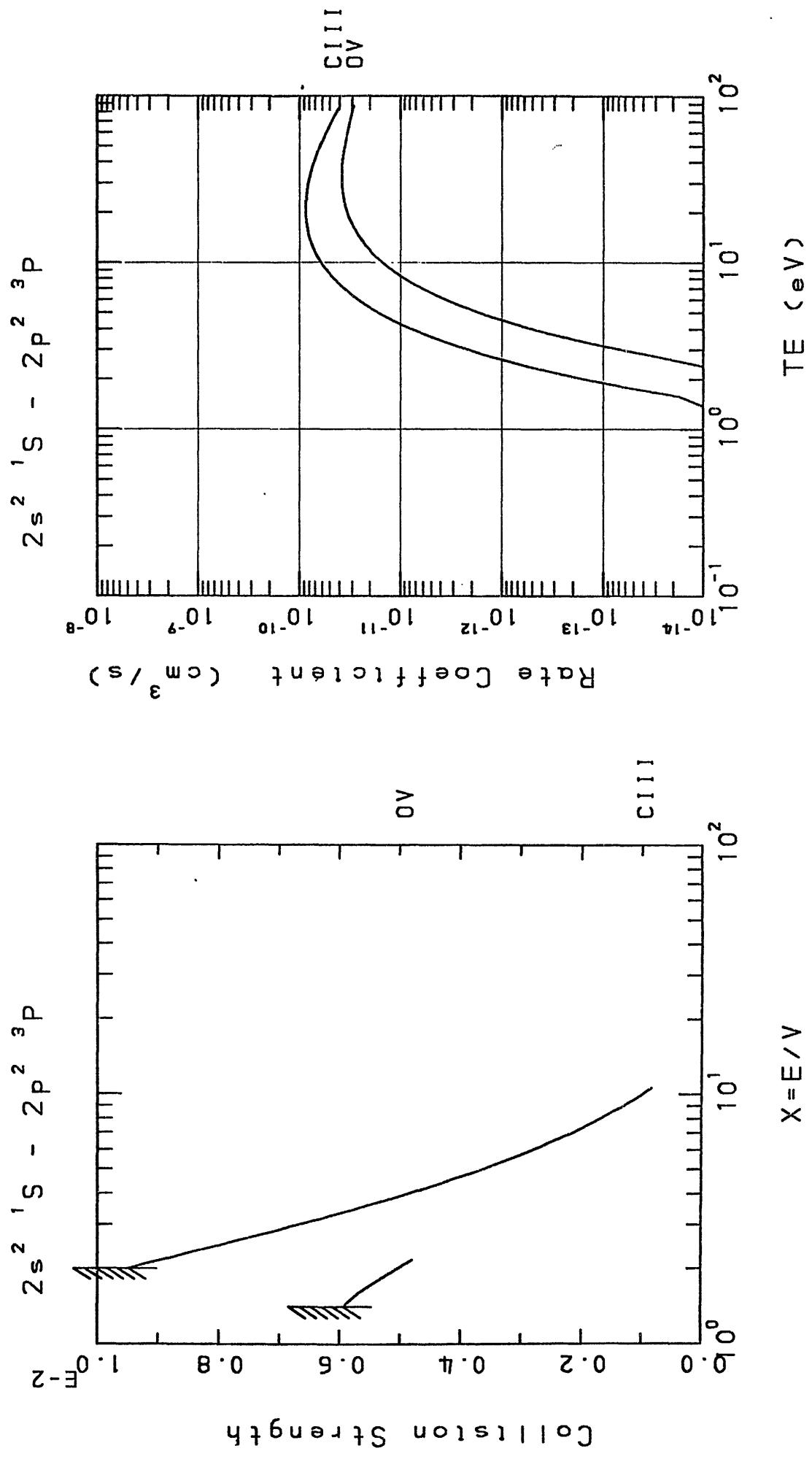


Fig. 35

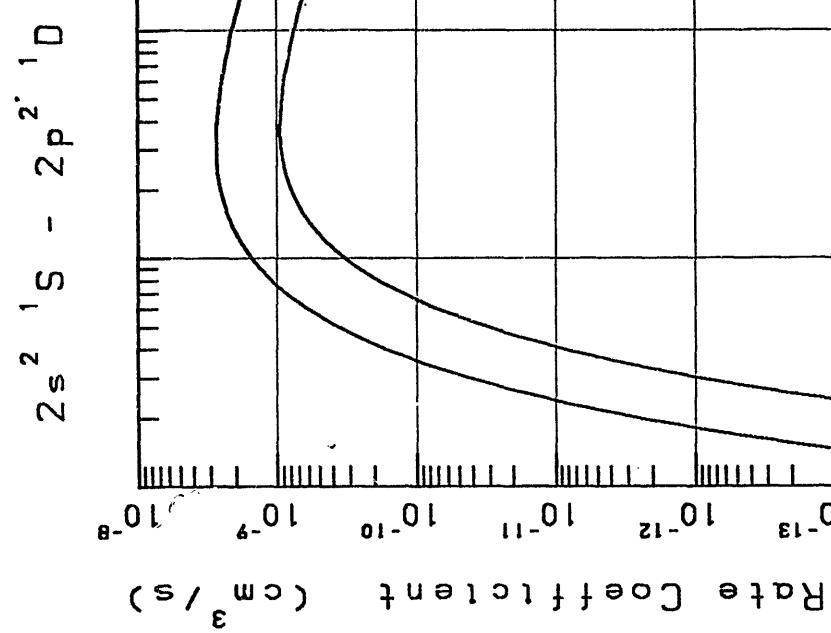
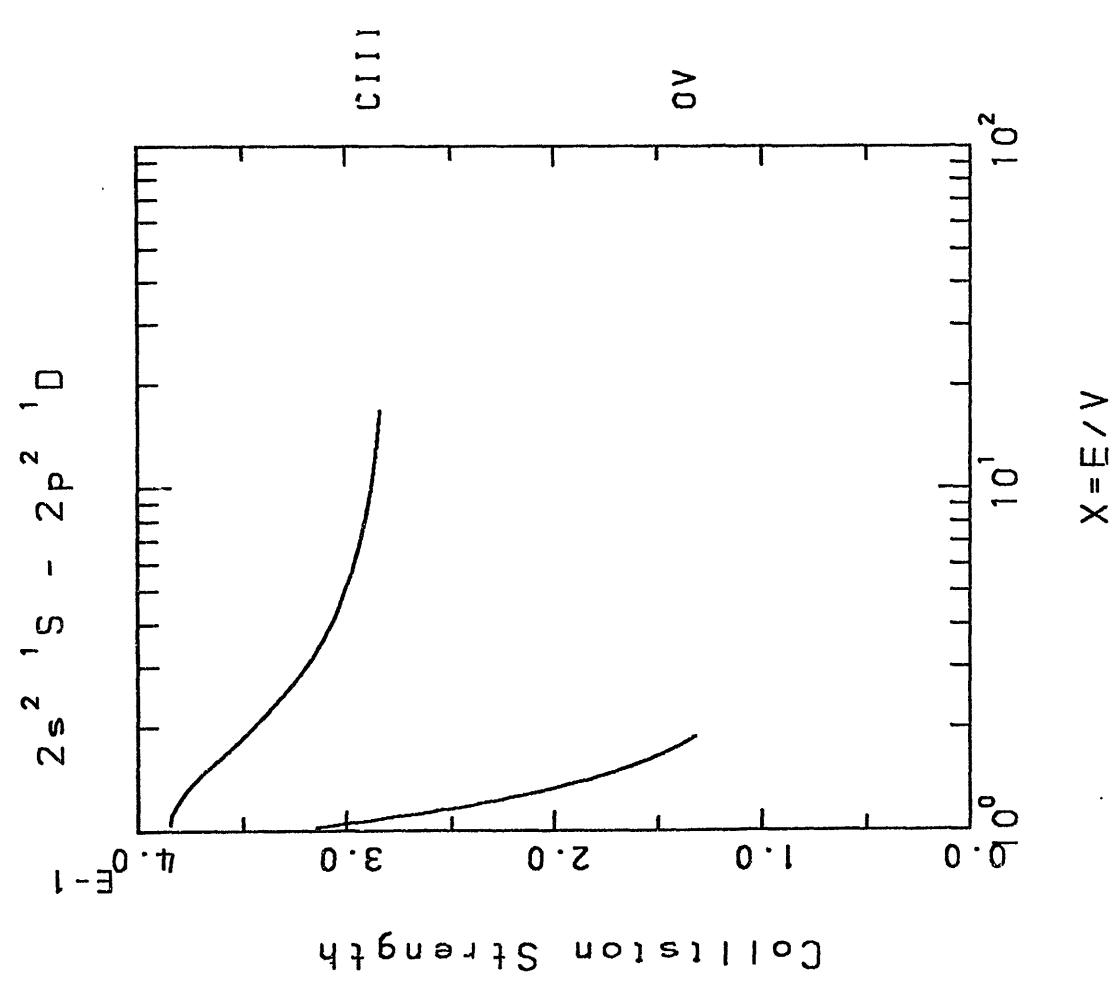


Fig. 36

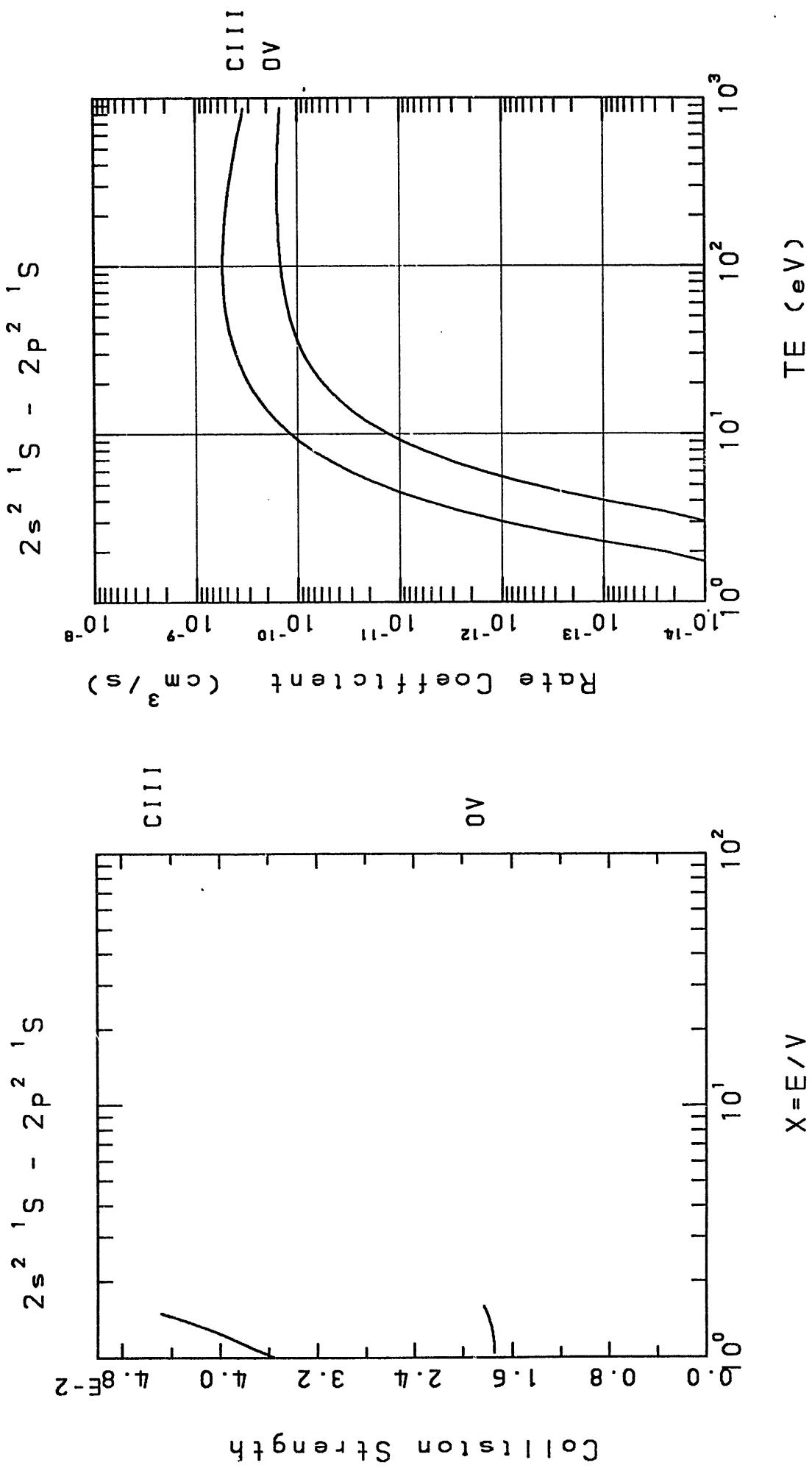


Fig. 37

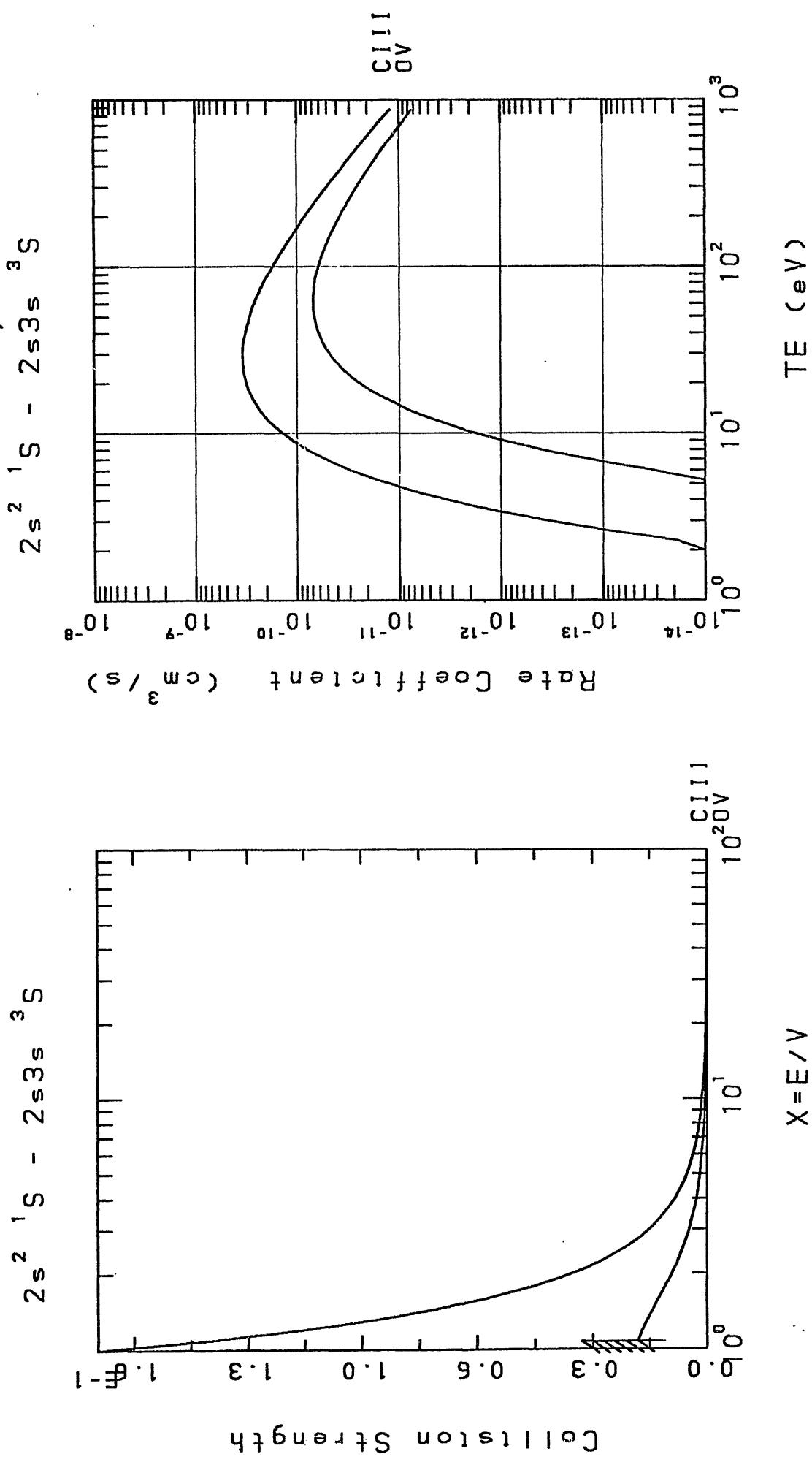


Fig. 38

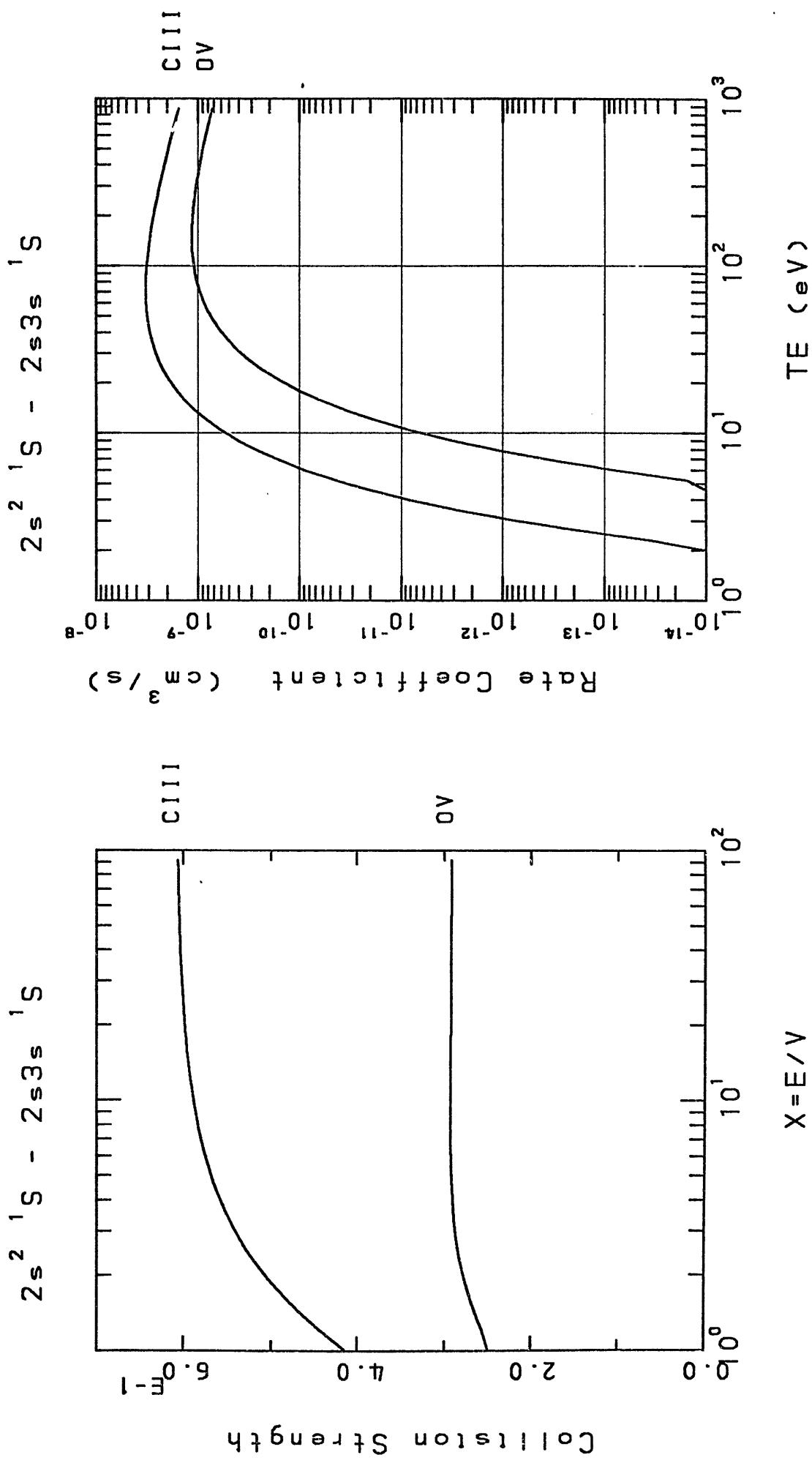


Fig. 39

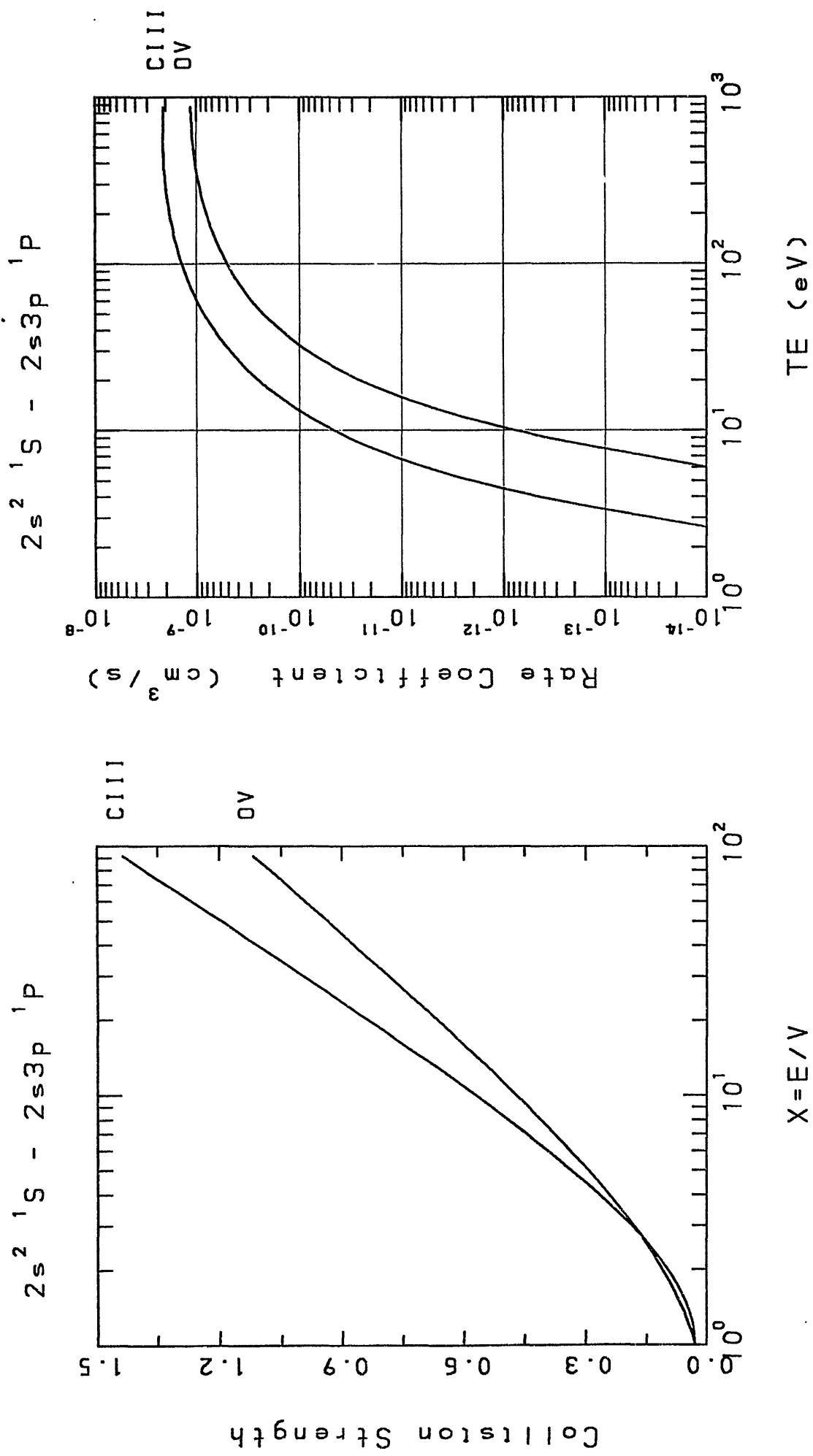


Fig. 40

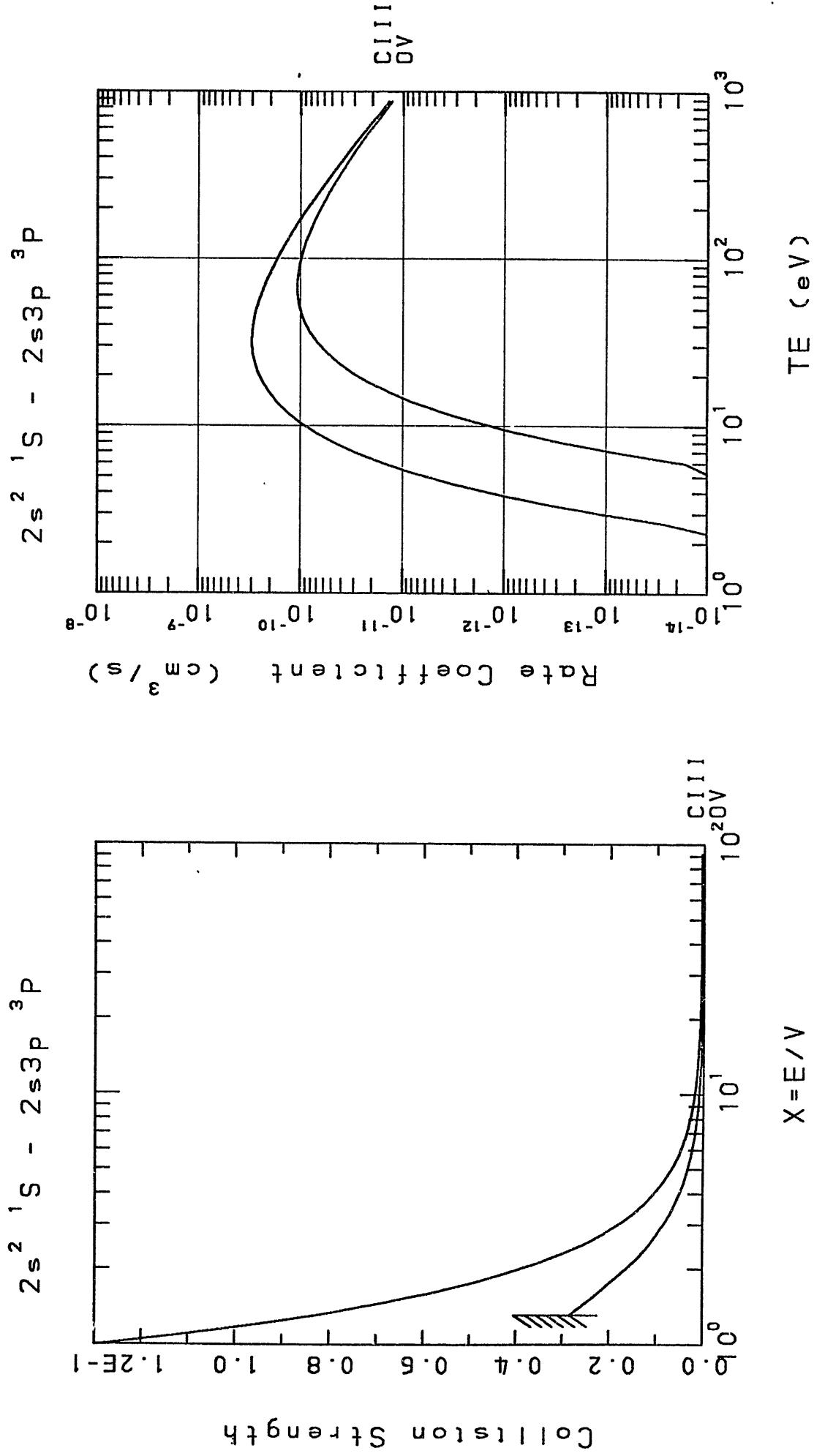


Fig. 41

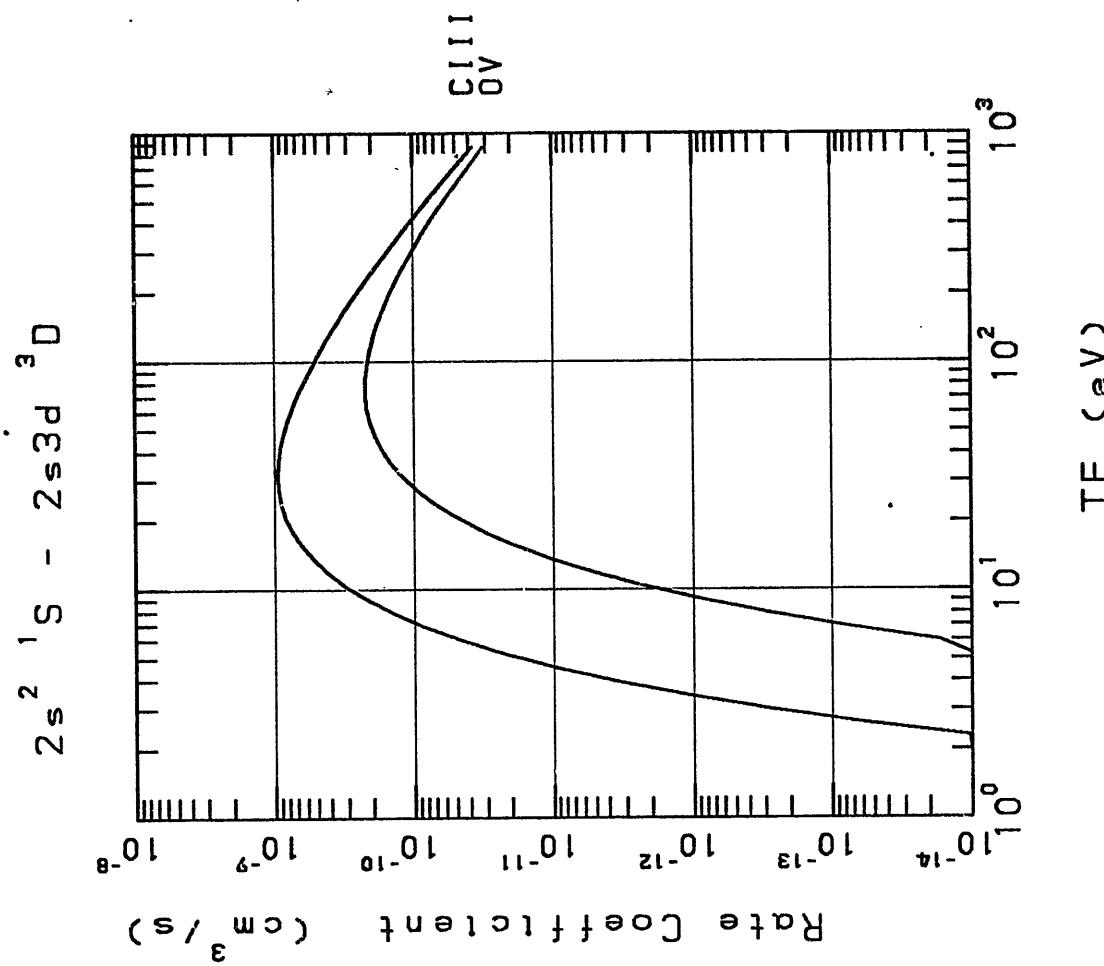
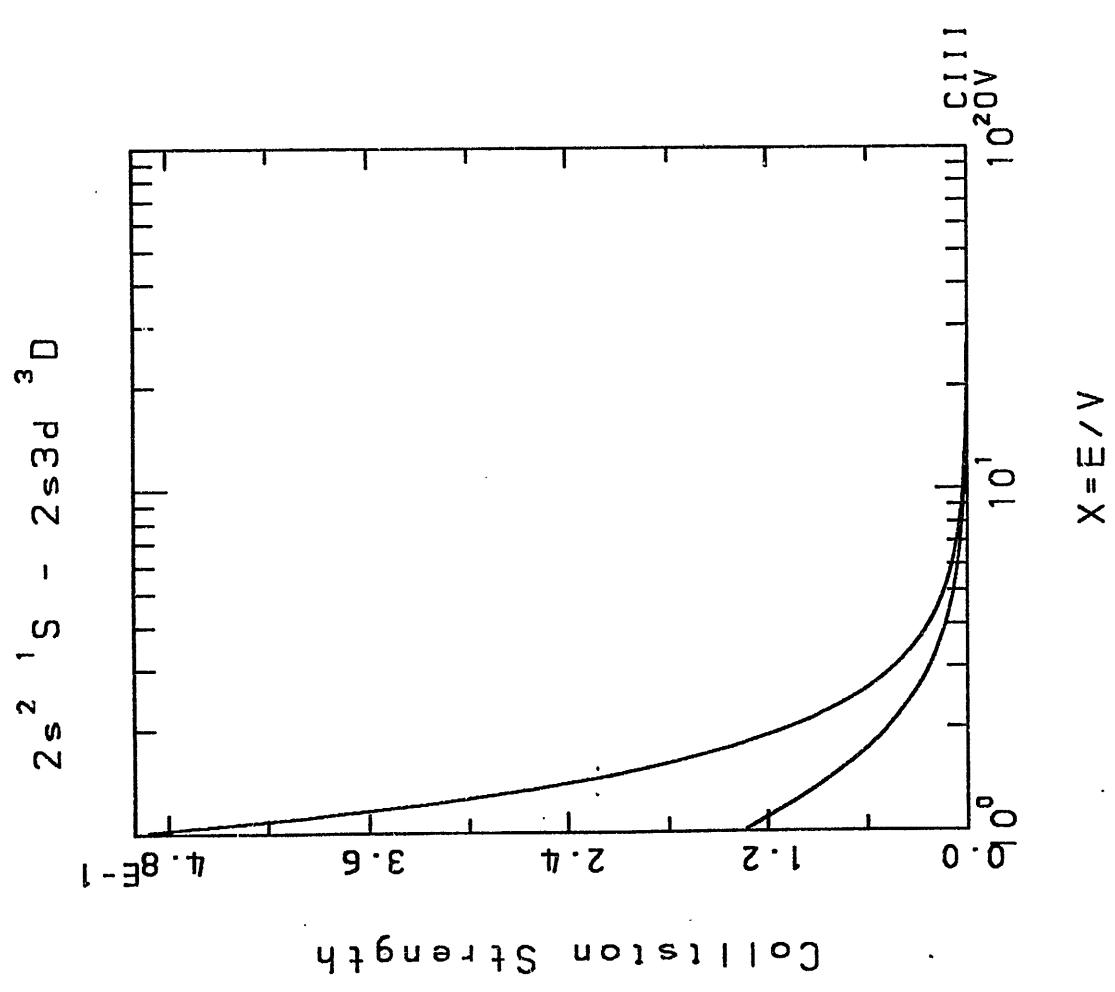


Fig. 42

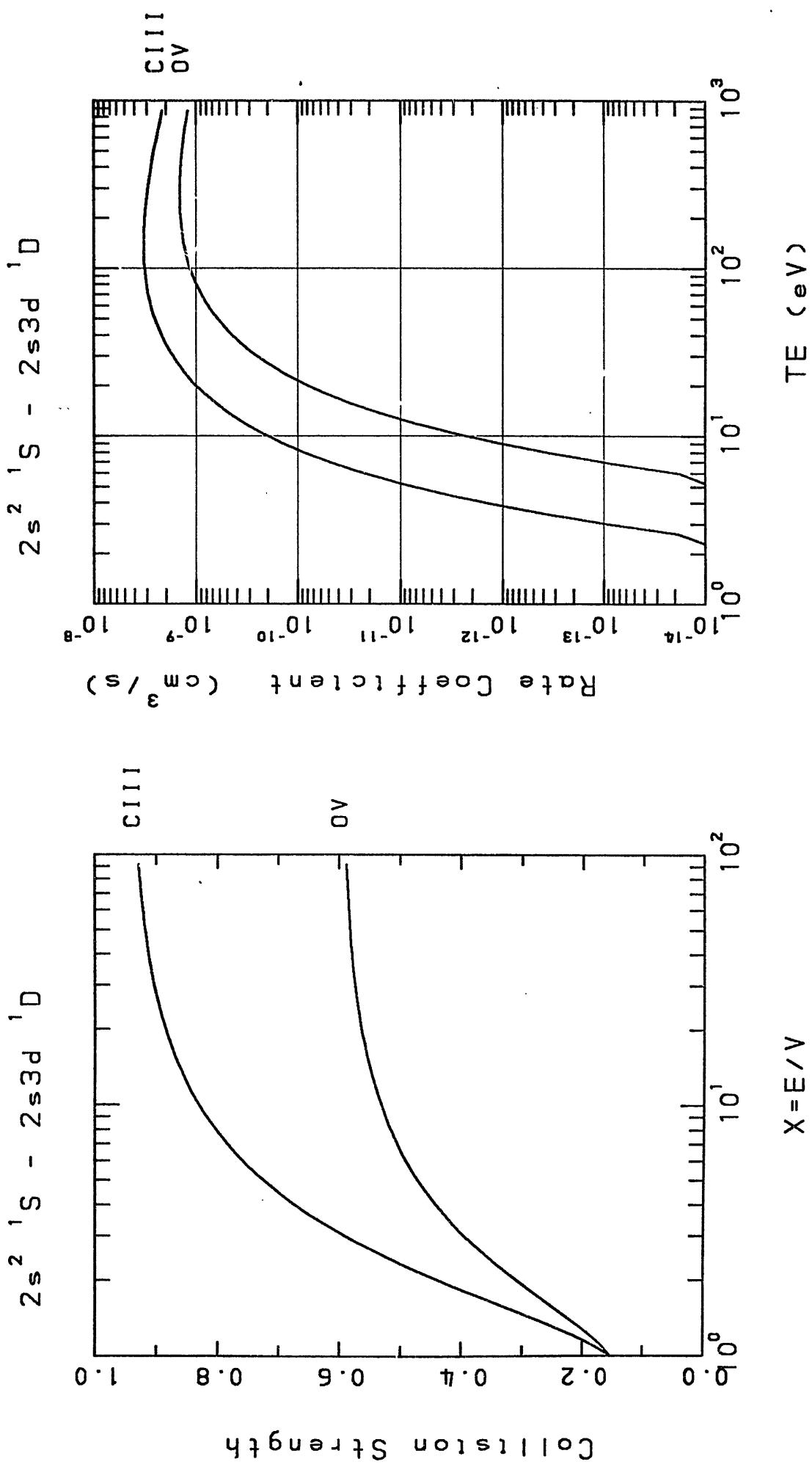


Fig. 43

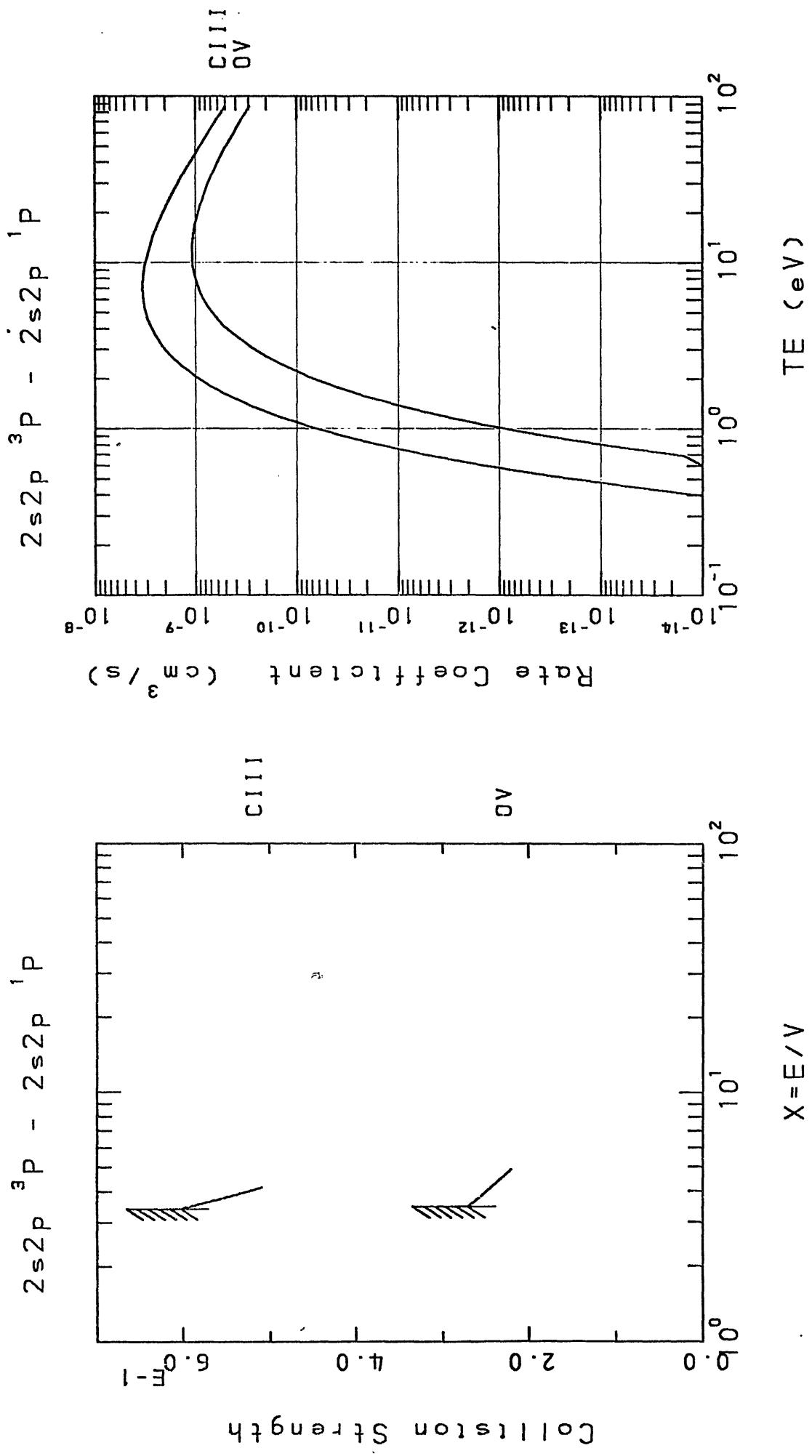


Fig. 44

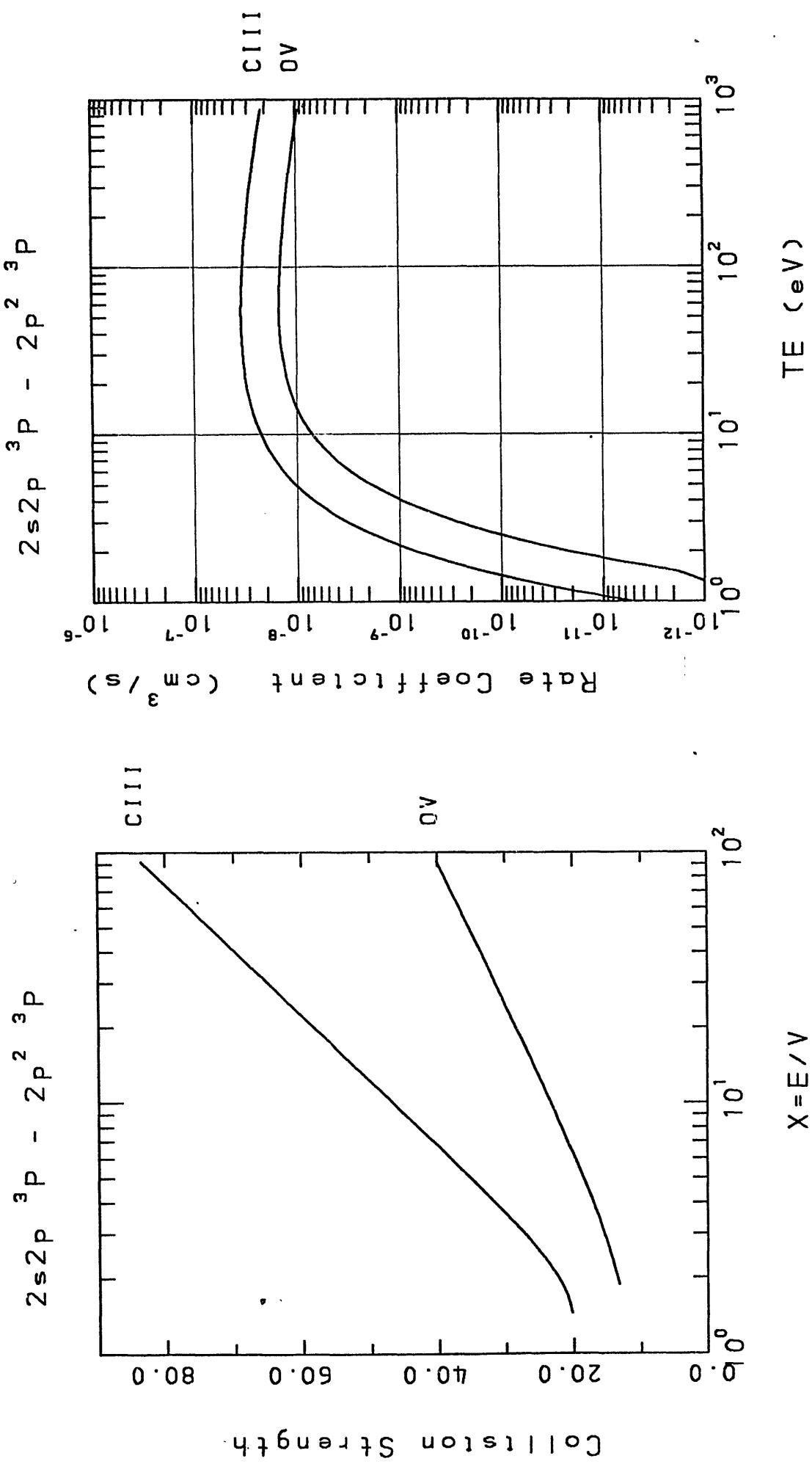


Fig. 45

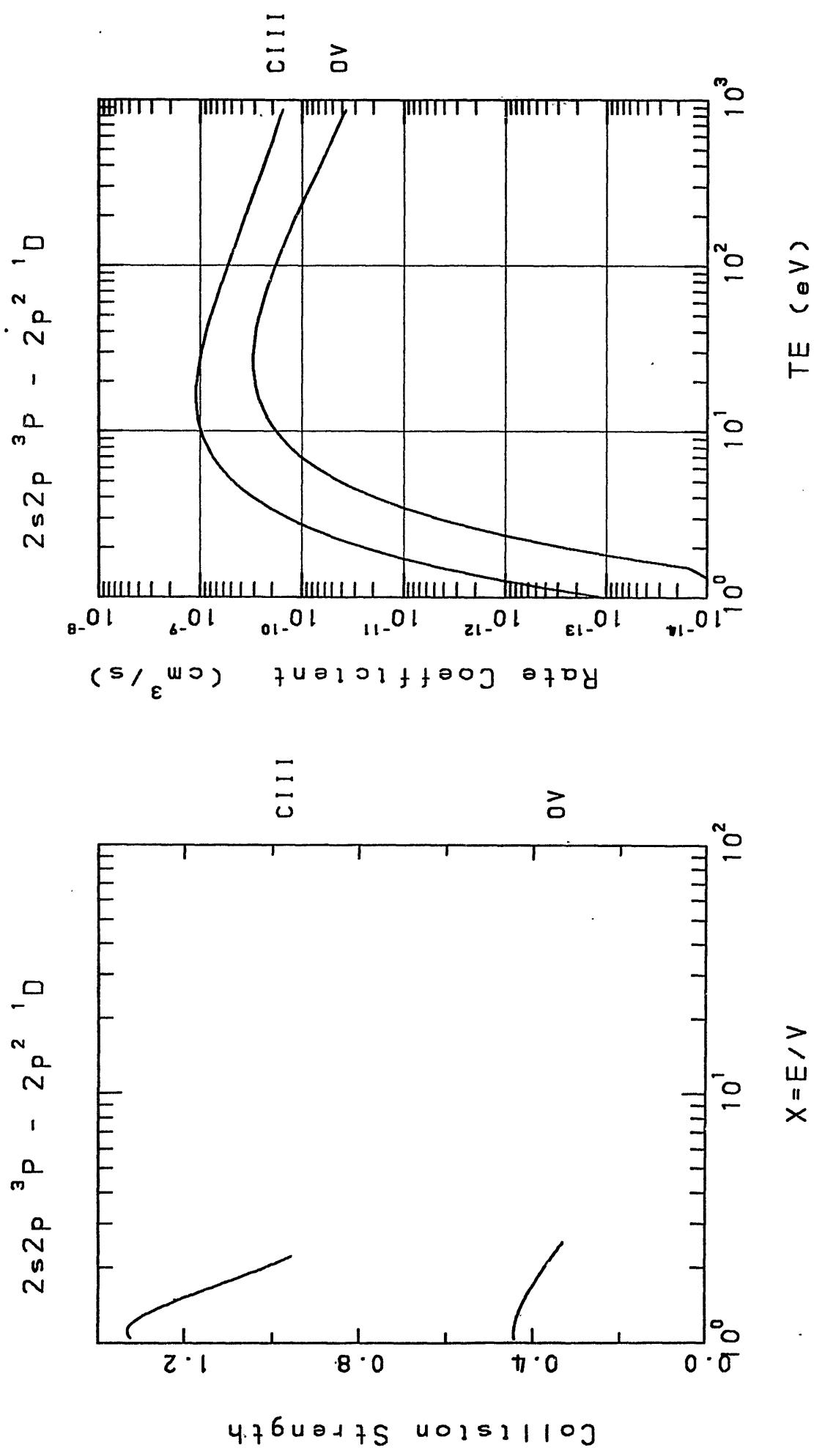


Fig. 46

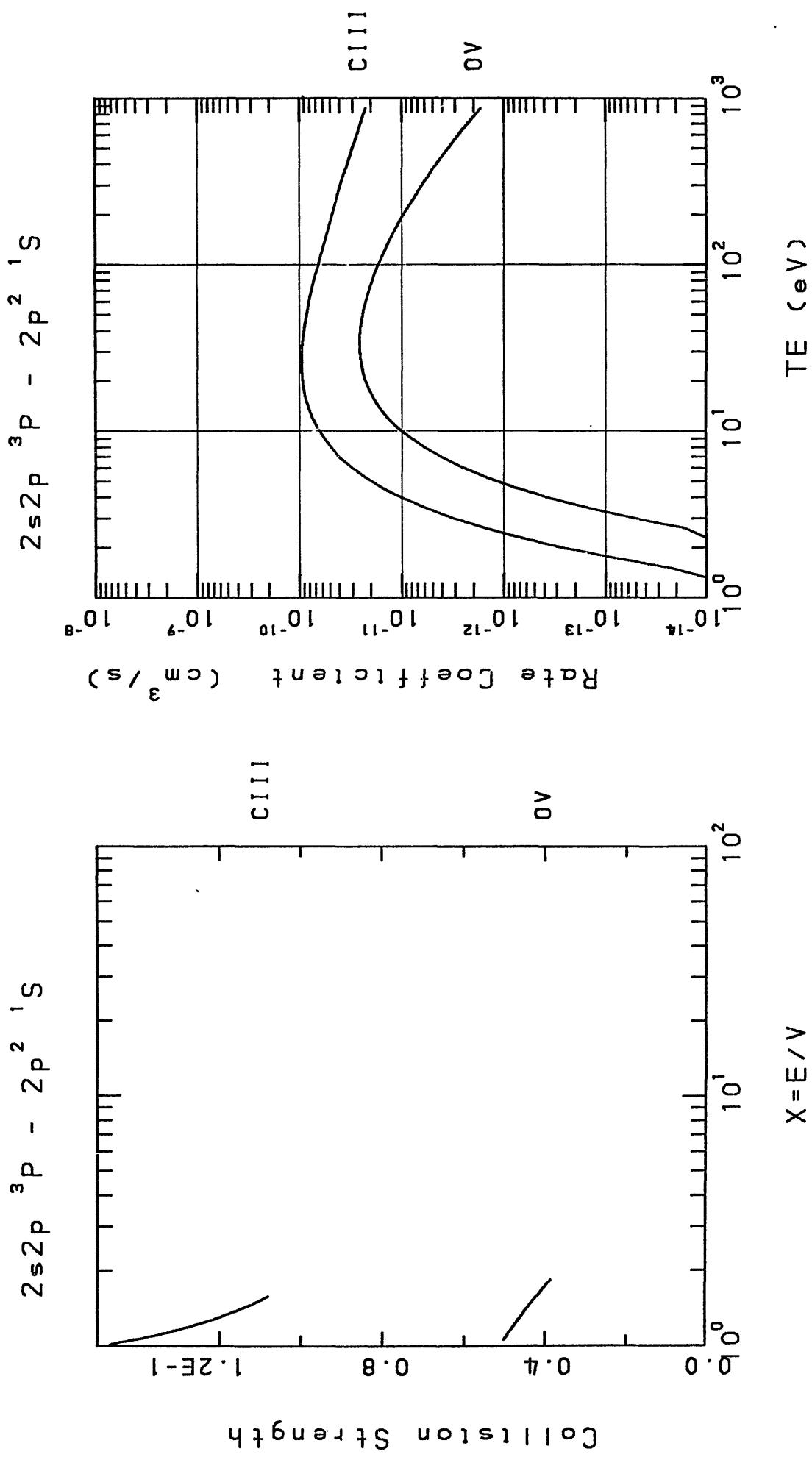


Fig. 47

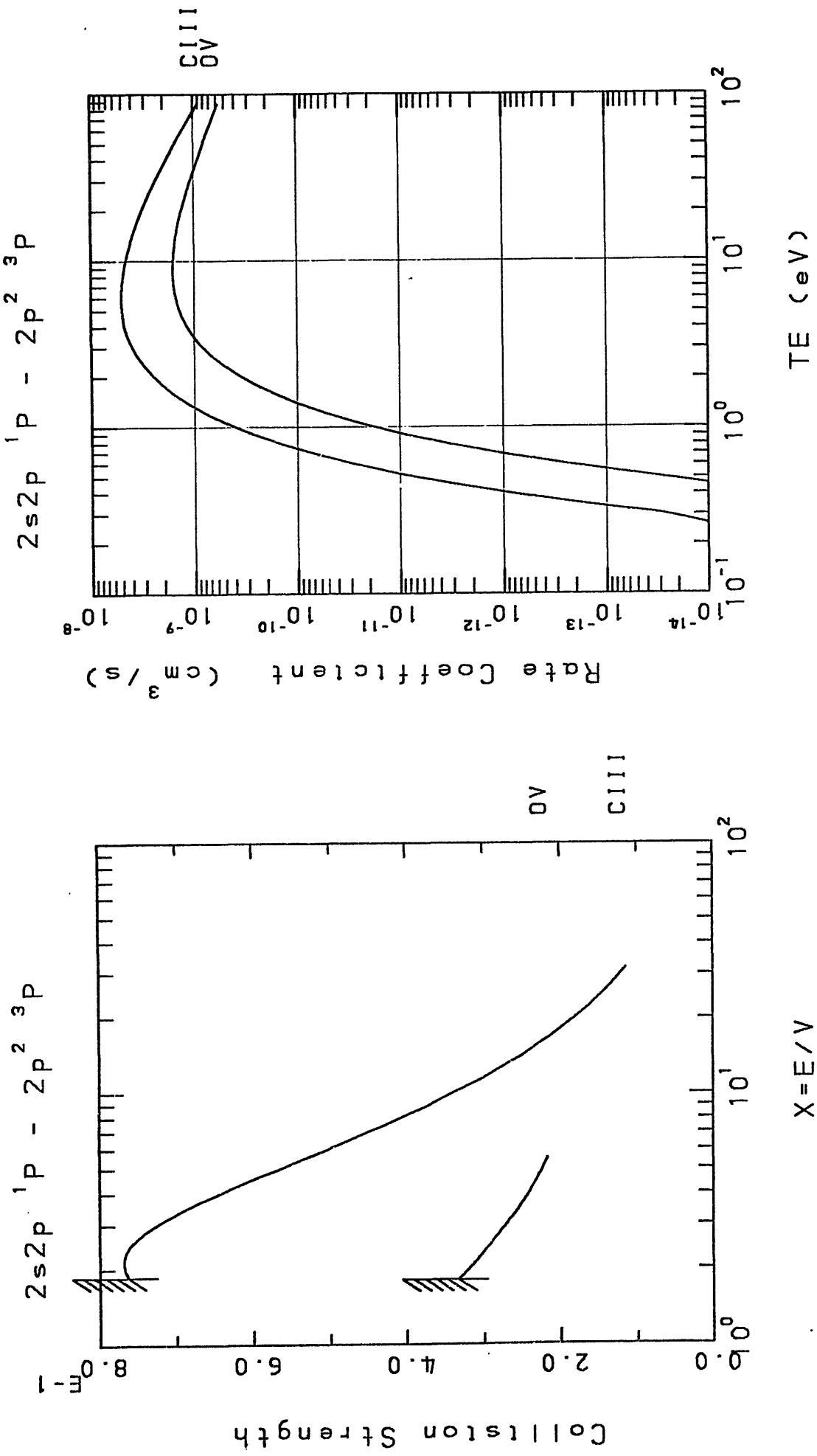


Fig. 48

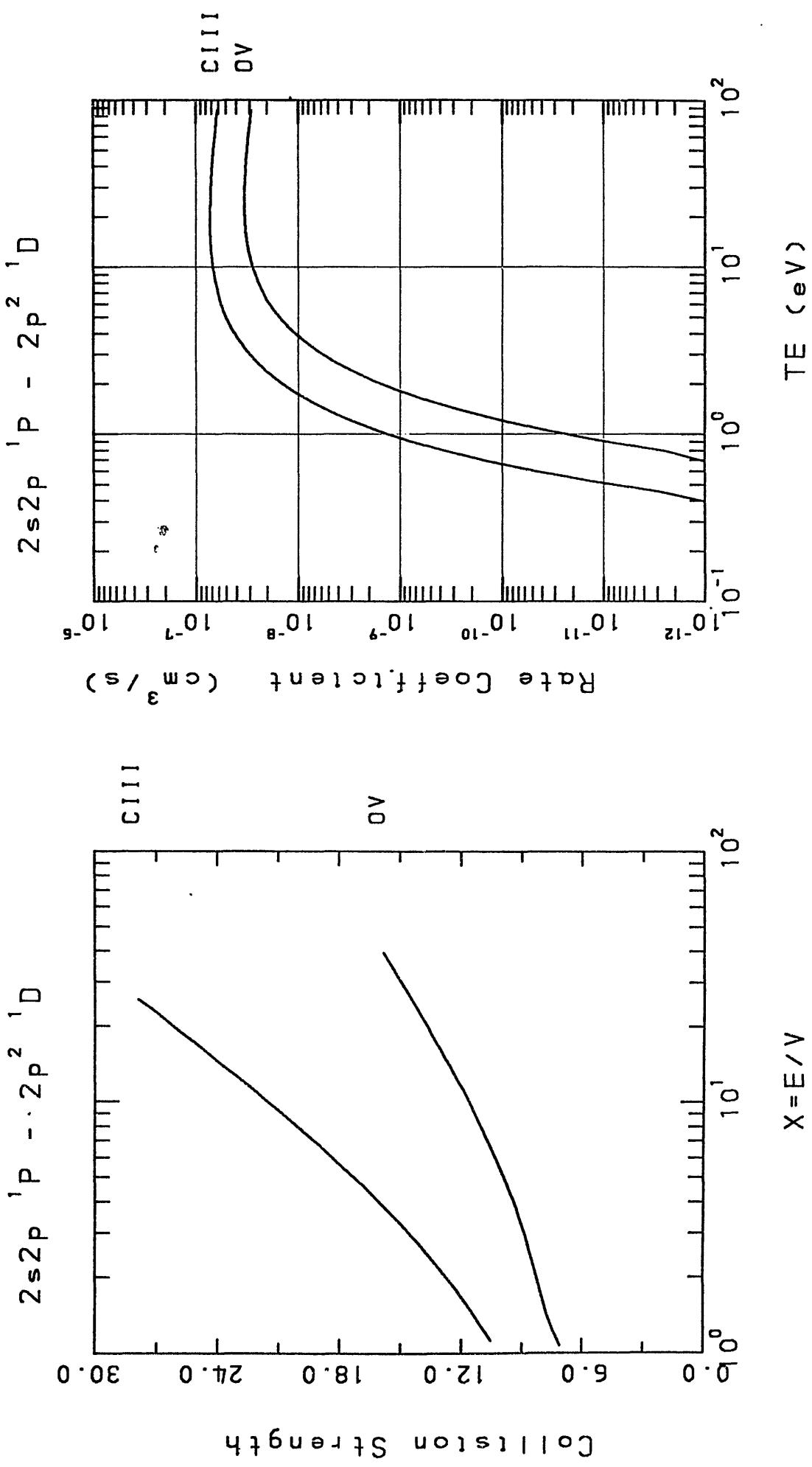


Fig. 4.9

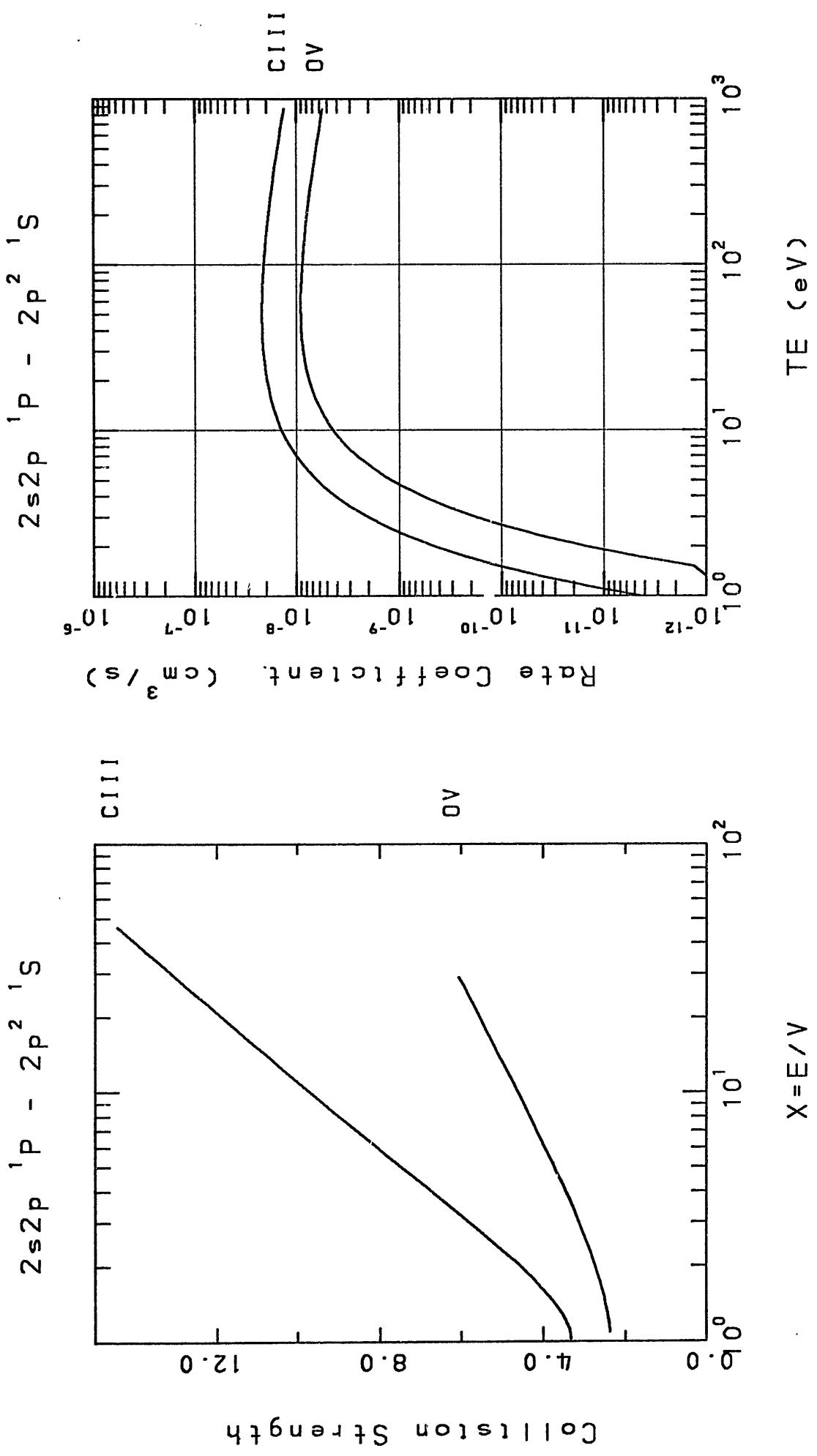


Fig. 50

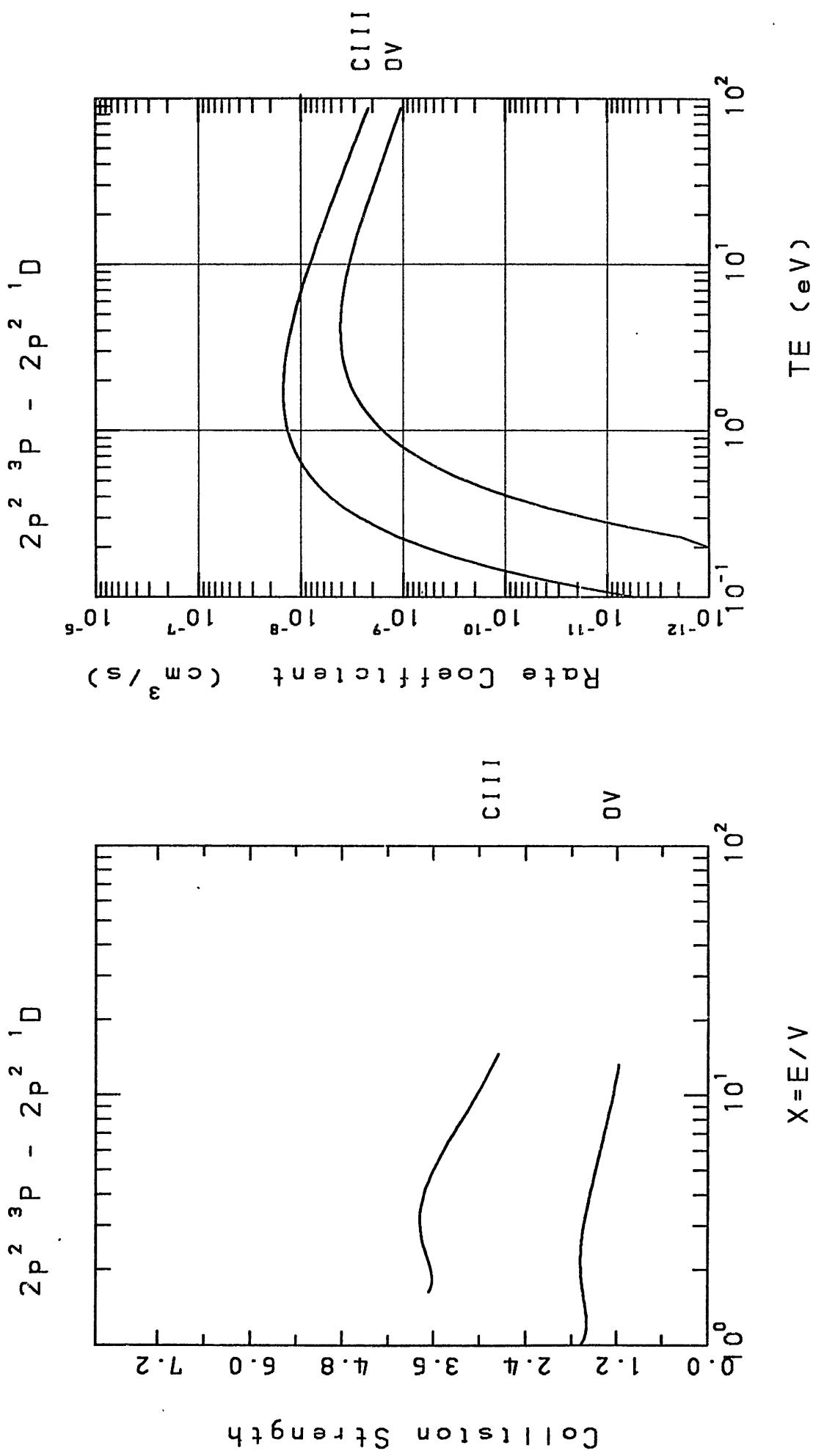


Fig. 51

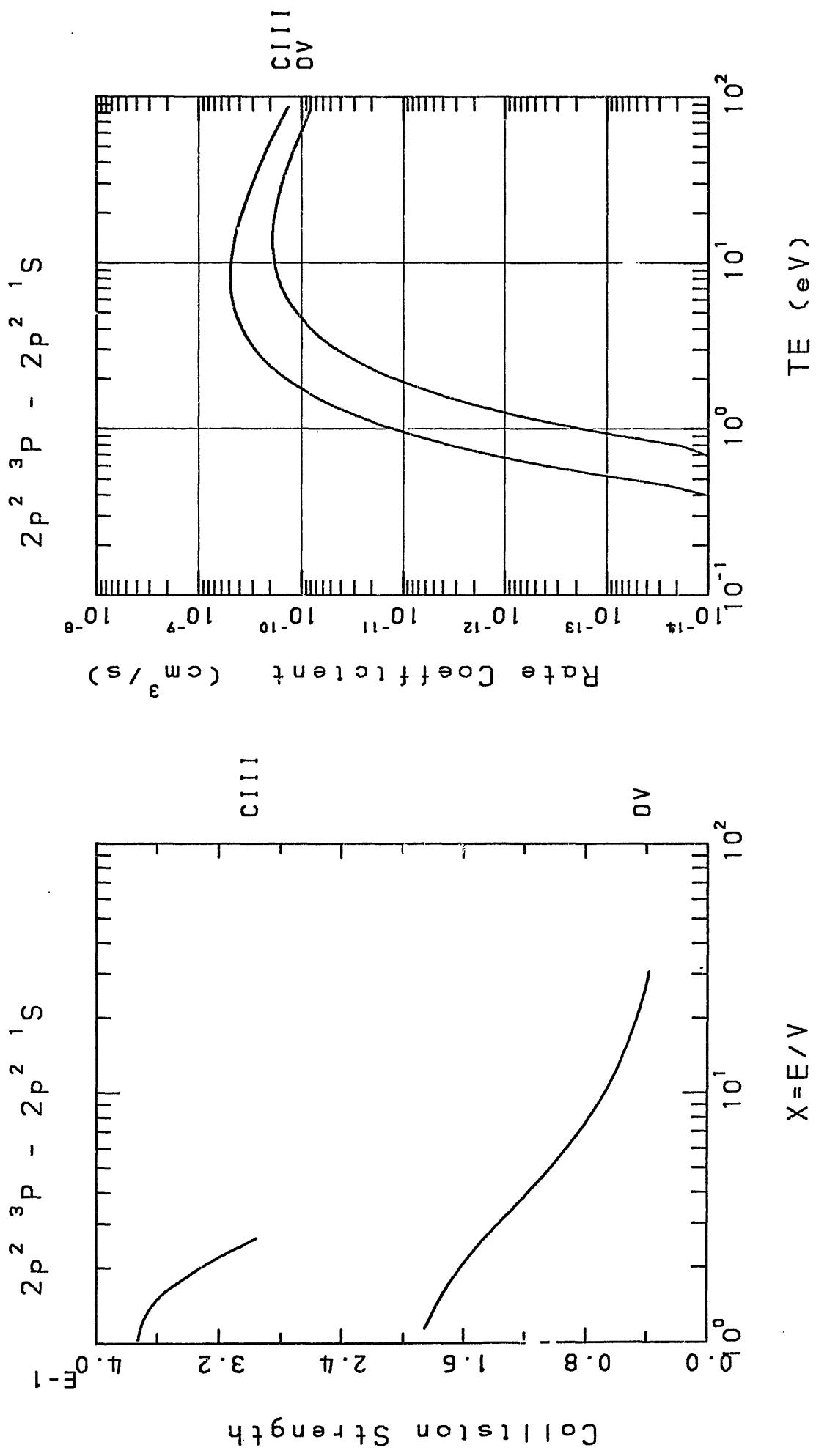
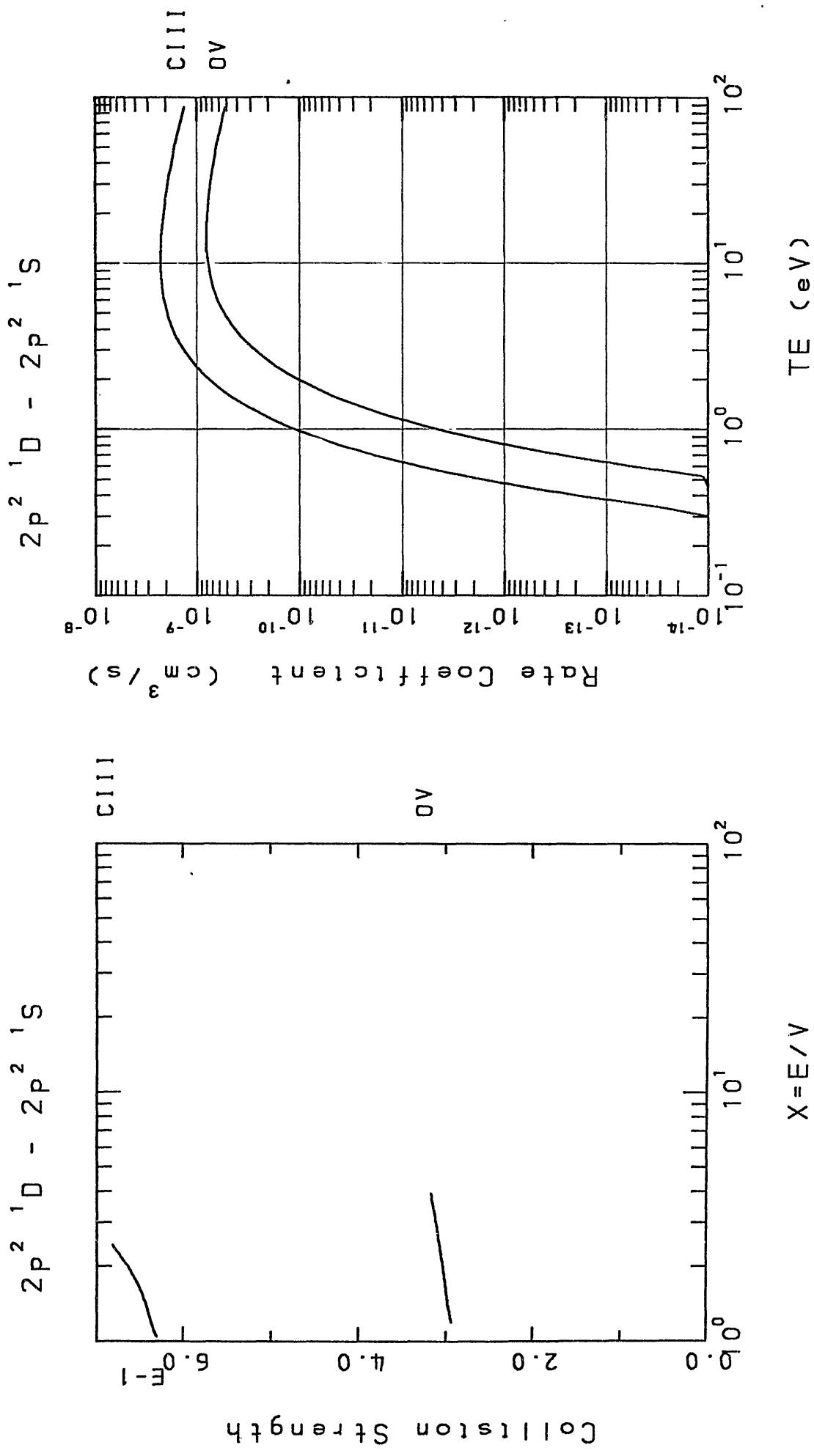


Fig. 52



B-like (C II, O IV)

Robb (1977) made a close-coupling (CC) calculation with five states ($2s^2 2p\ ^2P$, $2s2p^2\ ^4P, ^2D, ^2S, ^2P$). His calculation is employed here together with some less reliable data at higher energies and for highly excited states. It should be noted that Robb did not include closed-channel resonances in his calculation.

For C II, Robb's results are supplemented with the Coulomb-Born-Exchange cross sections obtained by Mann (1977). The agreement between the CBX and CC values is good for $X \geq 10$. For the excitations of $2s^2 3s$, $2s^2 3p$, $2s^2 3d$ states, only the CBX data are available.

In the case of O IV, the distorted-wave calculation by Mann (1981) is used to extend the data by Robb. For the excitation of the $n = 3$ states, only the scaling formula is available based on the DW calculation by Clarke et al. (1982).

Very recently Hayes (1983) has published a close-coupling calculation for O IV including $2s^2 2p\ ^2P$, $2s2p^2\ ^4P, ^2D, ^2S, ^2P$, $2p^3\ ^4S, ^2D, ^2P$ states. She took account of the effects of the closed-channel resonance, but reported only the rate coefficients for $(1.0 - 22.0) \times 10^4$ K. For the transitions $2s^2 2p\ ^2P - 2s2p^2\ ^4P$, $2s2p^2\ ^4P - 2s2p^2\ ^2D$ and $2s2p^2\ ^4P - 2s2p^2\ ^2P$, our original recommended values derived from the calculations of Robb (1977) and Mann (1981) have been modified to reproduce the Hayes rate coefficients. For the other transitions, such modification could not be made, but the present values of the rate coefficients are in fair agreement with the Hayes ones, except for $2s2p^2\ ^4P - 2s2p^2\ ^2S$. For the transitions to the states having $2p^3$, only the rate coefficients calculated by Hayes are available.

Data sources

Clarke, R.E.H., Magee, Jr., N.H., Mann, J.B. and Merts, A.L. (1982), *Astrophys. J.*

254 412

[$2s^2 p\ 2P - 2s^2 3s\ 2S, 2s^2 3d\ 2D$ of O IV, DW]

Hayes, M.A. (1983), *J. Phys. B* **16** 285

[$2s^2 2p\ 2P - 2s2p^2\ 4P, 2s2p^2\ 4P - 2s2p^2\ 2D, 2P$ of O IV, CC]

Mann, J.B. (1977), quoted in Los Alamos Scientific Laboratory Report, LA-6691-MS,

ed. N.H. Magee, Jr. et al.

[$2s^2 2p\ 2P - 2s2p^2\ 2D, 2S, 2P, 2s^2 3s\ 2S, 2s^2 3p\ 2P, 2s^2 3d\ 2D$ of C II, CBX]

Mann, J.B. (1981), private communication

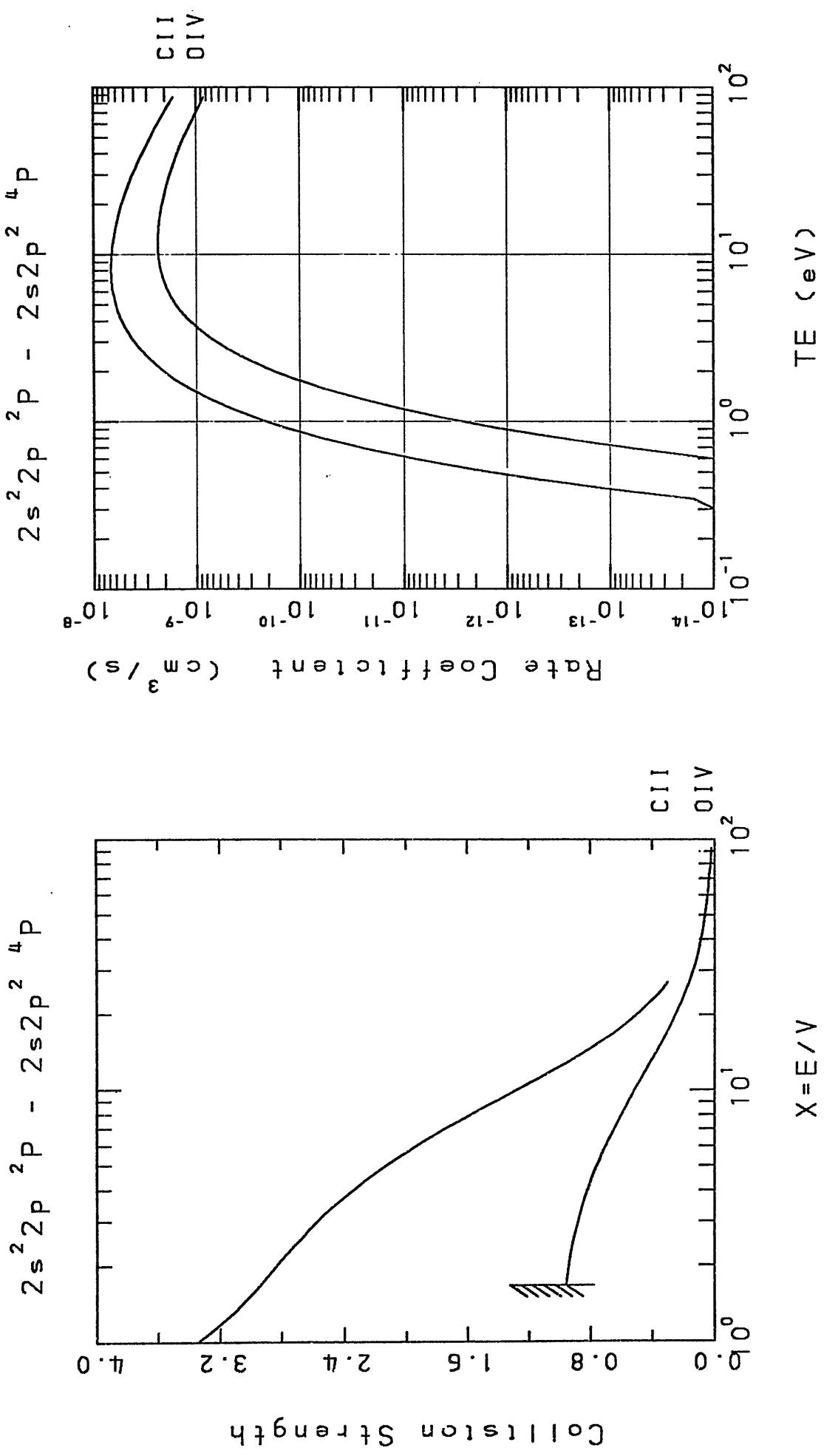
[$2s^2 p\ 2P - 2s2p^2\ 2S, 2P$ of O IV, DW]

Robb, W.D. (1977), quoted in Los Alamos Scientific Laboratory Report, LA-6691-MS,

ed. N.H. Magee, Jr. et al.

[transitions among $2s^2 2p\ 2P, 2s2p^2\ 4P, 2D, 2S, 2P$, CC]

Fig. 53



Collision Strength

Fig. 54

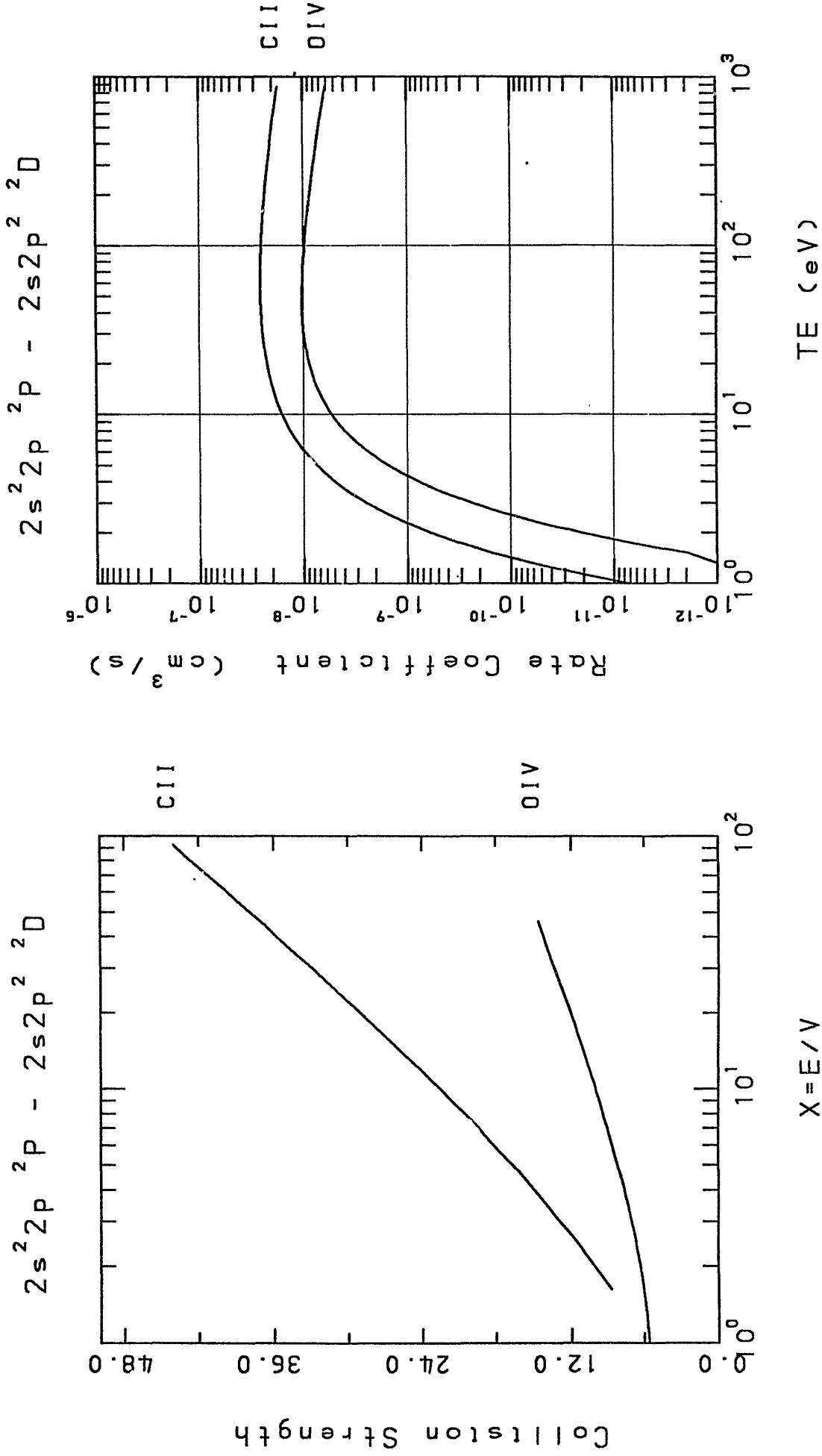
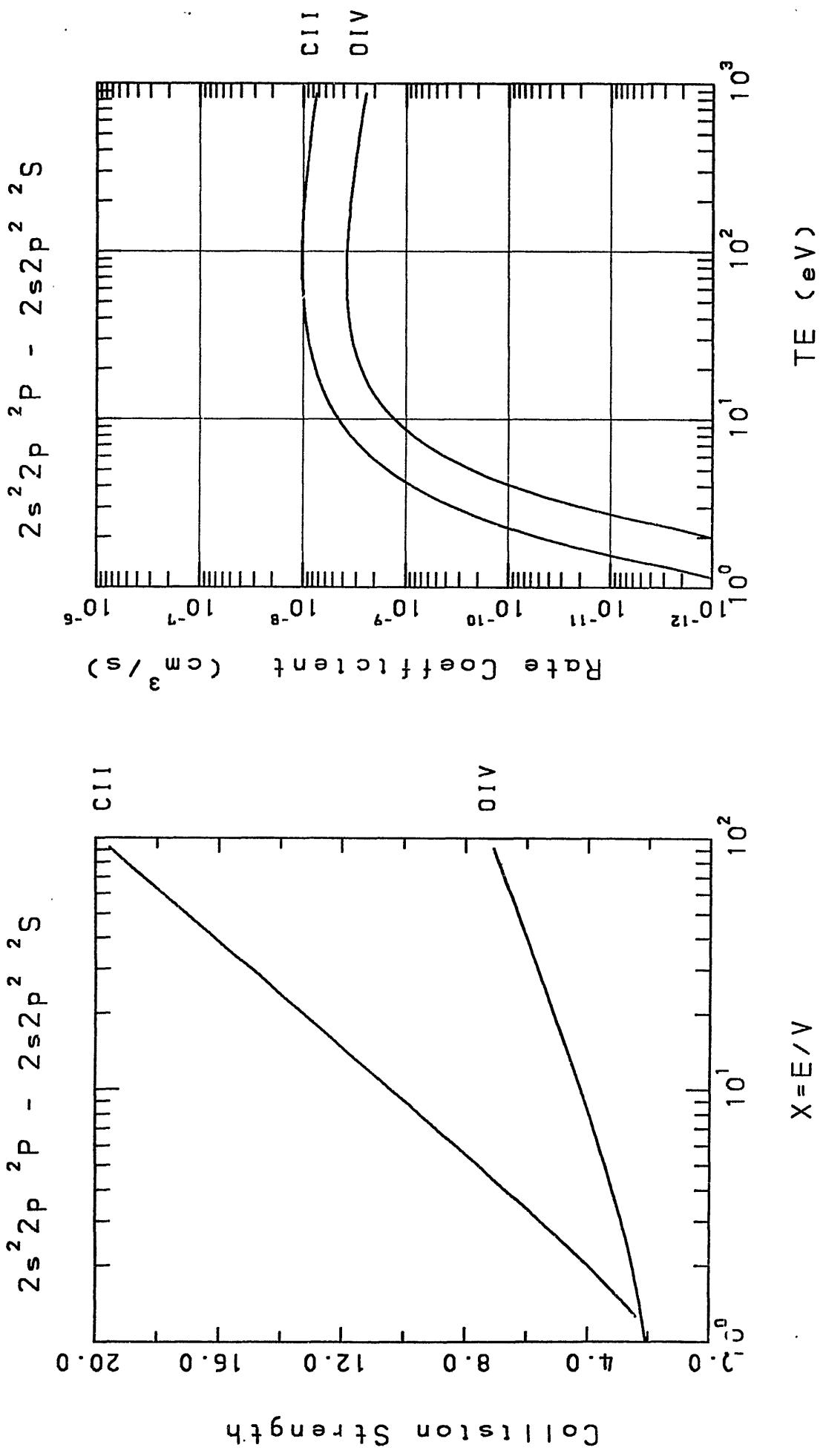


Fig. 55



Collision Strength

Fig. 56

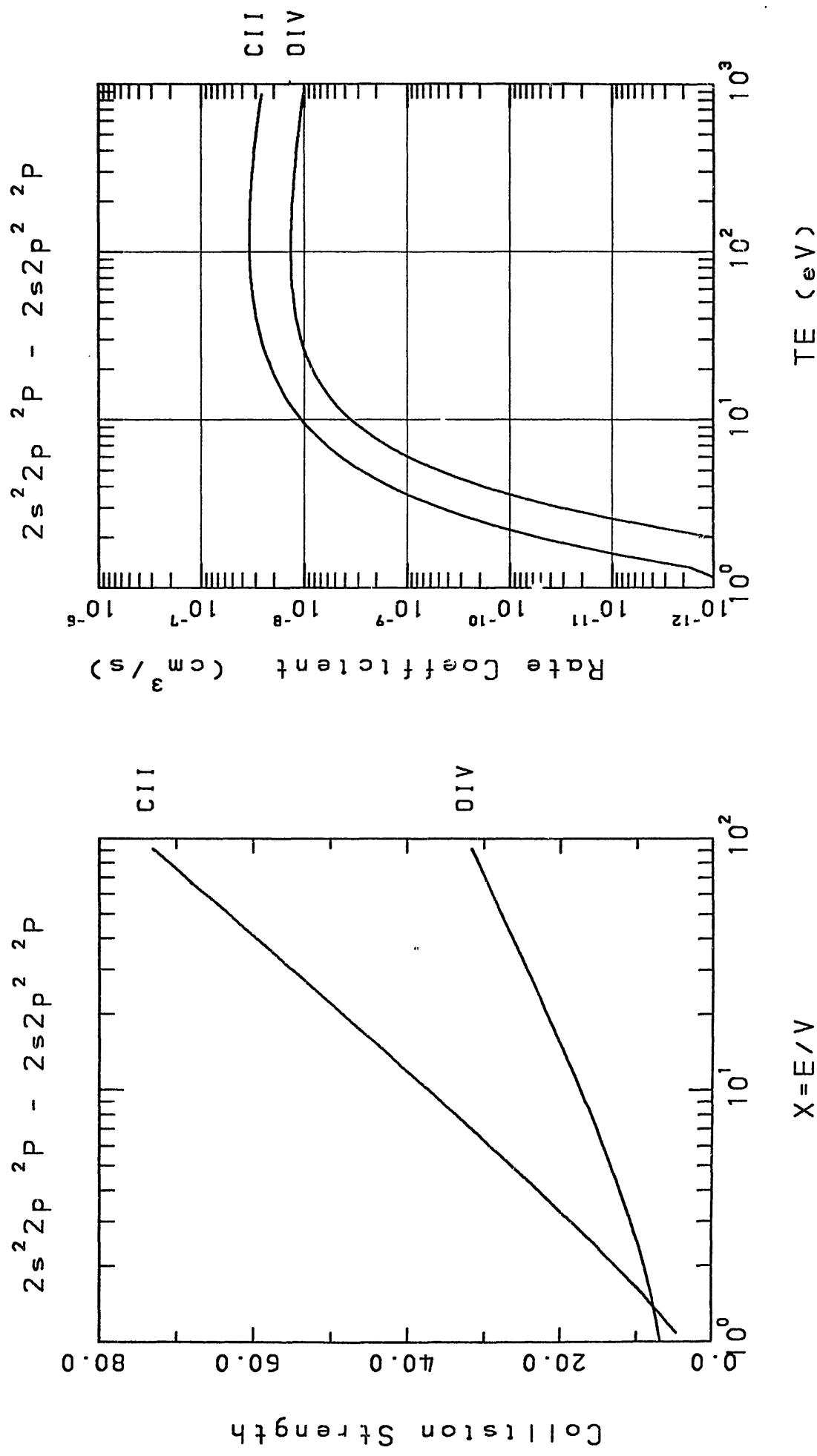


Fig. 57

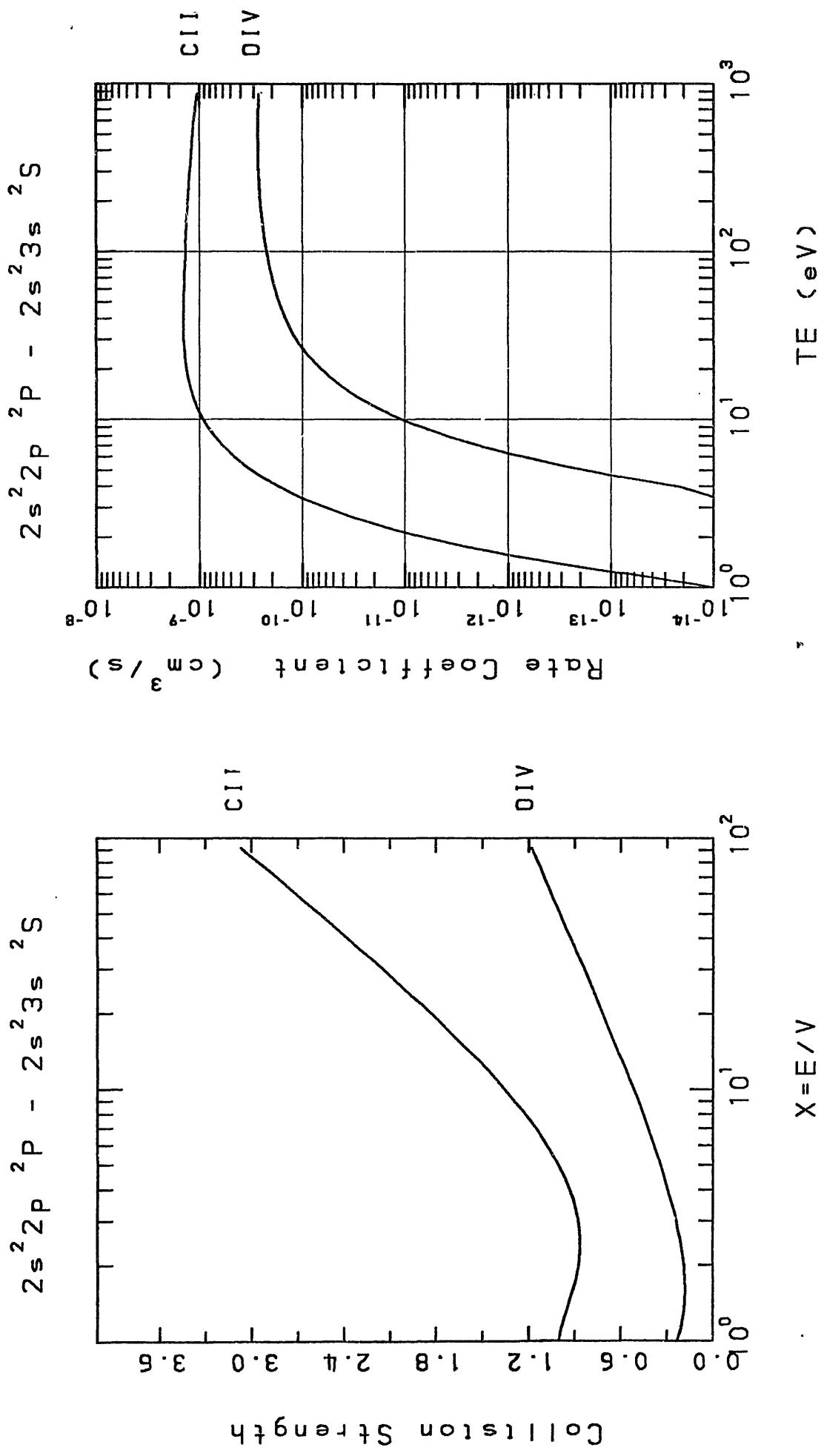


Fig. 58

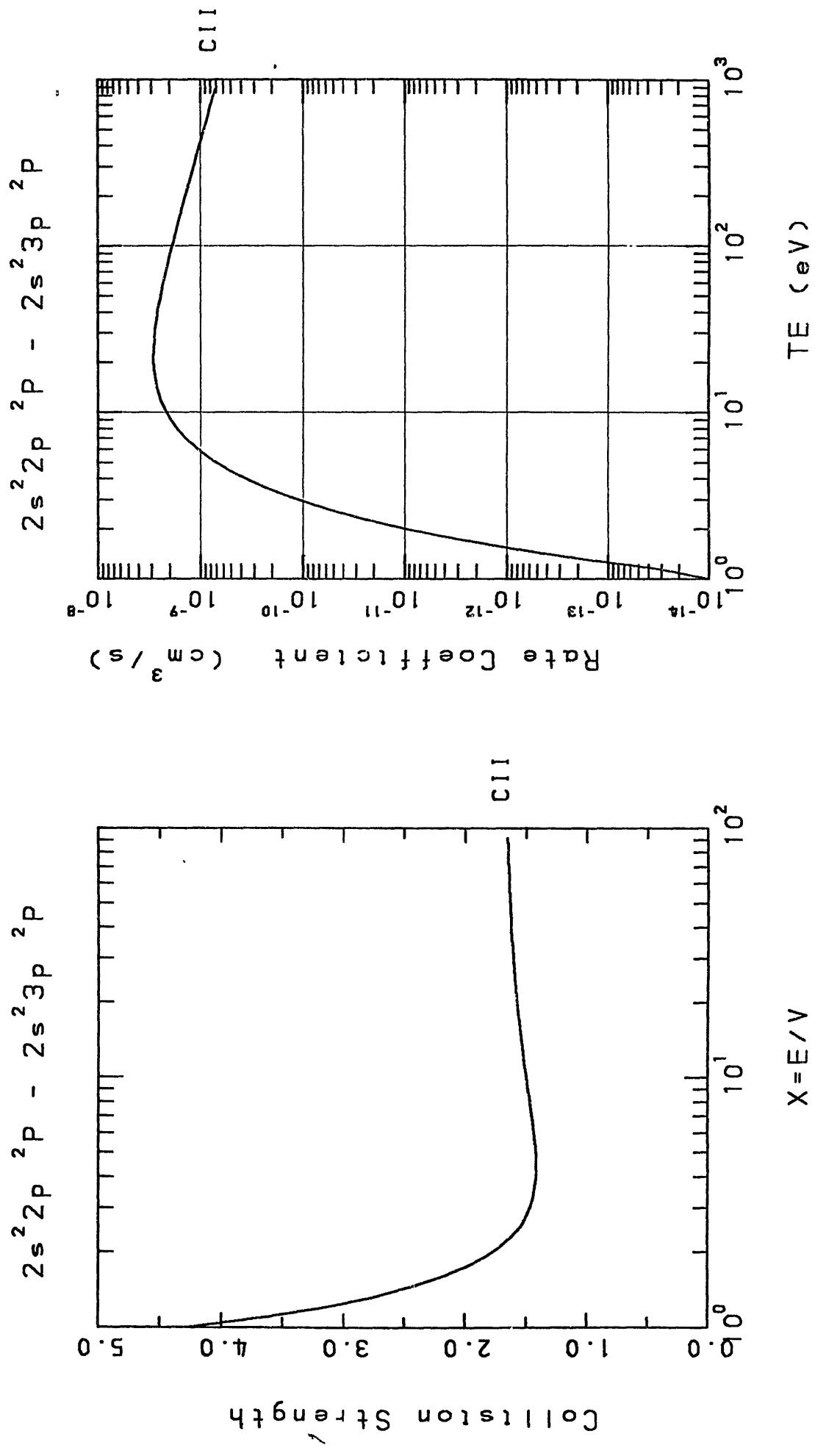
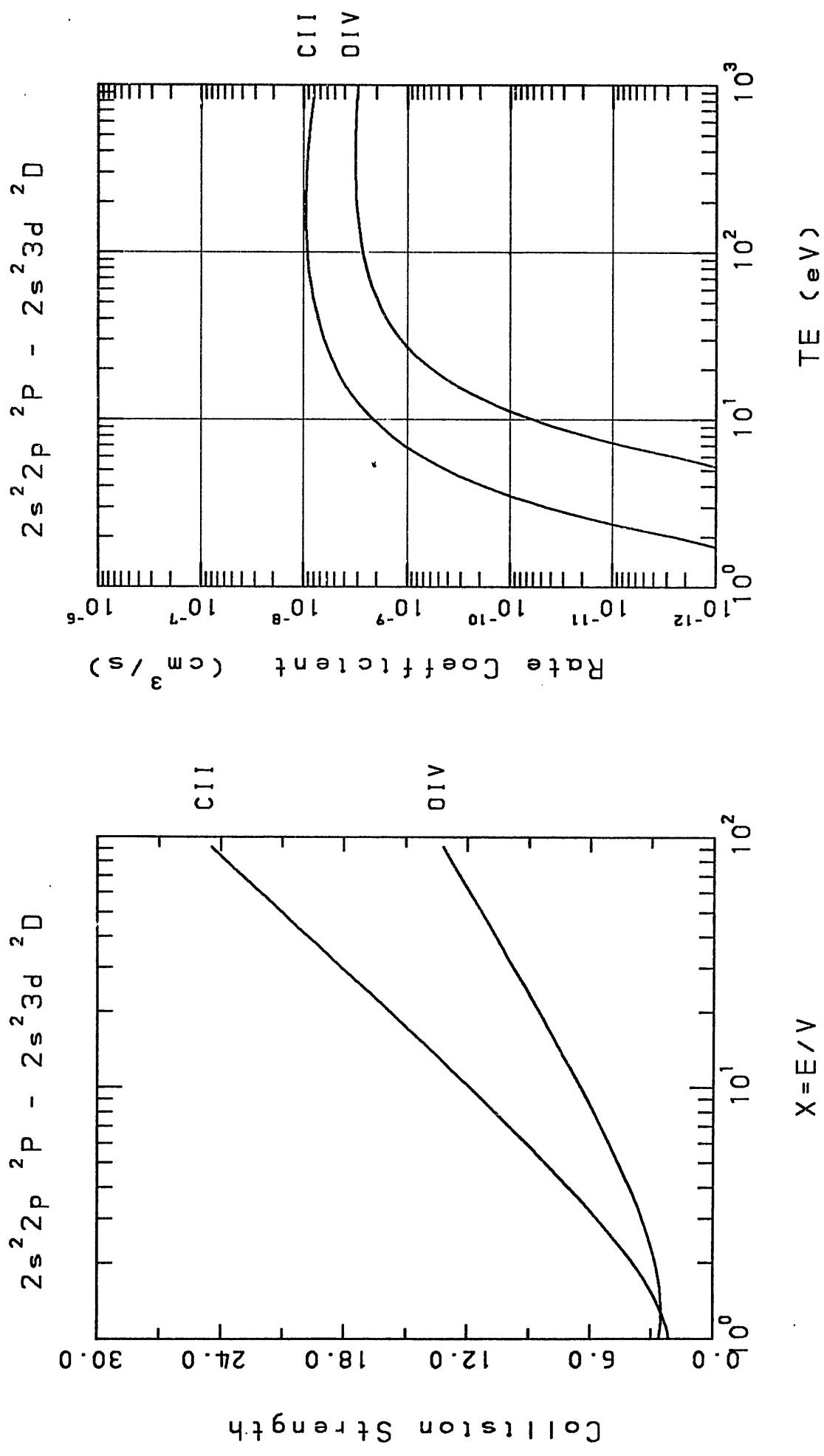


Fig. 59



Collision Strength

Fig. 60

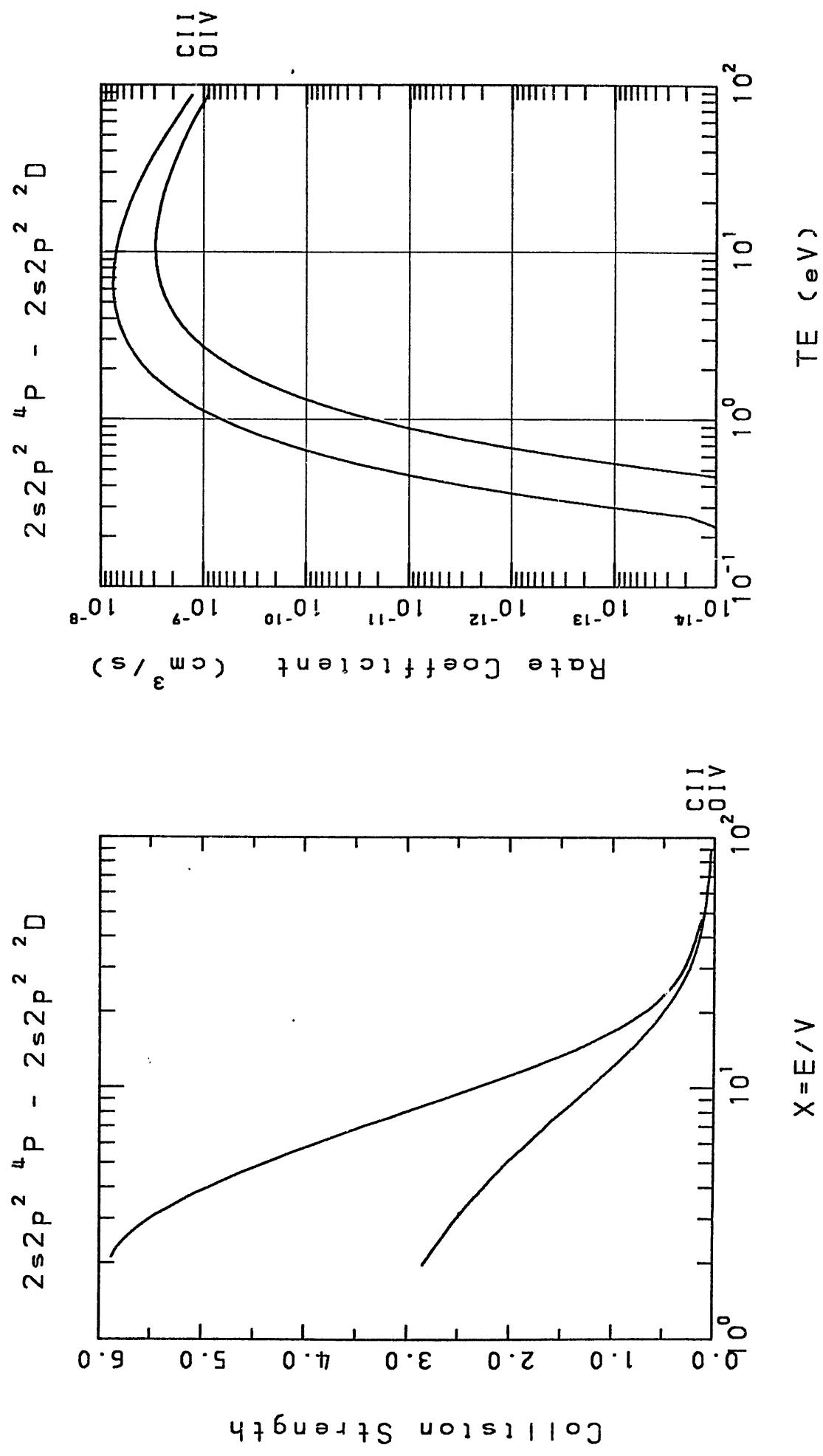


Fig. 61

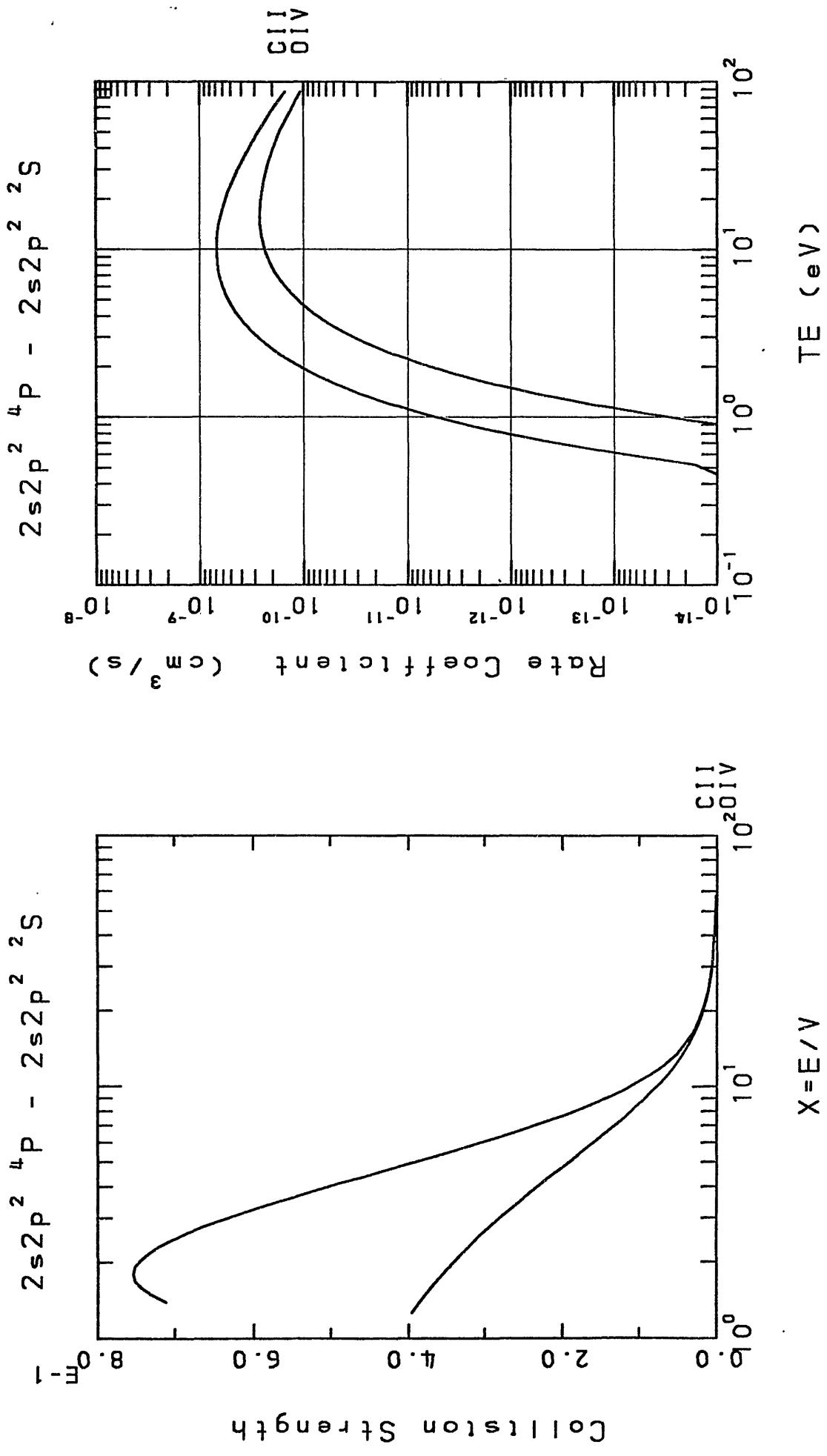


Fig. 62

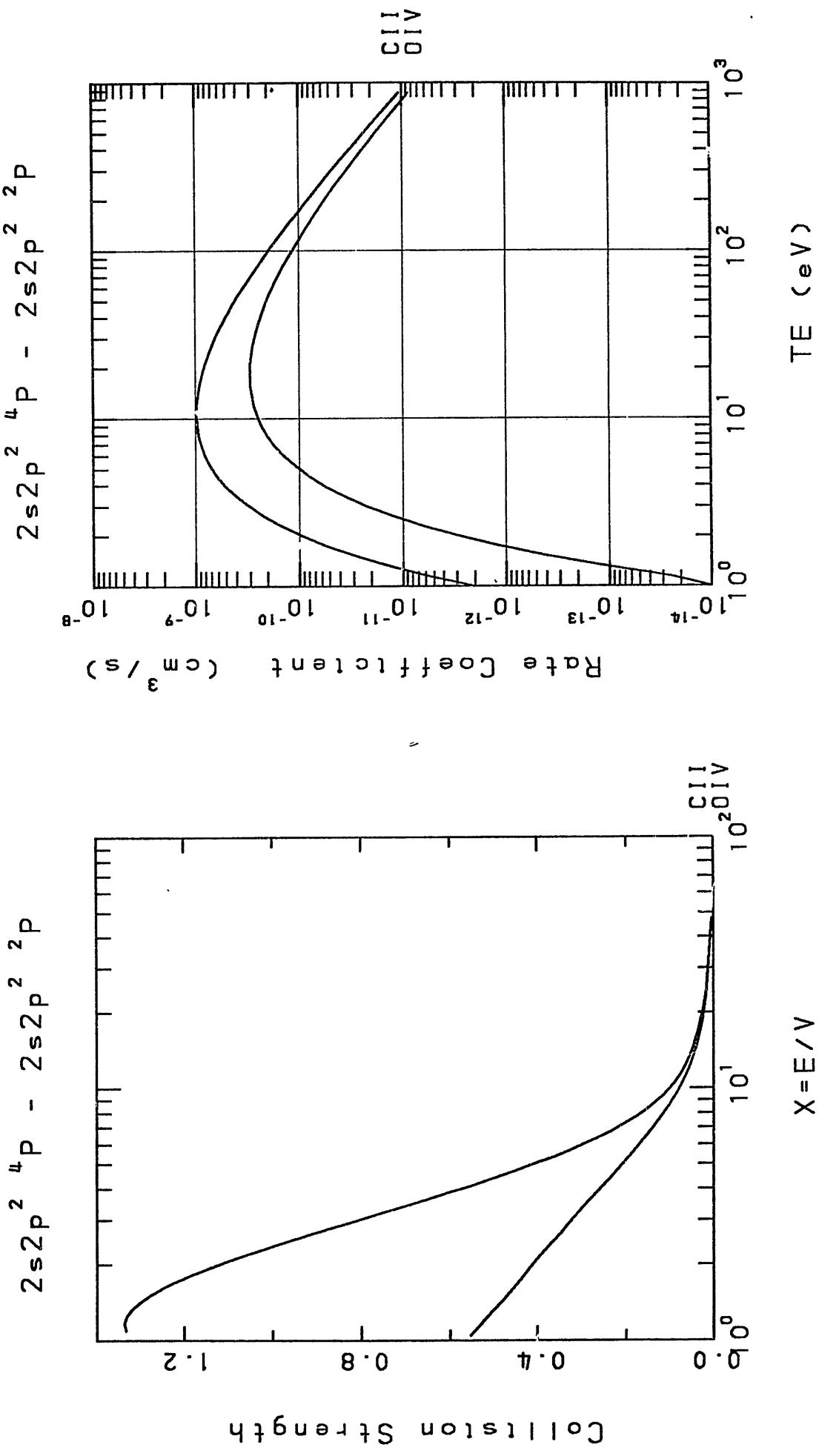


Fig. 63

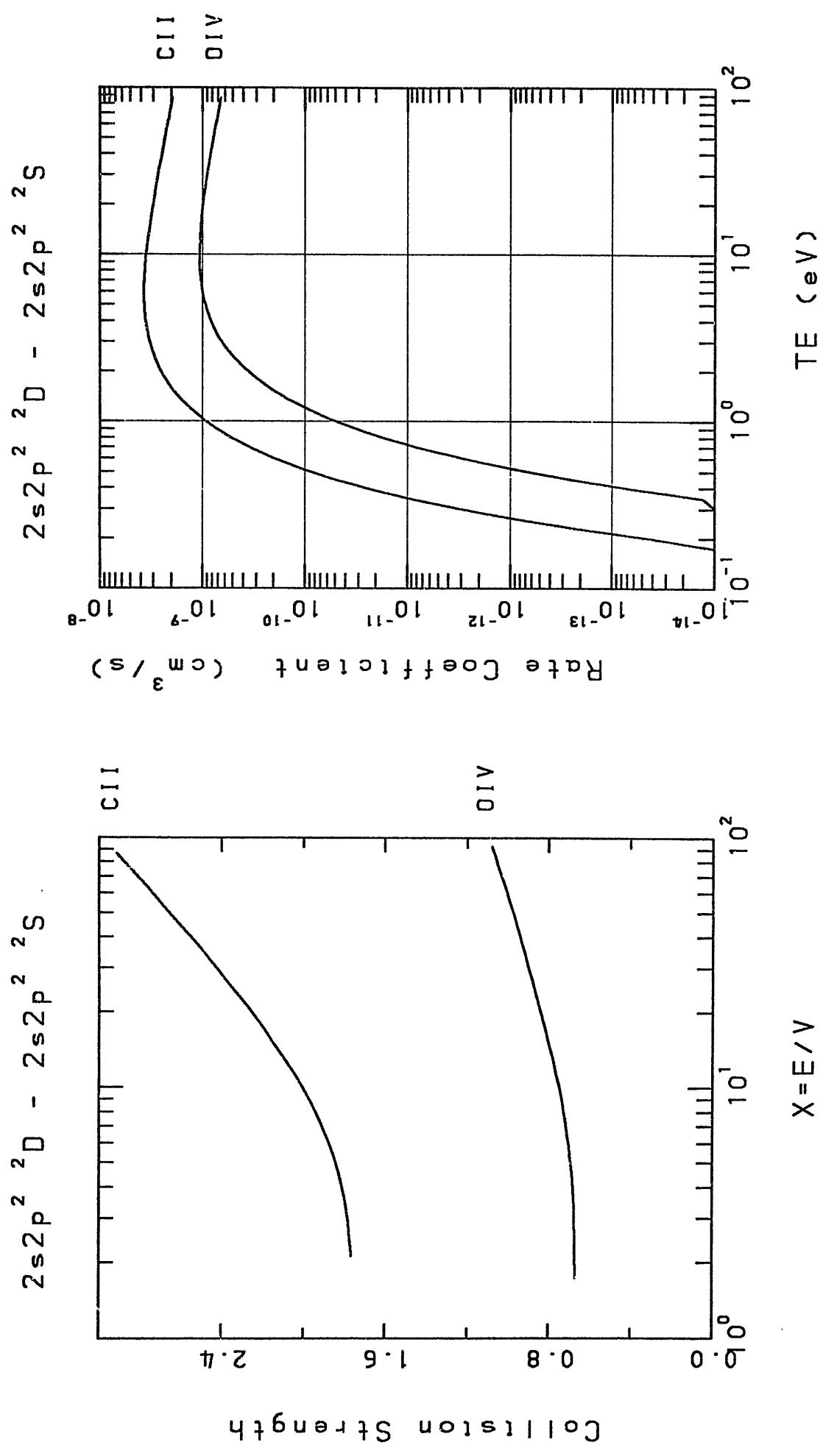


Fig. 64

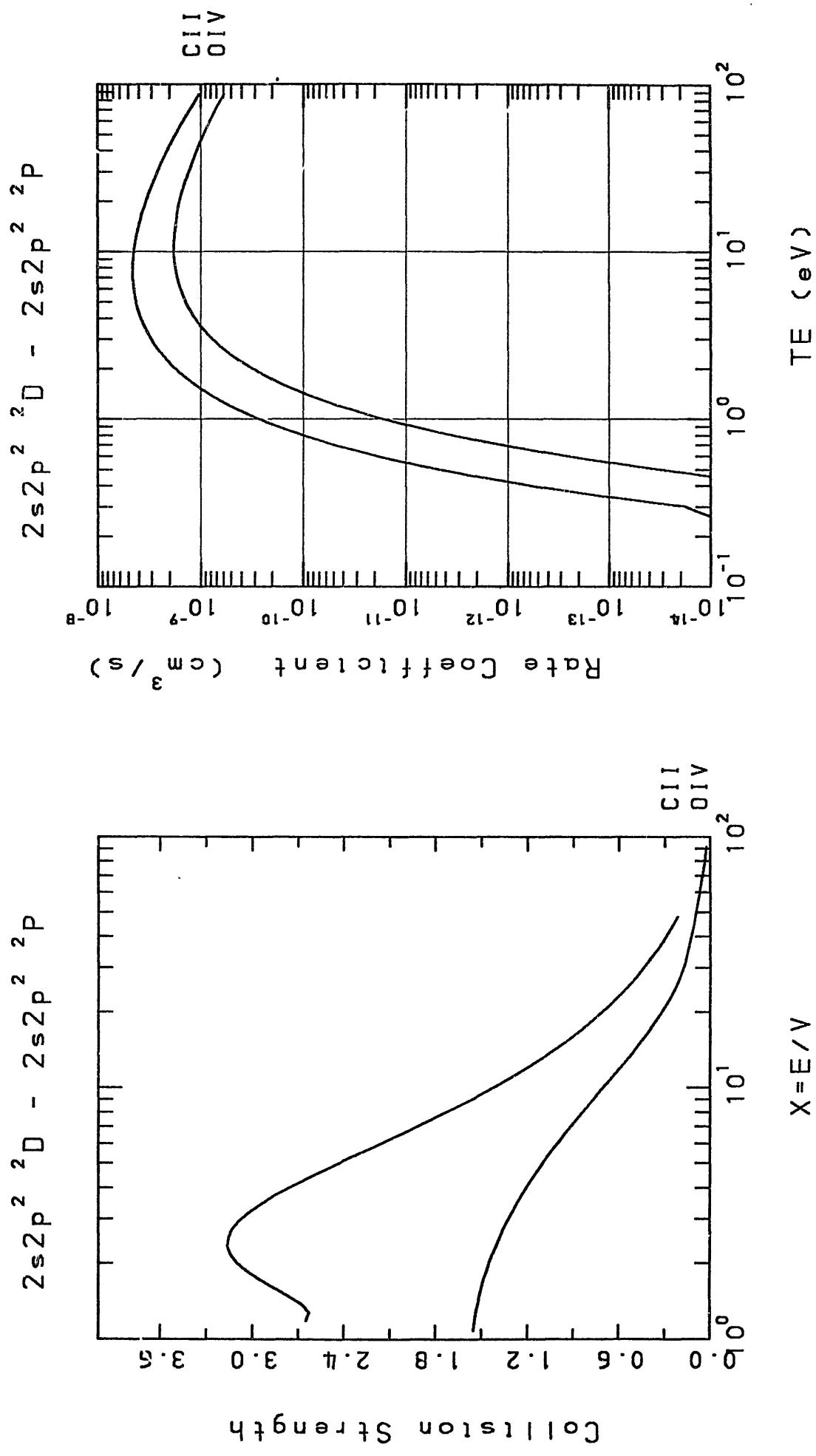
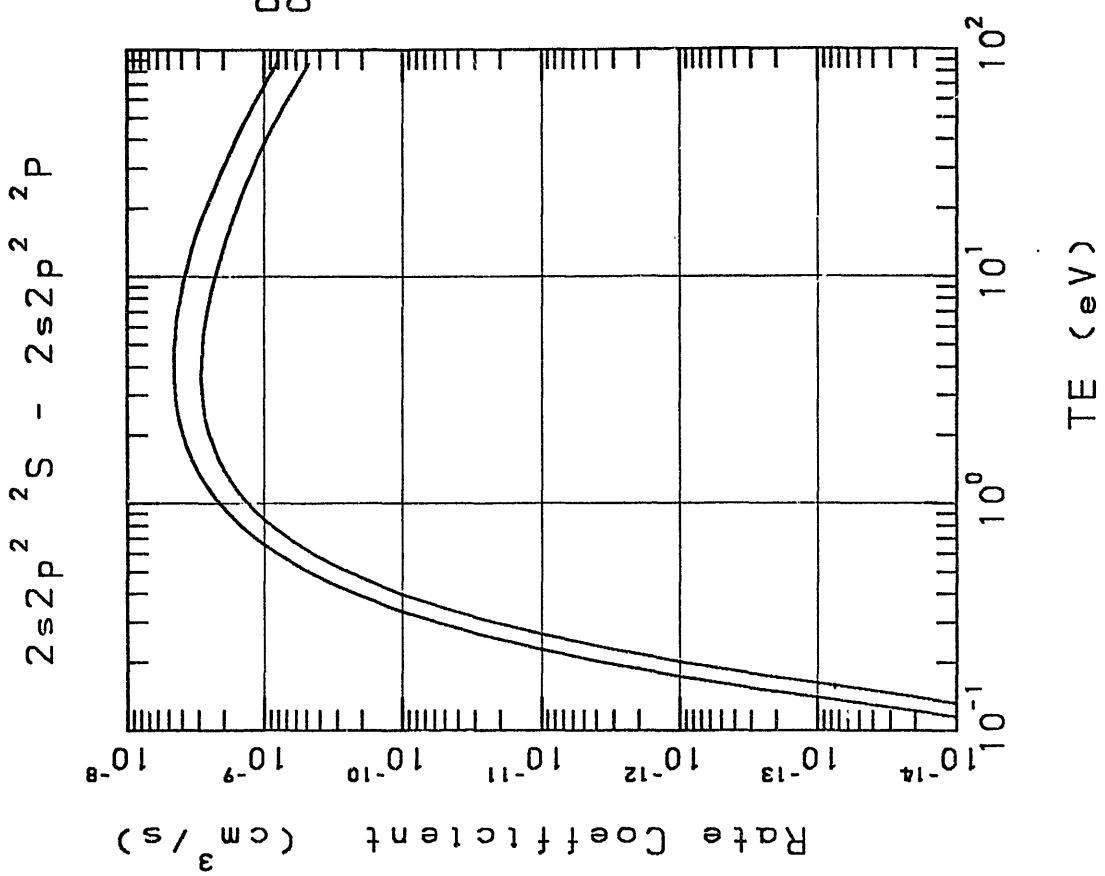
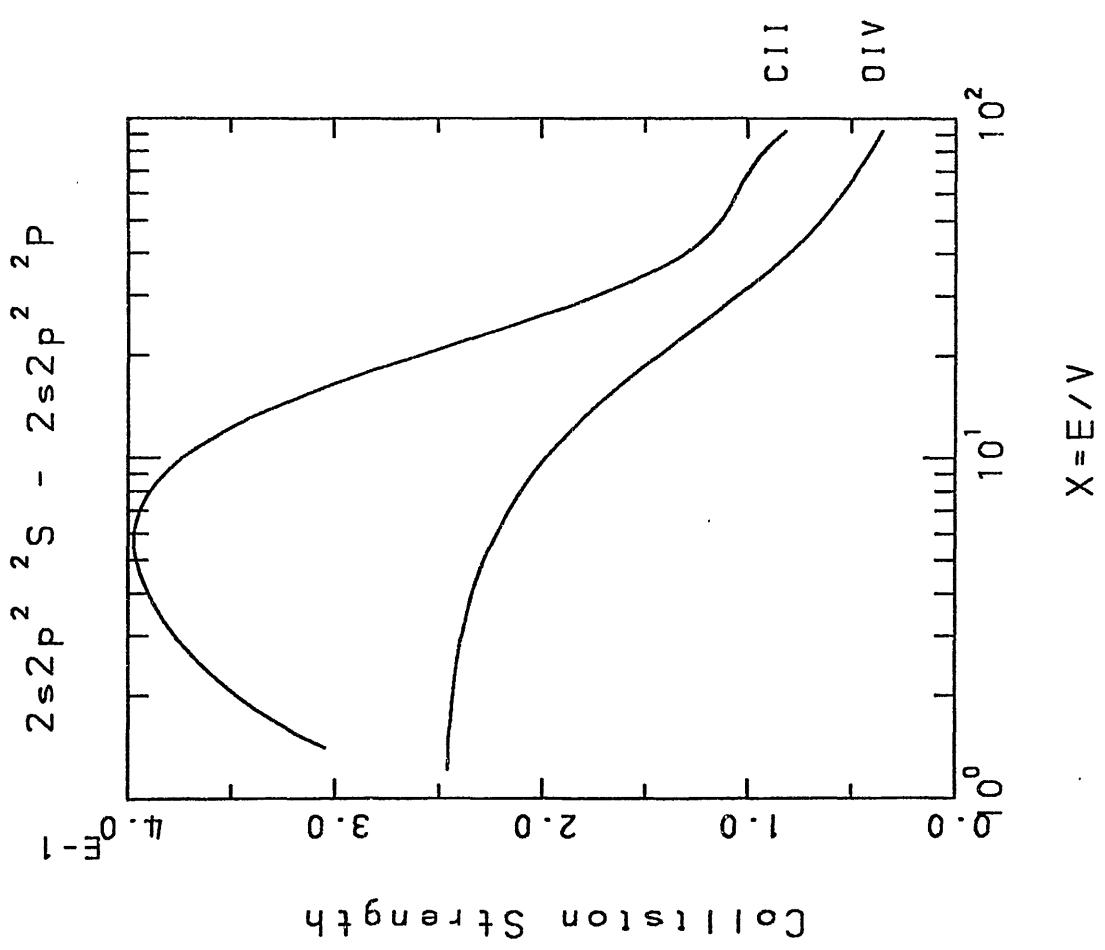


Fig. 65



C-like (O III)

Using the R-matrix method, Baluja et al. (1980, 1981) calculated the cross sections for various transitions among the states having the configurations $2s^22p^2$, $2s2p^3$ and $2p^4$. Their results included the resonance effect. They gave collision strengths only for the non-resonant part of the transitions among $2s^22p^2\ 3P, 1D, 1S$ and the excitations $2s^22p^2\ 3P - 2s2p^3\ 5S$, $2s2p^3\ 5S - 2s2p^3\ 3D$, $2s2p^3\ 5S - 2s2p^3\ 3P$. Otherwise rate coefficients were presented.

For the non-resonant part of the cross sections, the following data are adopted here. For $2s^22p^2\ 3P - 2s^22p^2\ 1D, 1S$, the values obtained by Baluja et al. (1981) are used with the cross sections calculated at the higher energies by the distorted wave method [Mann (1981)]. For $2s^22p^2\ 3P - 2s2p^3\ 5S$, Mann's DW values are used throughout the whole energy range, since the number of the data points given by Baluja et al. (1980) is very few. In general, the agreement between the DW and the R-matrix results is very good when a comparison can be made. For $2s^22p^2\ 1D - 2s^22p^2\ 1S$, the cross sections obtained by Baluja et al. (1981) are too small compared with other calculations. This may be the result of including an insufficient number of partial waves. The DW cross sections of Mann (1981), therefore, are adopted instead. The data given by Baluja et al. (1980) are used for $2s2p^3\ 5S - 2s2p^3\ 3D, 3P$ and the DW cross sections by Bhatia et al. (1979) for other transitions among $2s^22p^2\ 1S, 1D, 2s2p^3\ 3D, 3P$.

The resonance effect is incorporated according to the procedure described in the Introduction. The procedure has been successful except for $2s^22p^2\ 1D - 2s2p^3\ 3D$, $2s^22p^2\ 1S - 2s2p^3\ 3P$ and $2s2p^3\ 3D - 2s2p^3\ 3P$, for which the present recommended data should be less reliable.

For some of the excitations from the ground state to the states having the configuration $2s2p^3$, Ho and Henry (1983) have recently made a two-state CC calculation. Mann's DW results are adopted here for the excitations of the other states of $2s2p^3$.

Data sources

Baluja, K.L., Burke, P.G. and Kingston, A.E. (1980), J. Phys. B **13** 829

[$2s^2 2p^2 3P - 2s2p^3 5S$, $2s2p^3 5S - 2s2p^3 3D, 3P$, R-matrix]

Baluja, K.L., Burke, P.G. and Kingston, A.E. (1981), J. Phys. B **14** 119

[transitions among $2s^2 2p^2$, $2s2p^3$, $2p^4$, R-matrix]

Bhatia, A.K., Doschek, G.A. and Feldman, U. (1979), Astron. Astrophys. **76** 359

[$2s^2 2p^2 1D - 2s2p^3 3D, 3P$, $2s^2 2p^2 1S - 2s2p^3 3D, 3P$, $2s2p^3 3D - 2s2p^3 3P$, DW]

Ho, Y.K. and Henry, R.J.W. (1983), Astrophys. J. **264** 733

[$2s^2 2p^2 3P - 2s2p^3 3D, 3P, 3S$, CC]

Mann, J.B. (1981), private communication

[$2s^2 2p^2 3P - 2s^2 2p^2 1D, 1S$, $2s^2 2p^2 3P - 2s2p^3 5S, 1D, 1P$, $2s^2 2p^2 1D - 2s^2 2p^2 1S$, DW]

Fig. 66

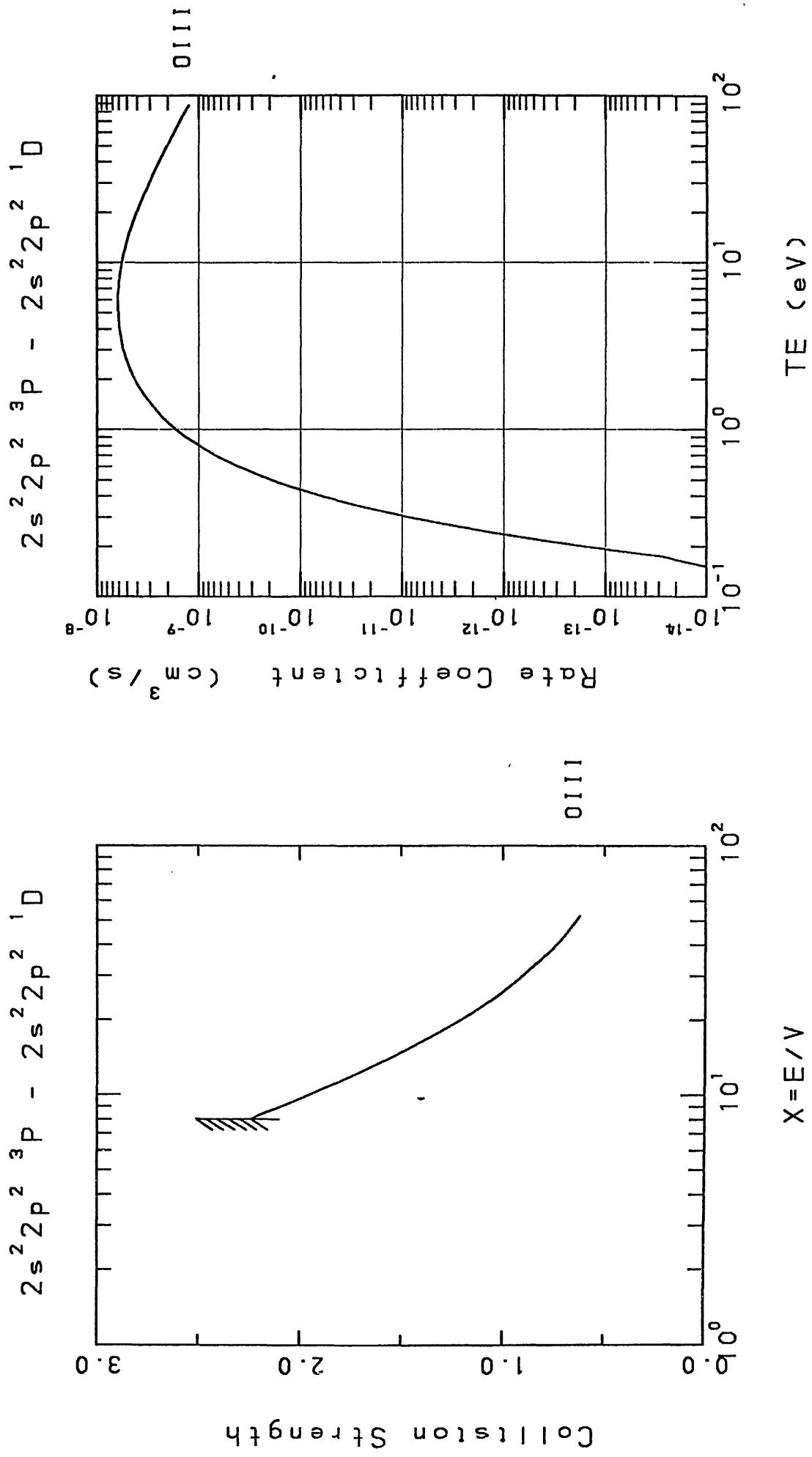


Fig. 67

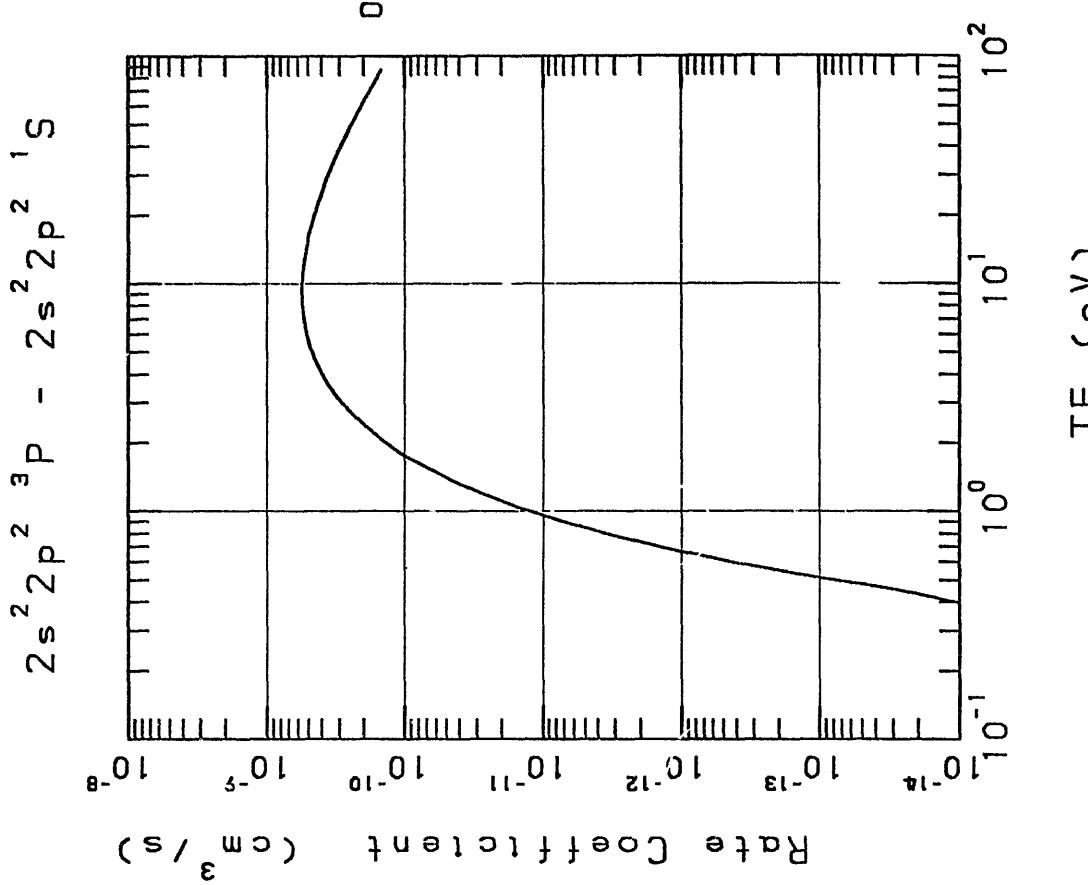
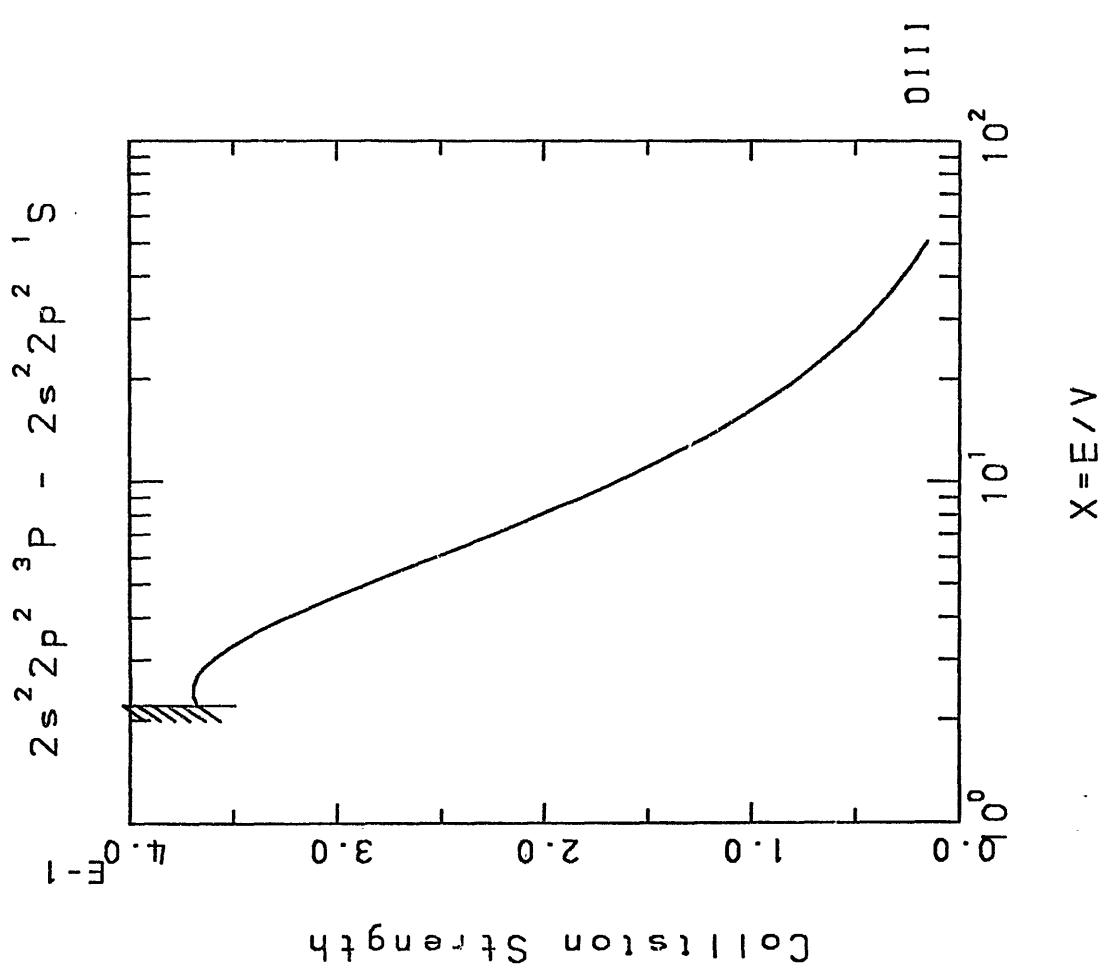


Fig. 68

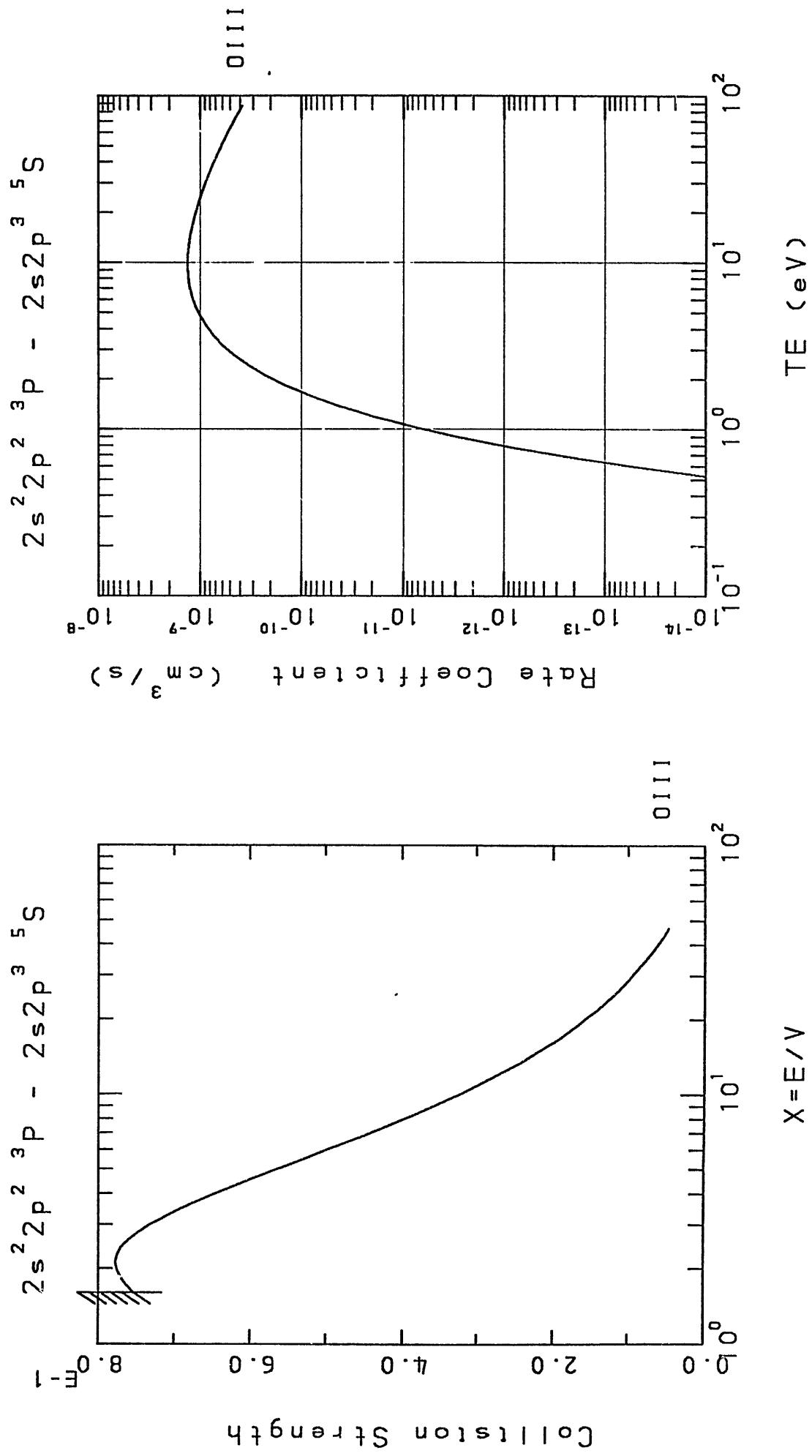


Fig. 69

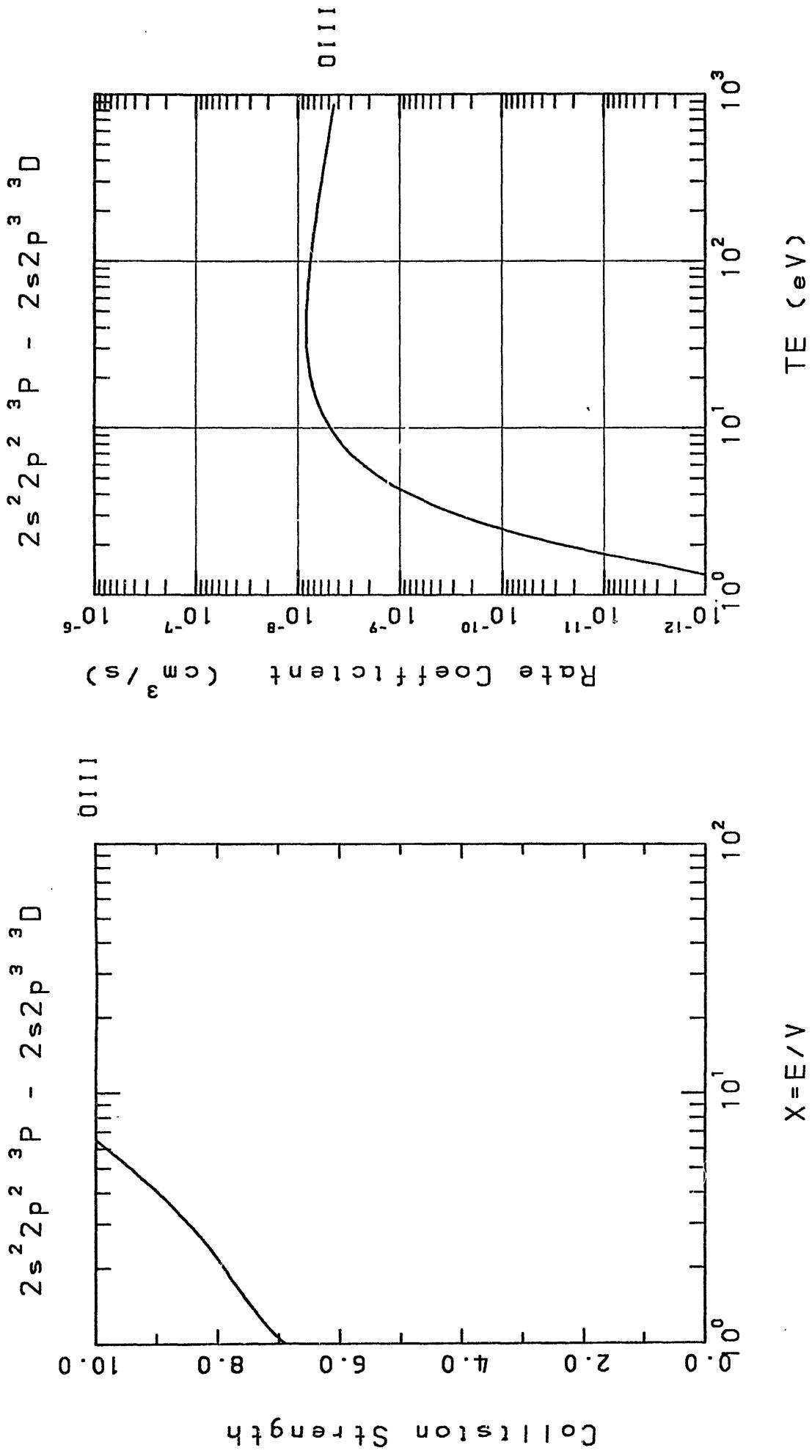


Fig. 70

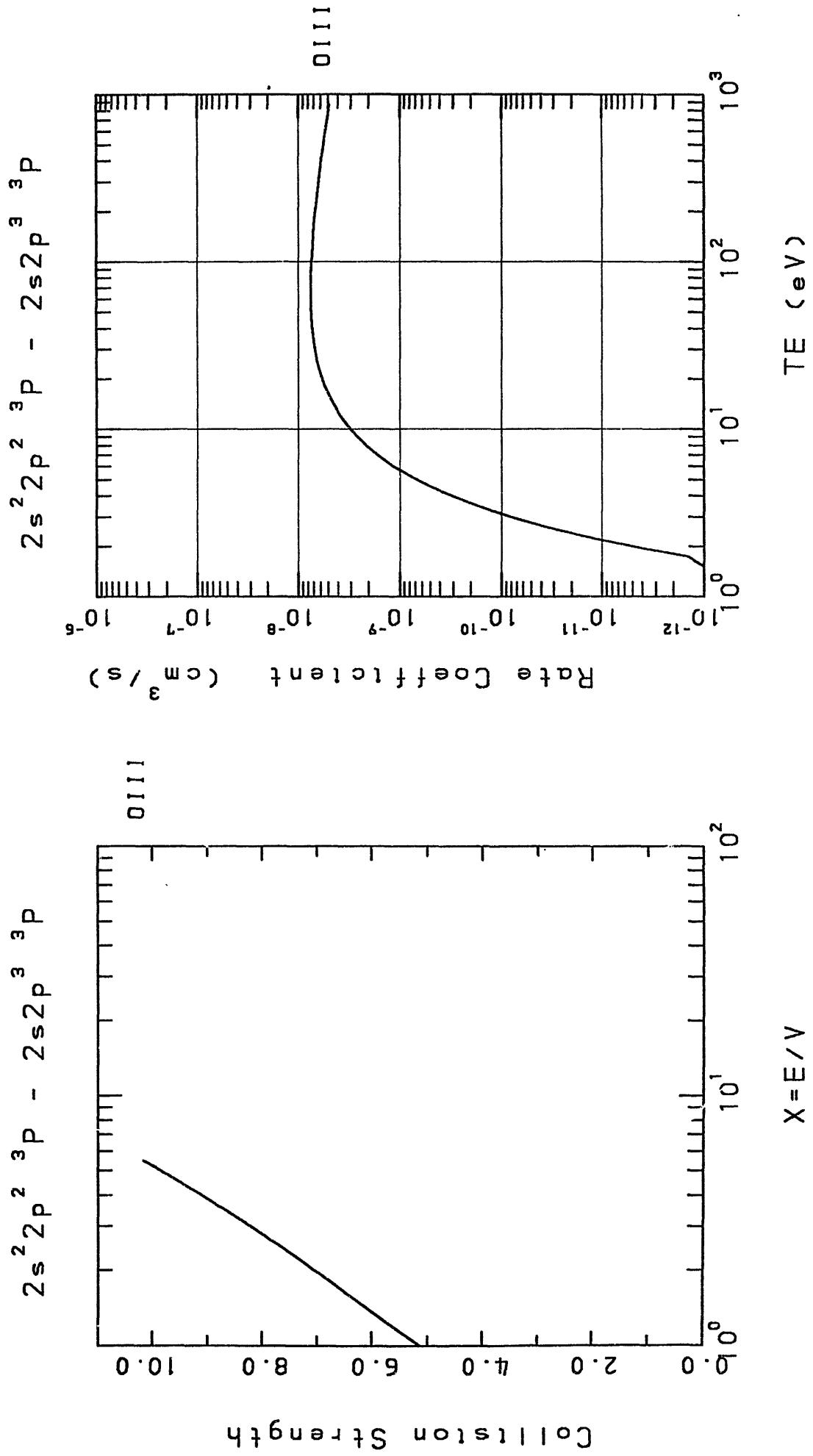


Fig. 71

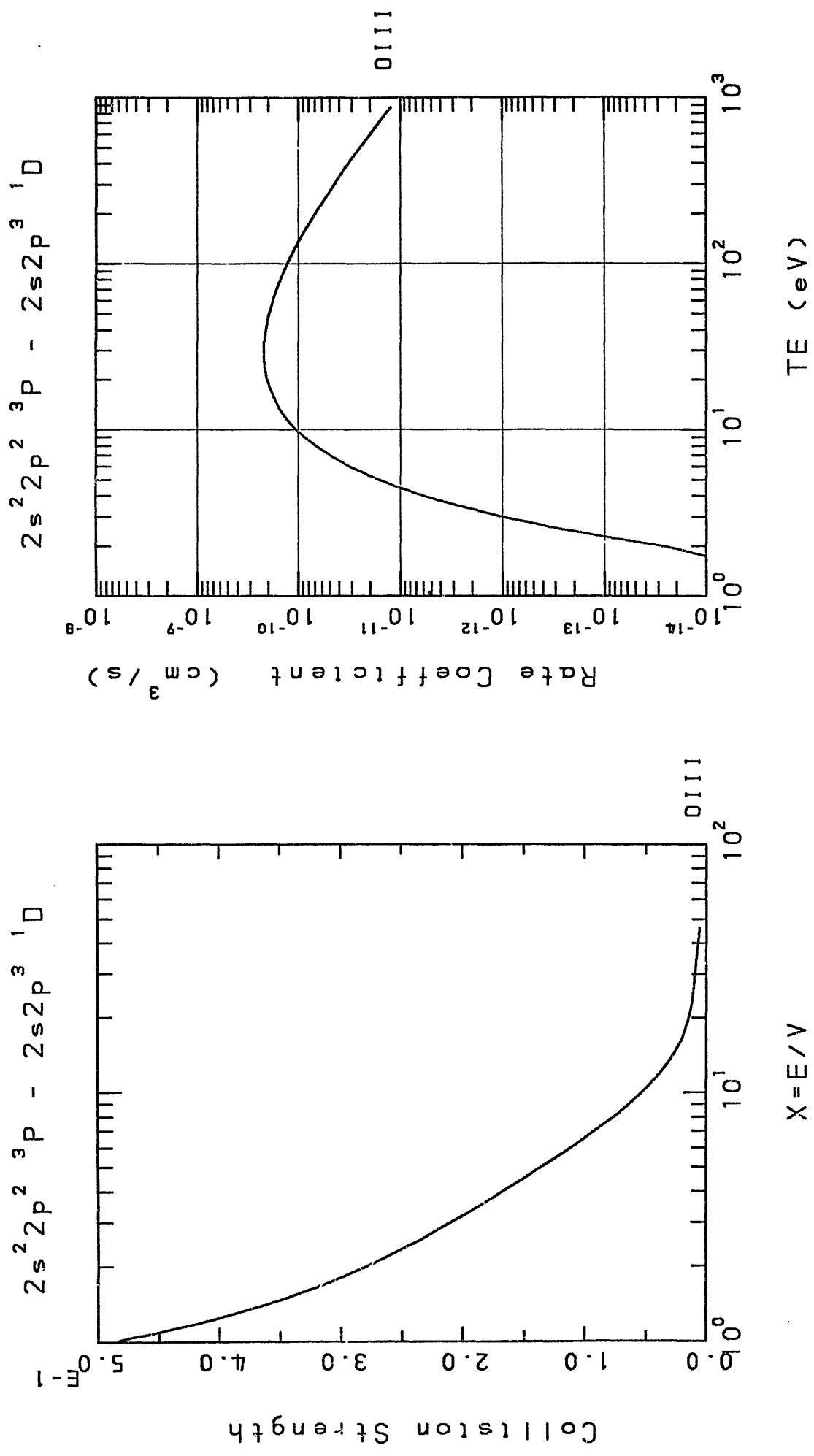


Fig. 72

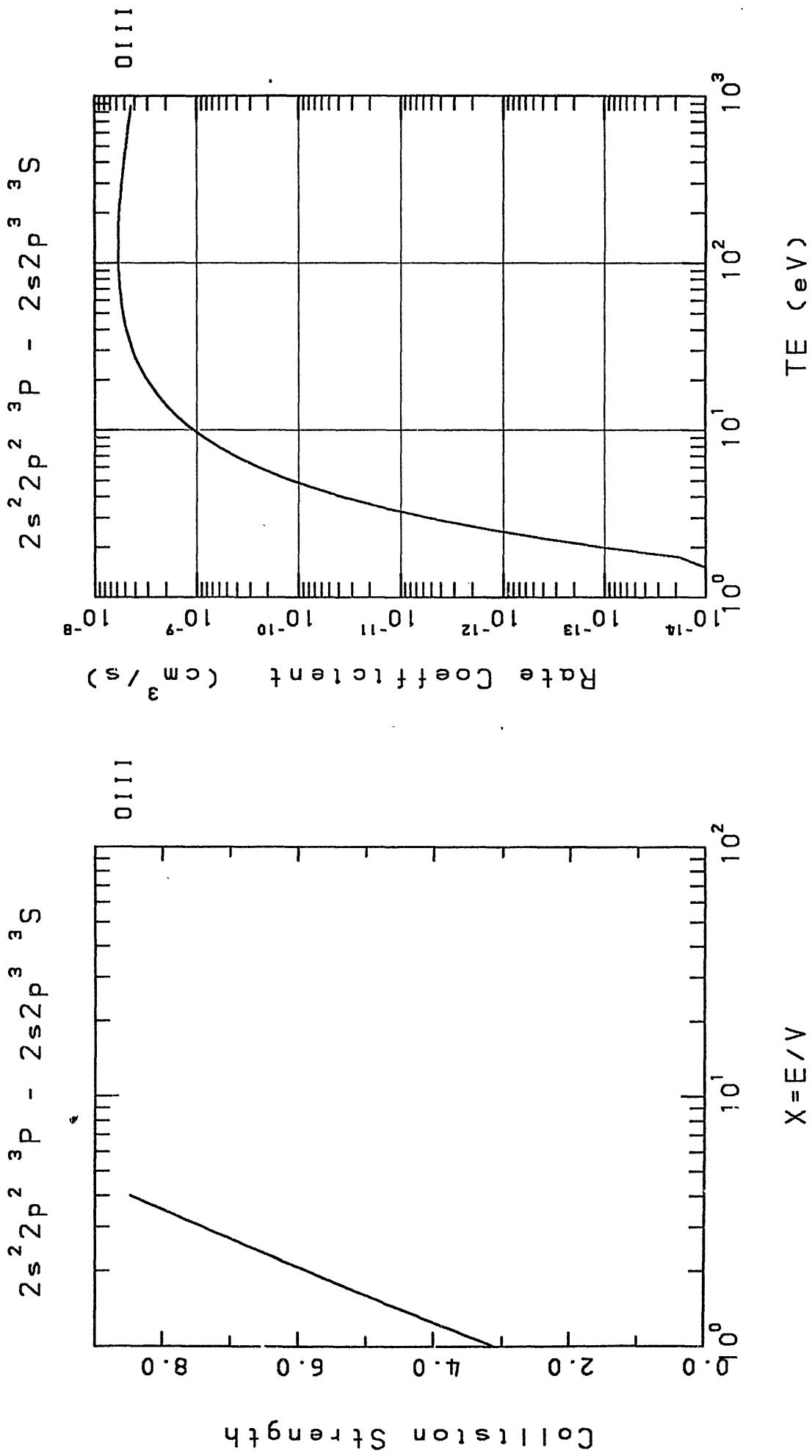


Fig. 73

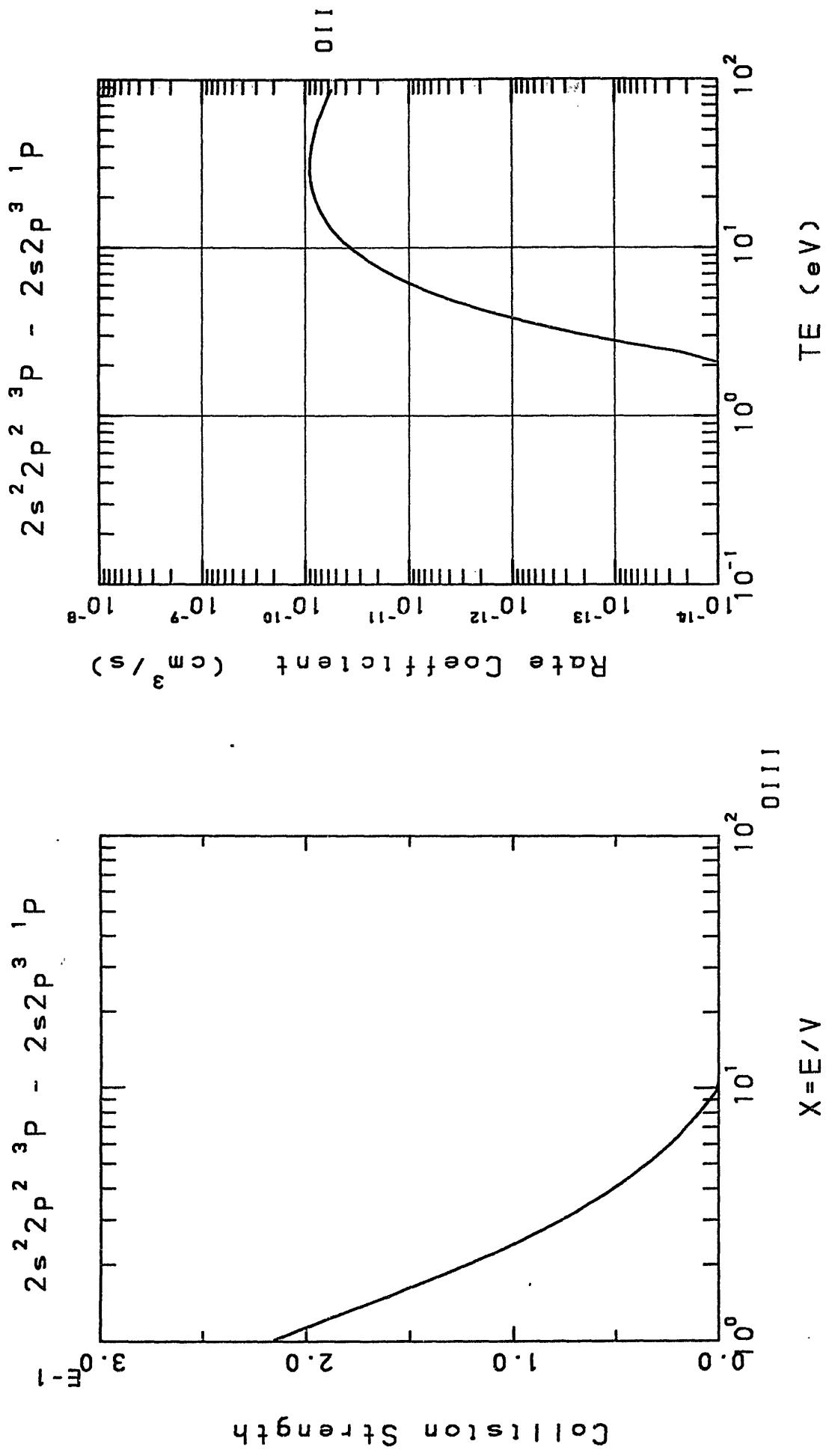


Fig. 74

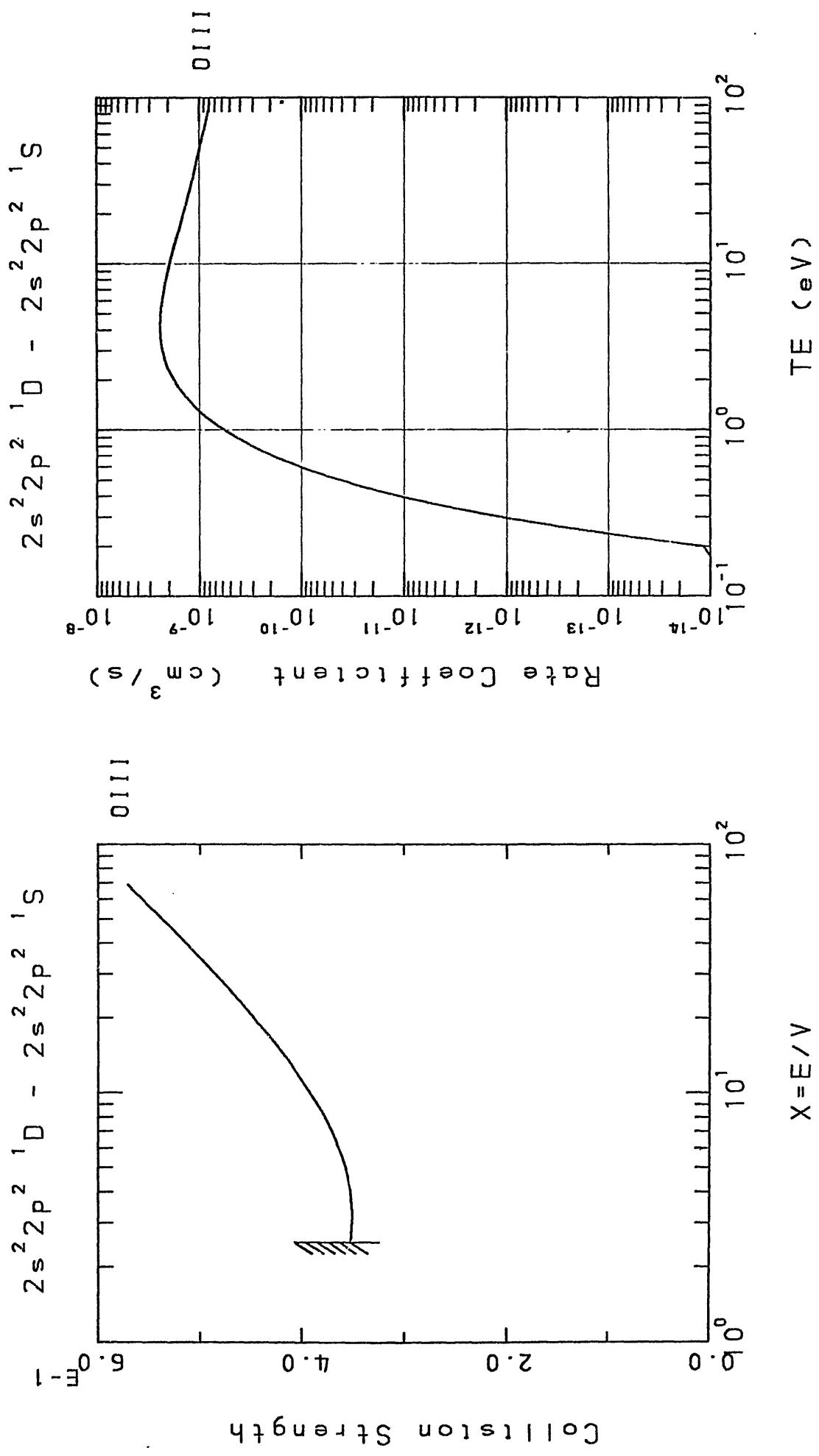


Fig. 75

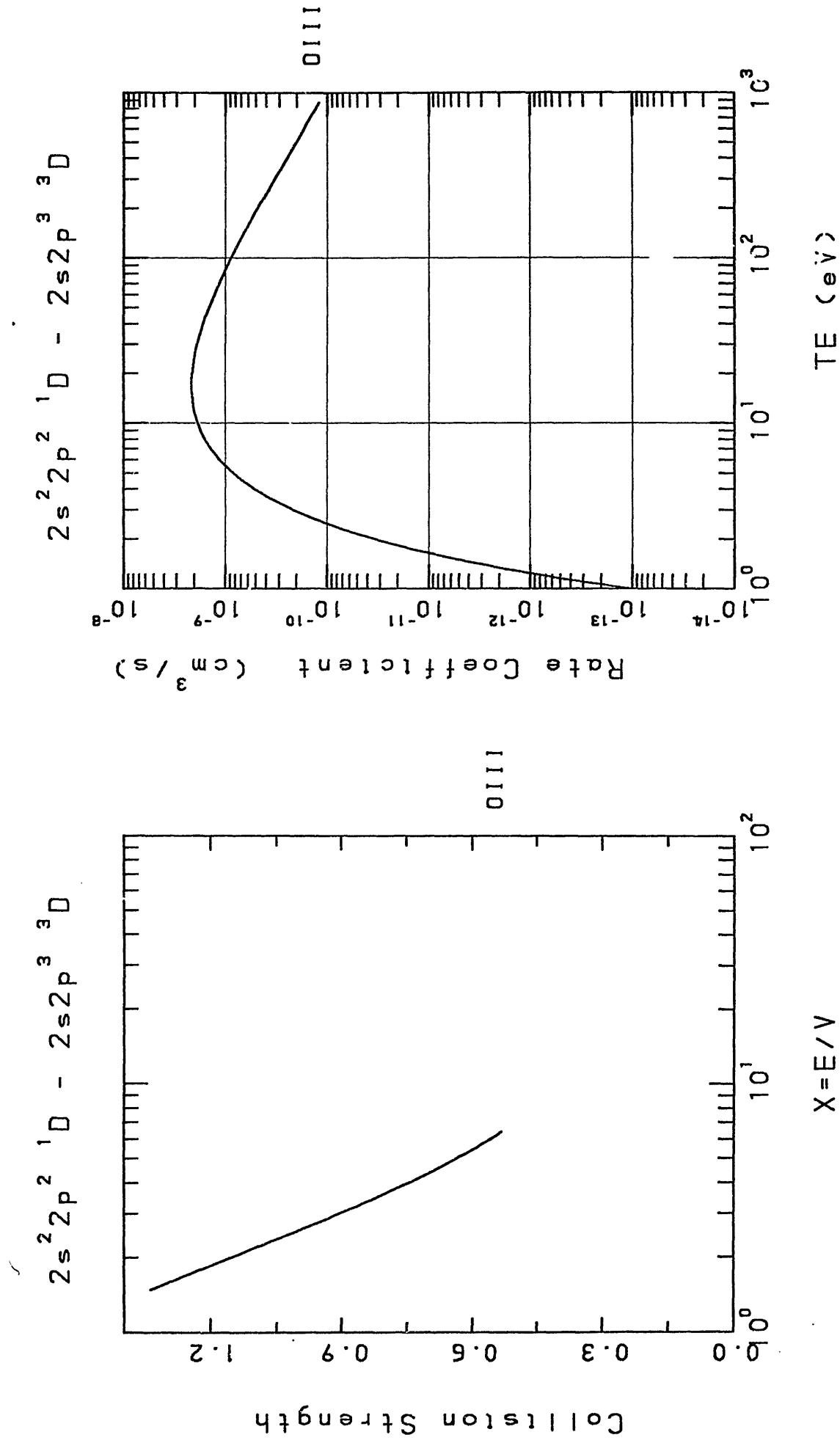


Fig. 76

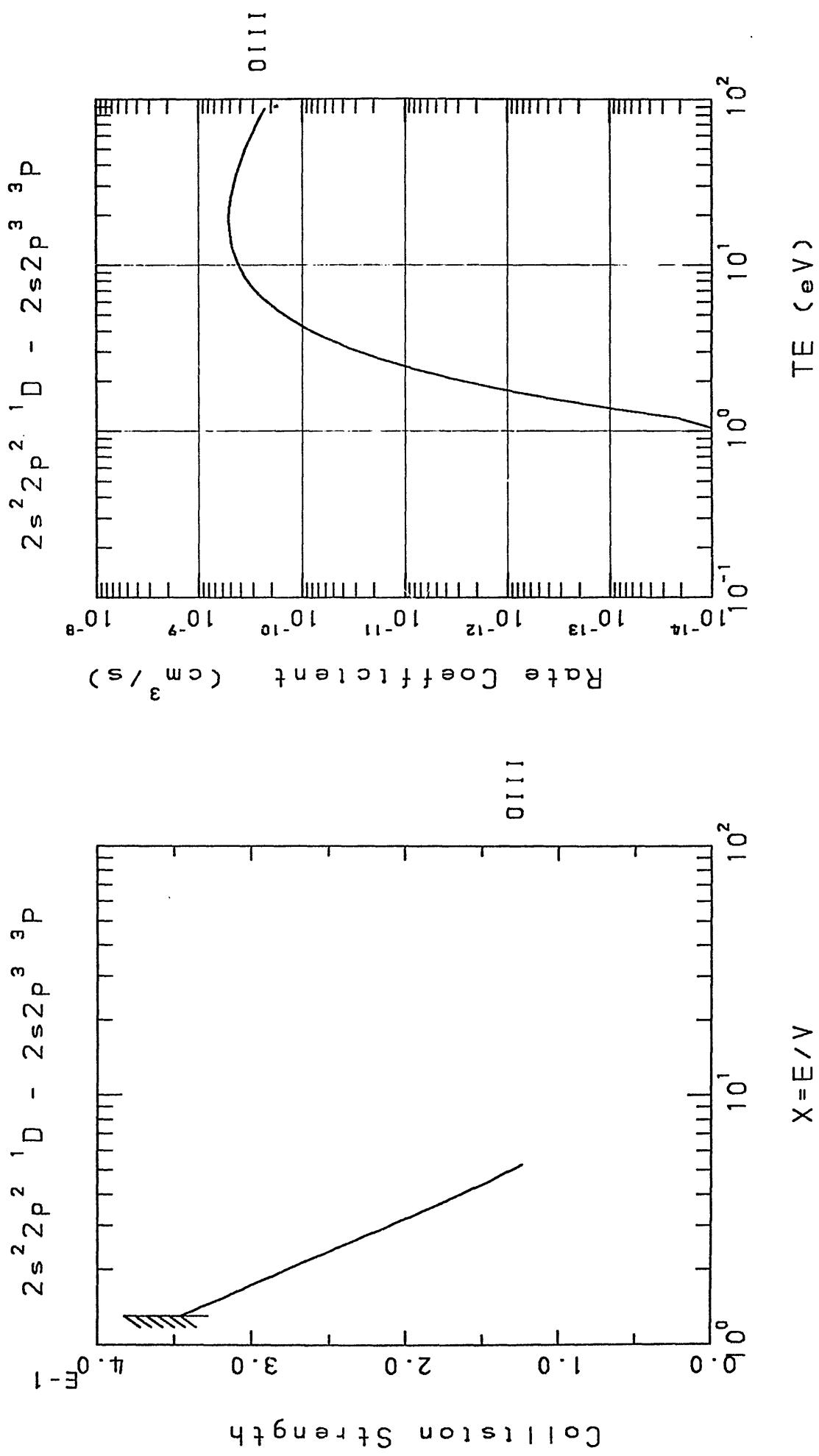


Fig. 77

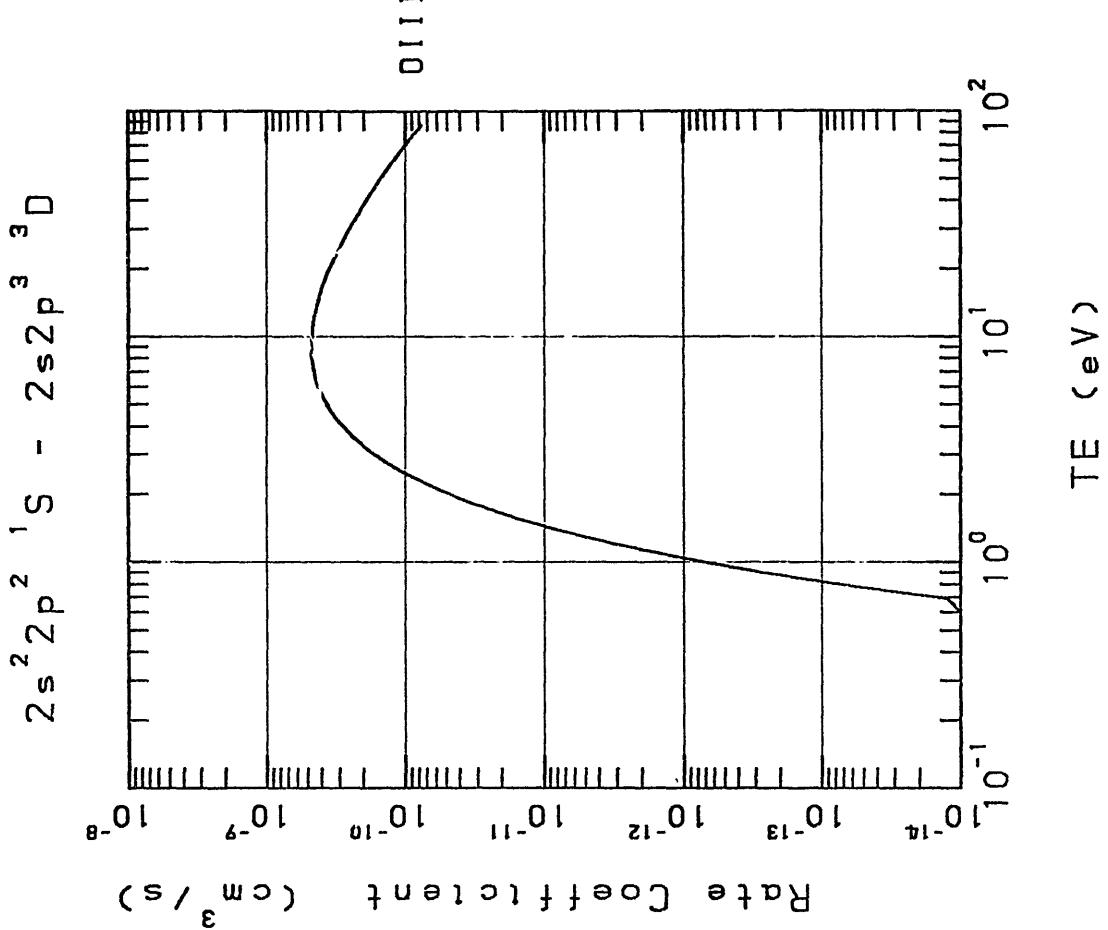
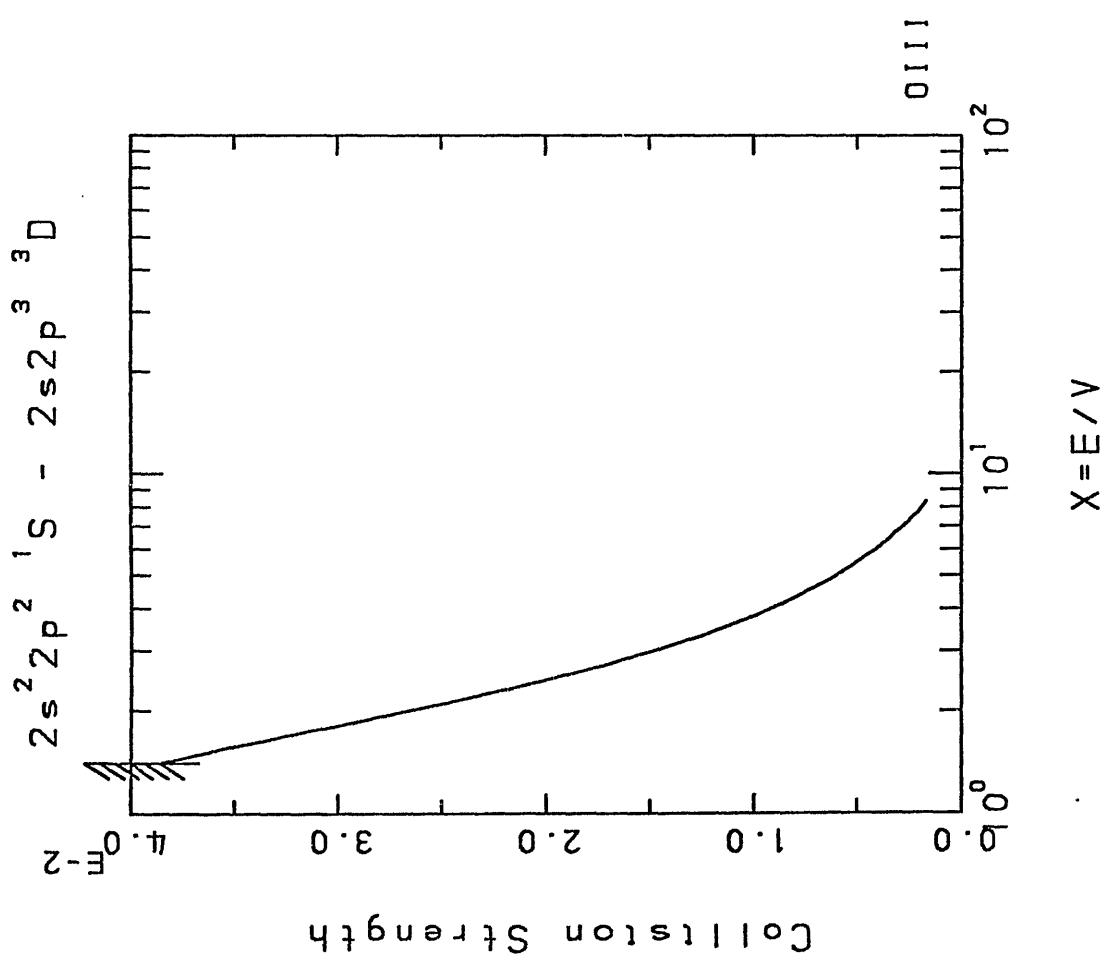


Fig. 78

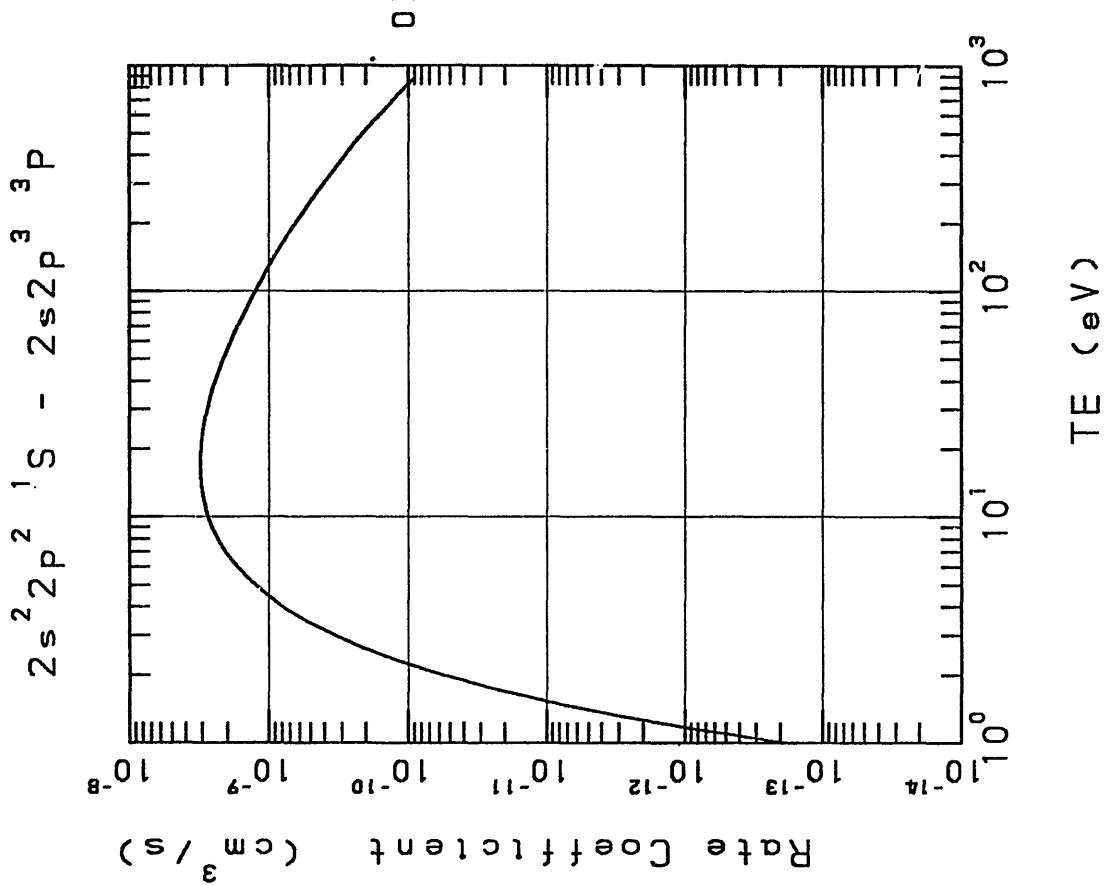
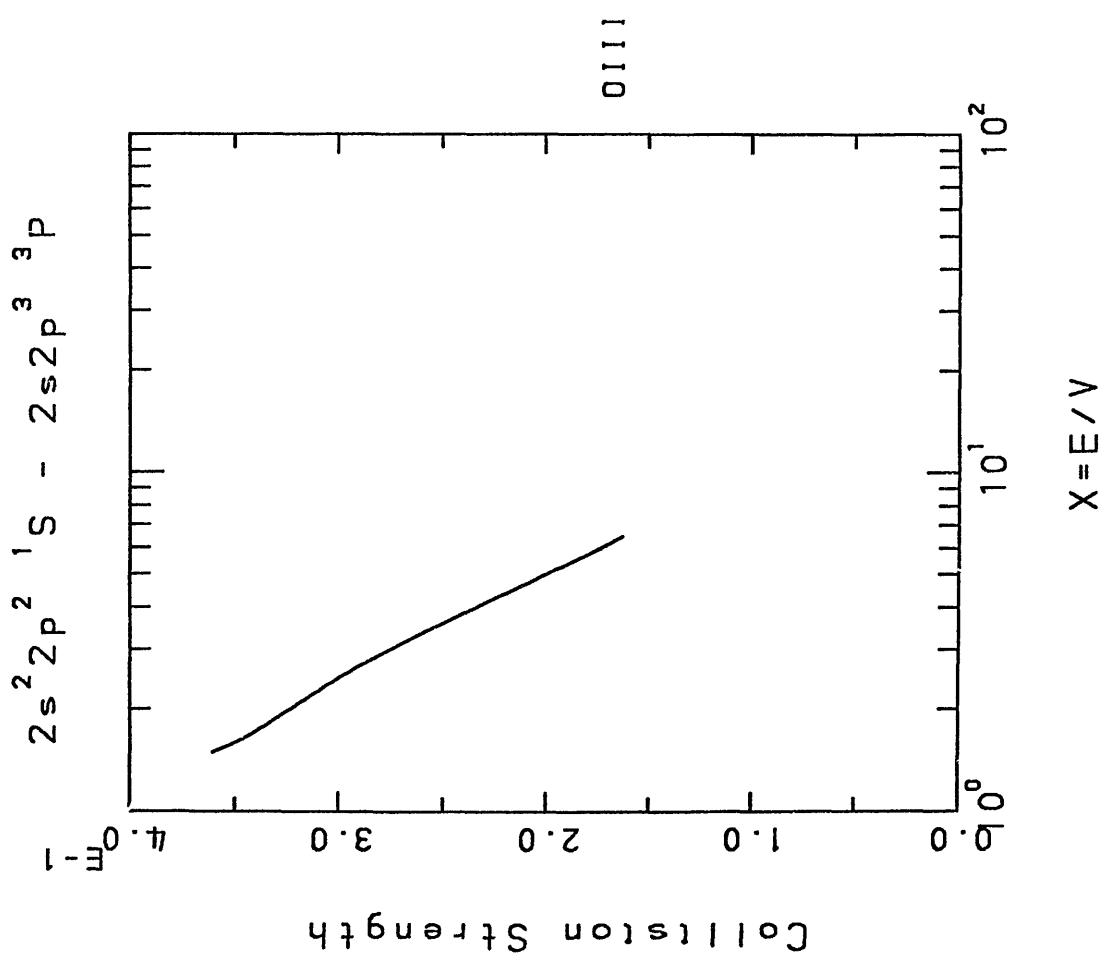


Fig. 79

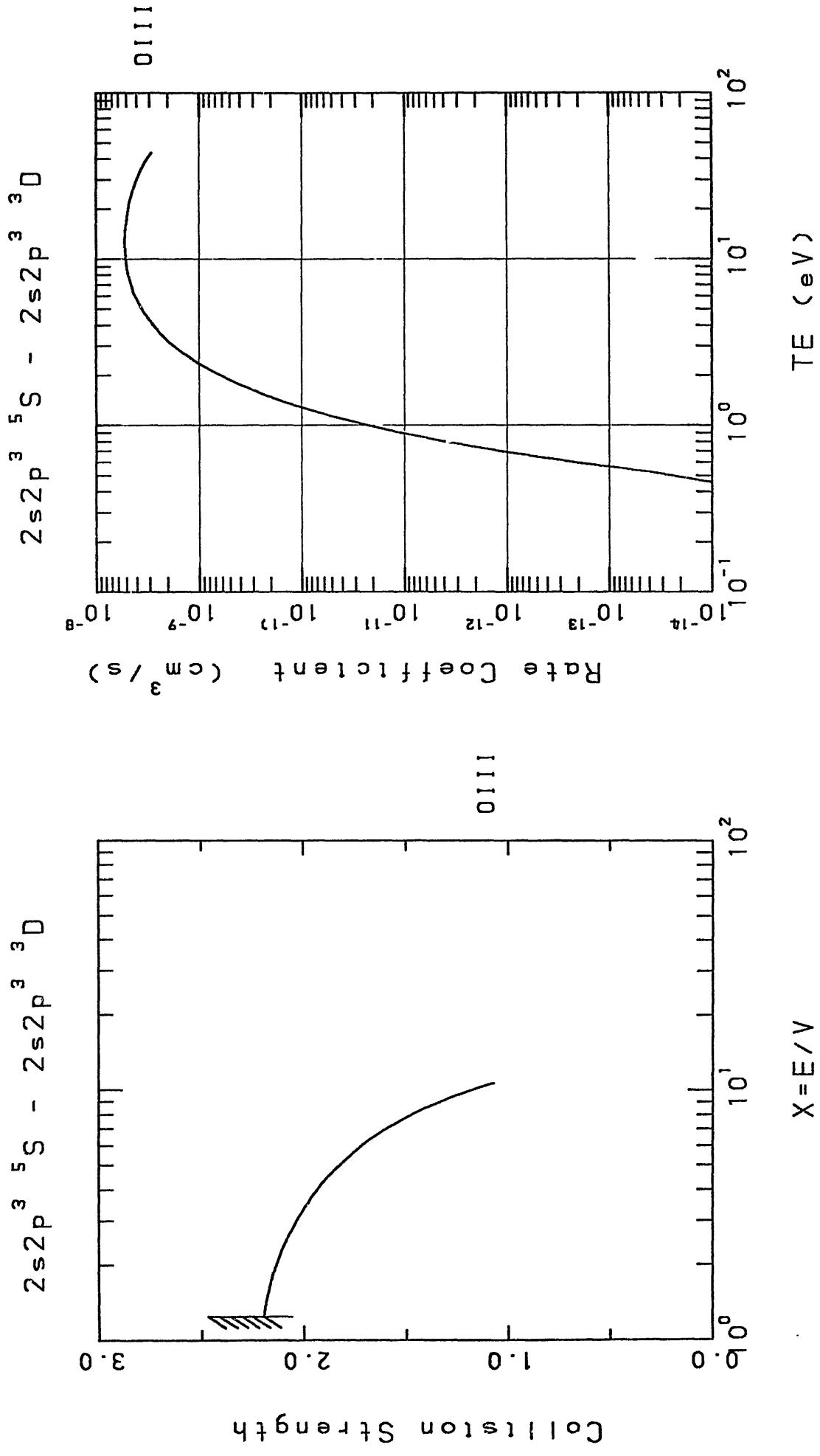


Fig. 80

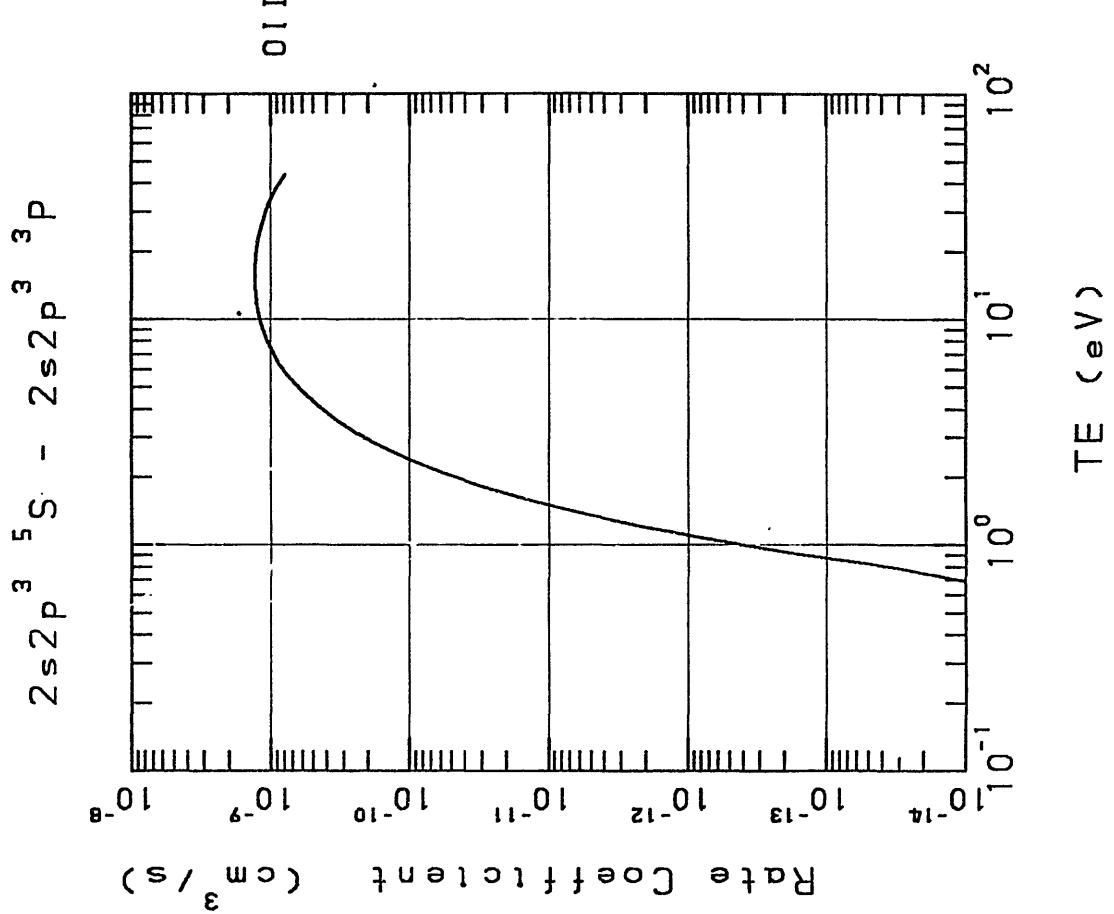
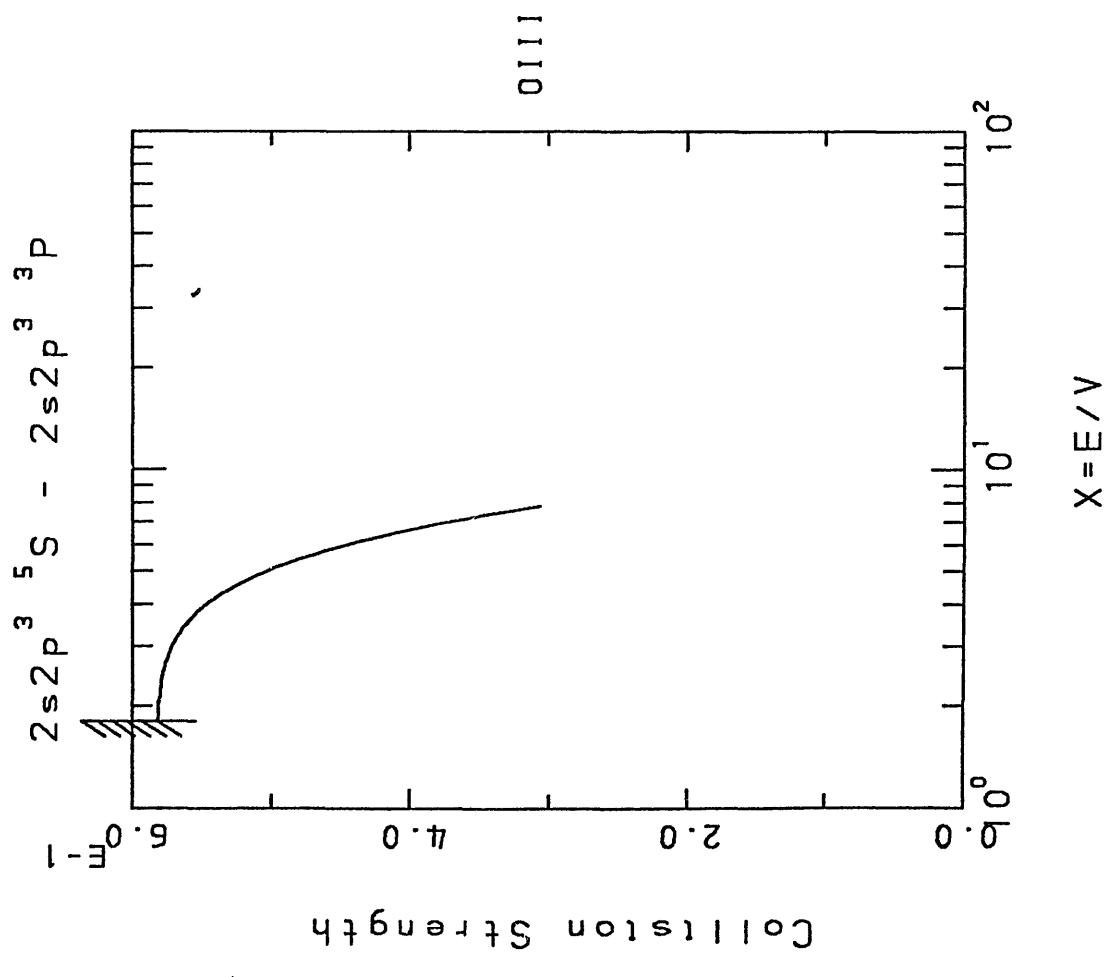
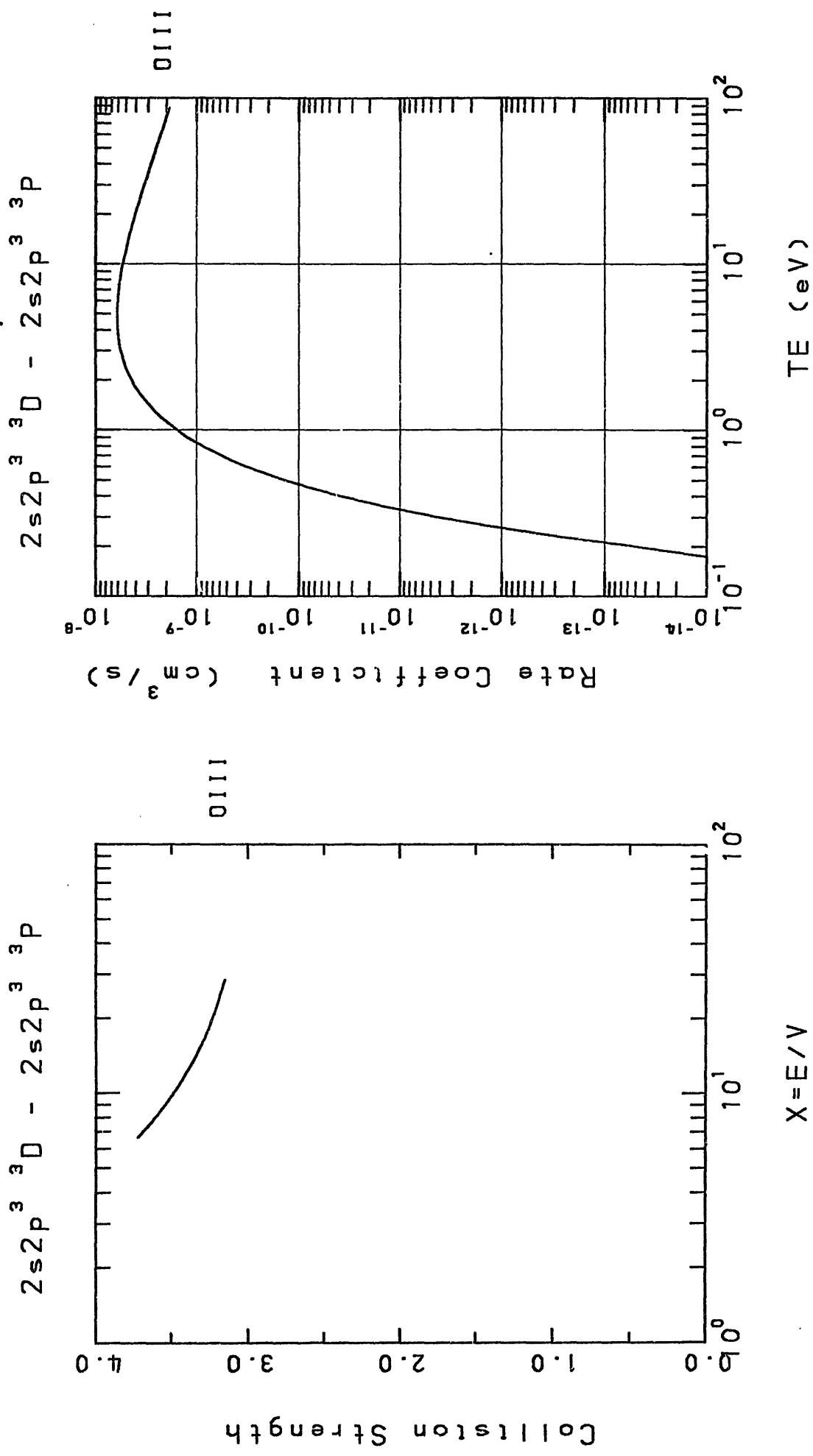


Fig. 81



N-like (O II)

Pradhan (1976a) made a close-coupling (CC) calculation with five states ($2s^2 2p^3 4S$, $2D$, $2P$, $2s 2p^4 4P$, $2D$) and obtained rate coefficients therefrom [Pradhan (1976b)]. His calculation includes the resonance effect, but gives the data over a very limited range of electron energy. Henry et al. (1969) performed a similar CC calculation but with only the lowest three states and no closed-channel resonances.

For $2s^2 2p^3 4S - 2s^2 2p^3 2D$, the values of Henry et al. are adopted for the non-resonant part of the cross section and the resonance effect is incorporated with the aid of Pradhan's rate coefficient. In the non-resonant region, both the CC calculations give almost the same cross sections.

For the transitions, $2s^2 2p^3 4S - 2s^2 2p^3 2P$ and $2s^2 2p^3 2P - 2s^2 2p^3 2D$, only the results of Henry et al. are used to give the present recommended data. The resulting rate coefficients are in a fair agreement with those of Pradhan. The present data, therefore, give collision strengths effectively including the resonance effect.

Recently Ho and Henry (1983) carried out a two-state CC calculation for $2s^2 2p^3 4S - 2s 2p^4 4P$ and $2s^2 2p^3 4S - 2s^2 2p^2 3s 4P$. Those data are included here.

Data sources

Henry, R.J.W., Burke, P.G. and Sinfailam, A.L. (1969), Phys. Rev. **178** 218

[transitions among $2s^2 2p^3 4S, 2D, 2P, CC$]

Ho, Y.K. and Henry, R.J.W. (1983), Astrophys. J. **264** 733

[$2s^2 2p^3 4S - 2s 2p^4 4P, 2s^2 2p^2 3s 4P, CC$]

Pradhán, A.K. (1976a), J. Phys. B **9** 433

[$2s^2 2p^3 4S - 2s^2 2p^3 2D, CC$]

Pradhan, A.K. (1976b), Mon. Not. R. Astr. Soc. **177** 31

[$2s^2 2p^3 4S - 2s^2 2p^3 2D, CC$]

Fig. 82

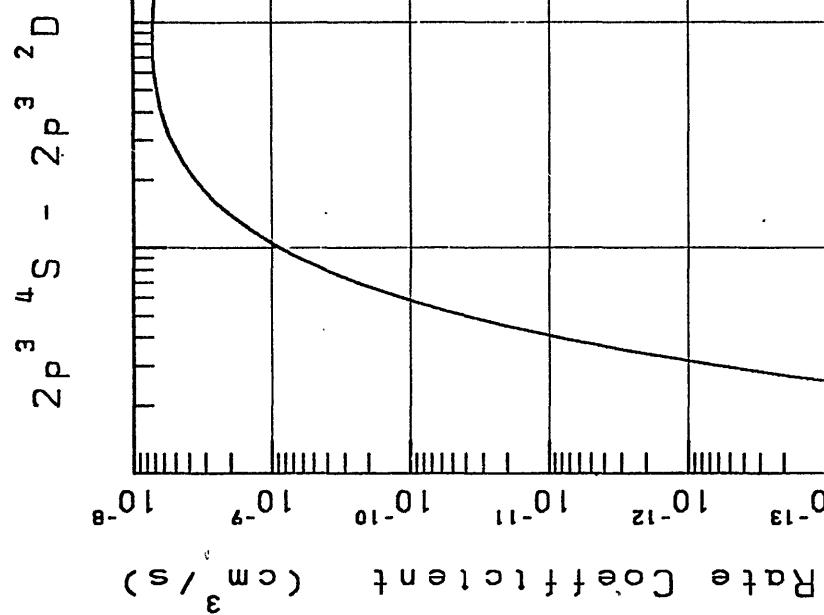
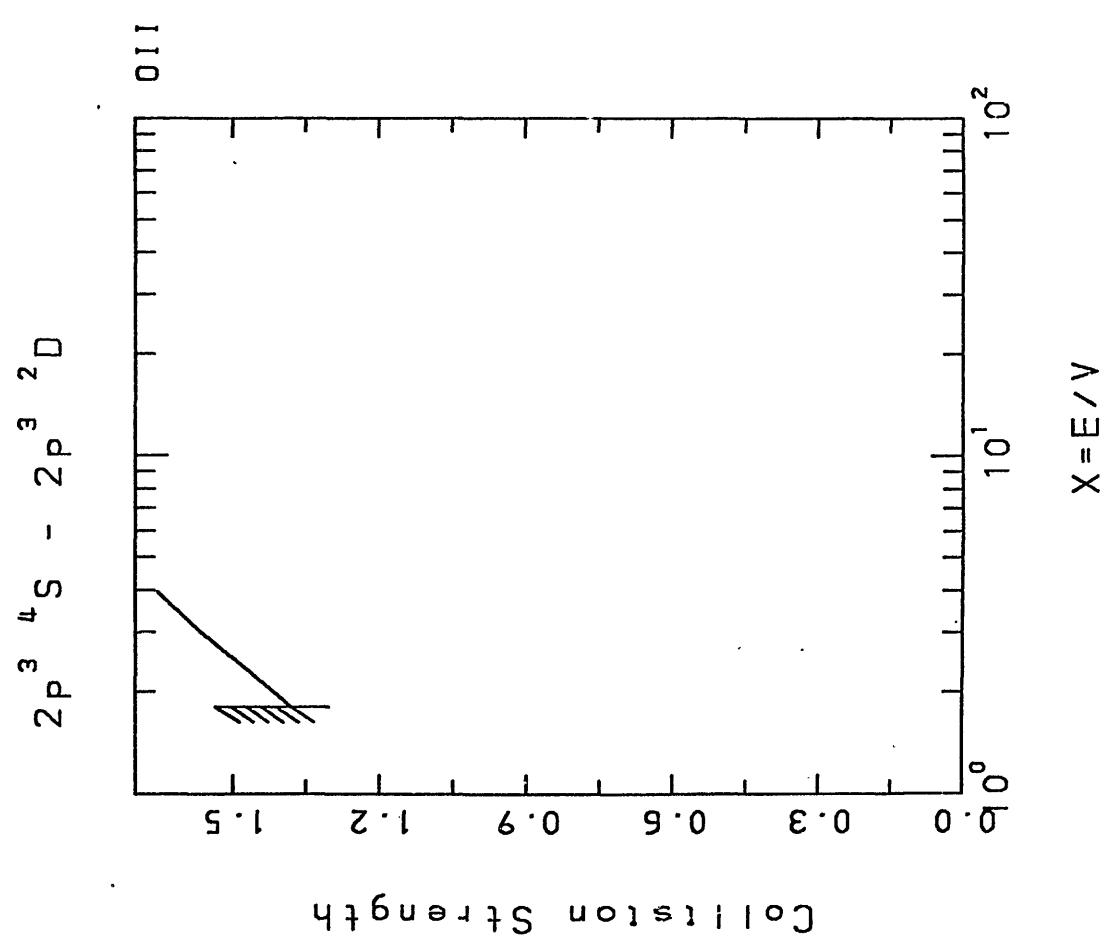


Fig. 83

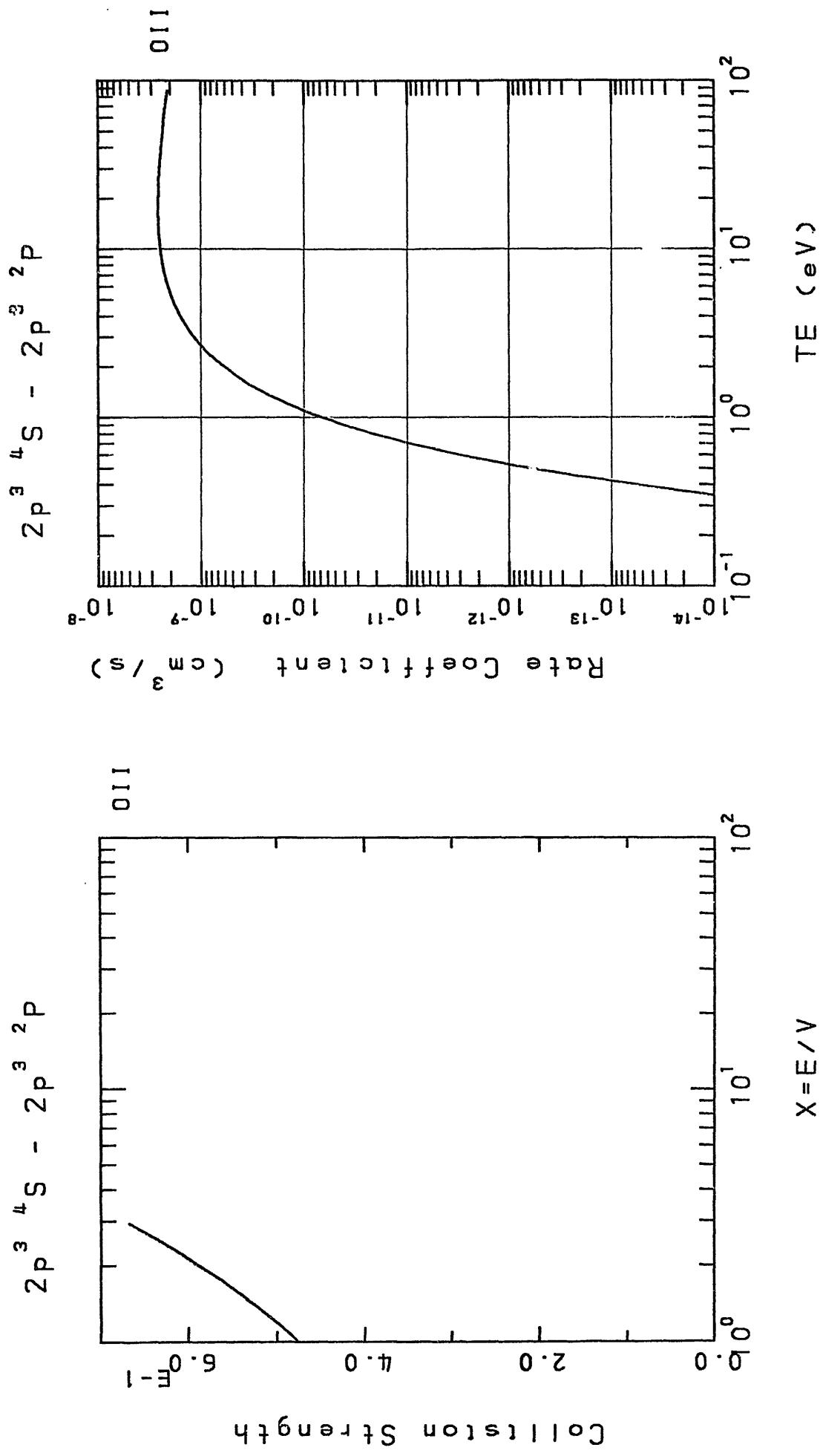


Fig. 84

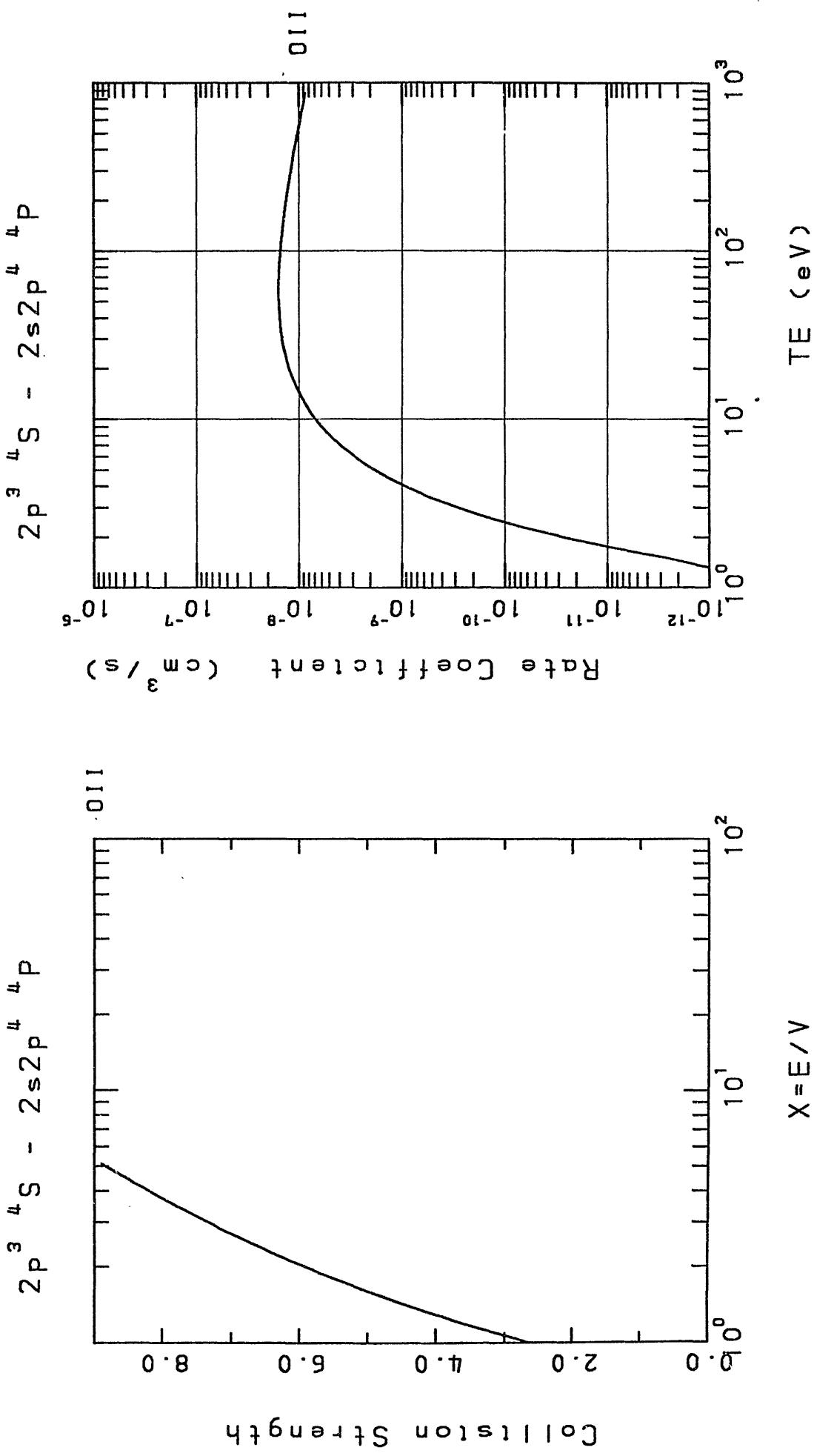


Fig. 85

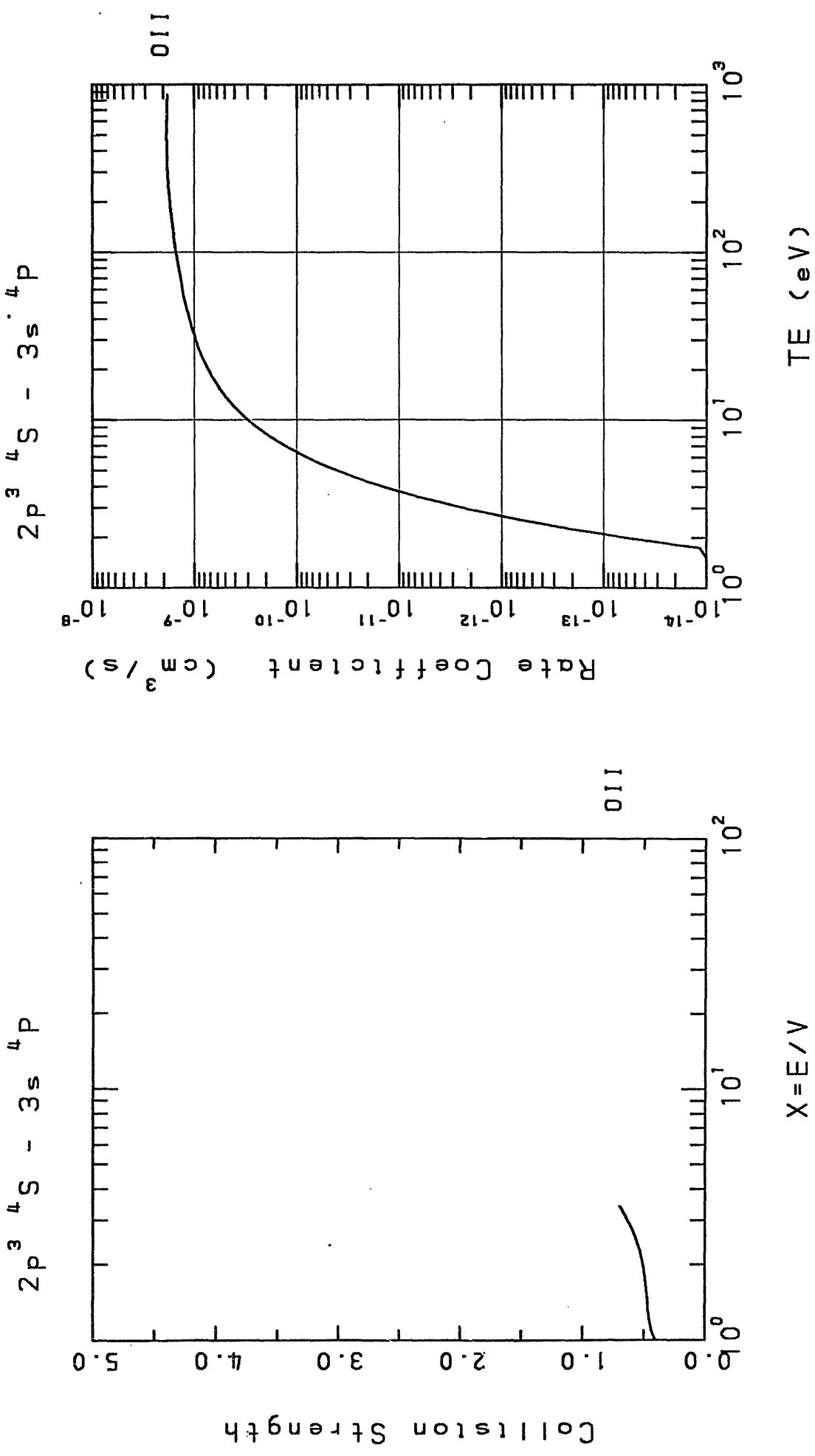
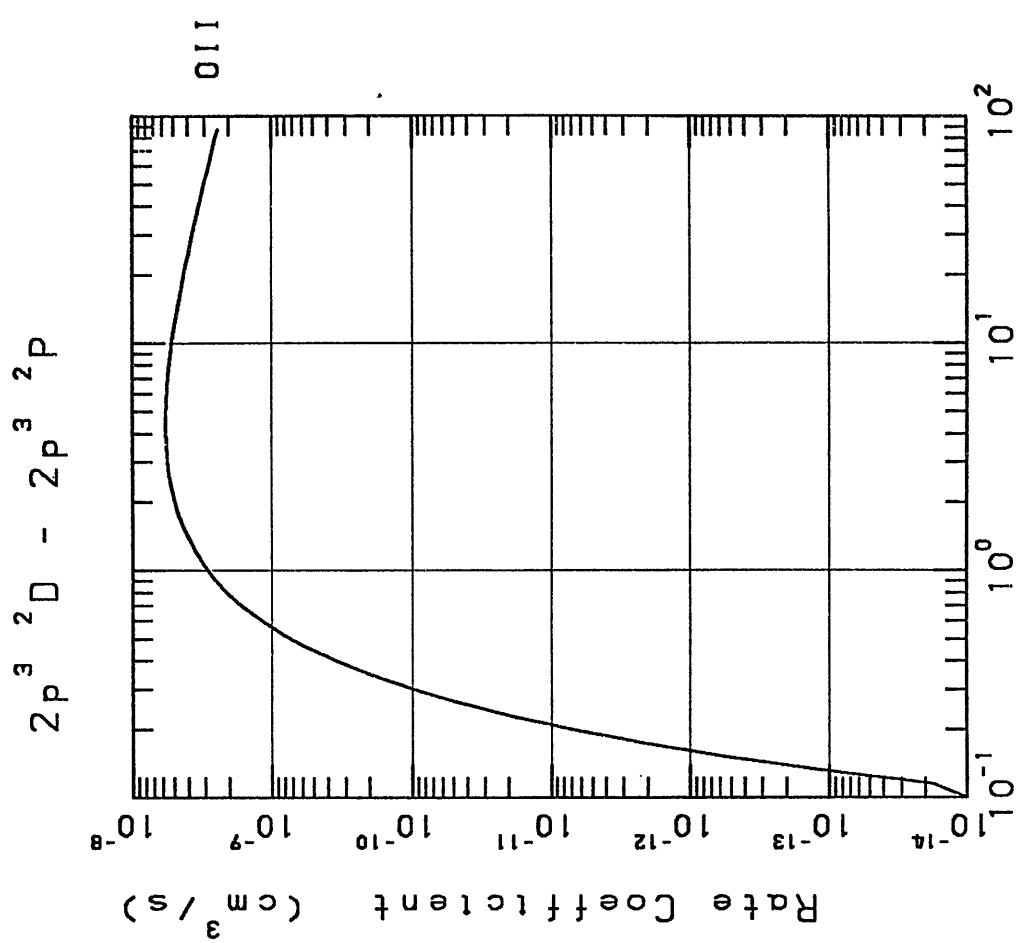
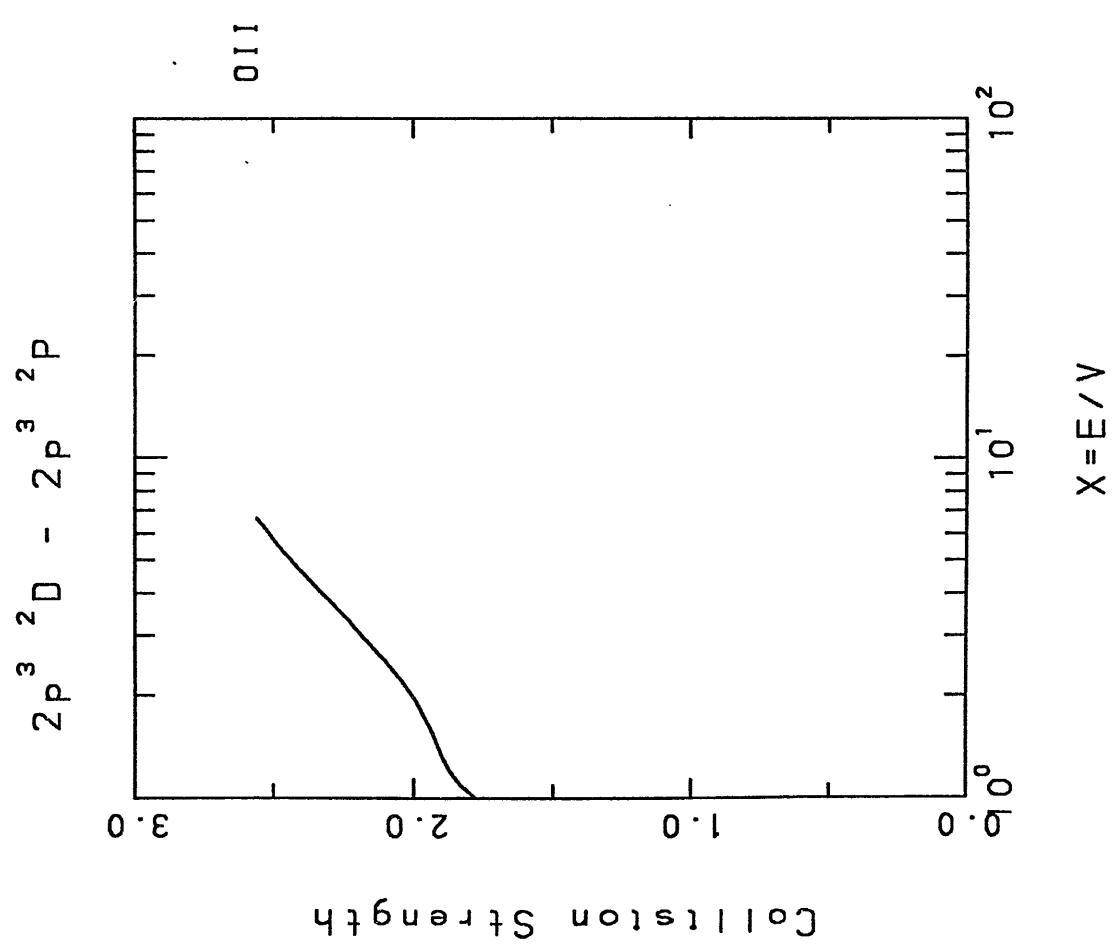


Fig. 86



Appendix

FORTRAN Program for the calculation of rate coefficients.

```
00010      FUNCTION RATEN(TEMP,EIJ,GI,ITYPE,A,B,C,D,E,F)
00020 C    --- RATE COEFFICIENT WITHOUT RESONANCES -----
00030 C    TEMP ..... TEMPERATURE IN EV
00040 C    EIJ ..... THRESHOLD ENERGY IN EV
00050 C    GI ..... STATISTICAL WEIGHT OF INITIAL STATE
00060 C    ITYPE =1 ...POWER - LOG TYPE
00070 C    =2 ...EXPONENTIAL TYPE
00080 C
00090      S=0.5
00100      CONST=8.010E-8/((SQRT(TEMP)*GI))
00110      Y=EIJ/TEMP
00130      IF(ITYPE.EQ.2) GO TO 10
00140 C   -- CASE OF TYPE=1 ---
00150      RA=A/Y+ C+ S*D*(1.-Y)
00160      RB=B- C*Y+ S*D*Y*Y+ E/Y
00170      RATEN=CONST*EXP(-Y)*Y*(RA+EIEXP(Y)*RB)
00180      RETURN
00190 C   -- CASE OF TYPE=2 ---
00200      10 RA=A*(1.-EIEXP(Y)*Y)
00210      RB=B*EXP(-F)/(F+Y)+ C*EXP(-2.*F)/(2.*F+Y)+D*EXP(-3.*F)/(3.*F+Y)
00220      1 + E*EXP(-4.*F)/(4.*F+Y)
00230      RATEN=CONST*EXP(-Y)*Y*(RA+RB)
00240      RETURN
00250      END
00251 C
00260 C
00270      SUBROUTINE RATER(TEMP,EIJ,GI,ITYPE,A,B,C,D,E,F,P,Q,X1)
00280 C   -- RATE COEFFICIENT WITH RESONANCES -----
00290 C    TEMP ..... TEMPERATURE IN EV
00300 C    EIJ ..... THRESHOLD ENERGY IN EV
00310 C    GI ..... STATISTICAL WEIGHT OF INITIAL STATE
00320 C    ITYPE =1 ...POWER - LOG TYPE
00330 C    =2 ...EXPONENTIAL TYPE
00340 C
00350      S=0.5
00360      CONST=8.010E-8/((SQRT(TEMP)*GI))
00370      Y=EIJ/TEMP
00380      Y1=Y*X1
00390      IF(ITYPE.EQ.2) GO TO 10
00400 C   -- CASE OF TYPE=1 ---
00410      RA=A/Y+C/X1+S*D*(1./(X1*X1)-Y/X1)+E*LOG(X1)/Y
00420      RB=B-C*Y+S*D*Y*Y+E/Y
00430      RNOR=CONST*Y*EXP(-Y1)*(RA+EIEXP(Y1)*RB)
00440      GO TO 20
00450 C   -- CASE OF TYPE=2 ---
00460      10 RA=A*(1./X1-EIEXP(Y1)*Y)
00470      RB= B*EXP(-F*X1)/(F+Y)+C*EXP(-2.*F*X1)/(2.*F+Y)
00480      1 + D*EXP(-3.*F*X1)/(3.*F+Y)+E*EXP(-4.*F*X1)/(4.*F+Y)
00490      RNOR=CONST*Y*EXP(-Y1)*(RA+RB)
00500      20 RRES=CONST*EXP(-Y)*(P*(1.+1./Y)*(1.-EXP((1.-X1)*Y)*(X1+1./Y)/
00510      1 (1.+1./Y))+Q*(1.-EXP((1.-X1)*Y)))
00520      RATE=RNOR + RRES
00540      RETURN
00550      END
00551 C
00560 C
```

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00570 C
00580      FUNCTION EIEXP(X)
00590 C
00600 C      EIEXP=E1(X)*EXP(X)
00610 C      HANDBOOK OF MATHEMATICAL FUNCTIONS, PAGE 231
00620 C      BY M. ABRAMOWITZ AND I.A. STEGUN
00630 C
00640      IF(X.GT.1.0) GO TO 10
00650      A0=-0.57721566
00660      A1=0.99999193
00670      A2=-.24991055
00680      A3=0.05519968
00690      A4=-0.00976004
00700      A5=0.00107857
00710      EIEXP=(A0+A1*X+A2*X**2+A3*X**3+A4*X**4+A5*X**5-LOG(X))*EXP(X)
00720      RETURN
00730 10   A1=8.5733287401
00740      A2=18.0590169730
00750      A3=8.6347608925
00760      A4=.2677737343
00770      B1=9.5733223454
00780      B2=25.6329561486
00790      B3=21.0996530827
00800      B4=3.9584969228
00810      EIEXP=(X**4+A1*X**3+A2*X**2+A3*X+A4)/
00820      1      (X**4+B1*X**3+B2*X**2+B3*X+B4)/X
00830      RETURN
00840      END
00850 C

```

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