Electron-Impact Excitation of the B $^1\Sigma^+$, C$^1\Sigma^+$ and E$^1\Pi$ States of CO at 100eV

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Abstract

Electron impact excitation of CO plays an important role in planetary atmospheres and interstellar clouds. At the present time, serious discrepancies exist among excitation cross sections reported in the literature for this molecule. We measured electron impact excitation cross sections for $B^1\Sigma^+ \rightarrow X^1\Sigma^+$, $C^1\Sigma^+ \rightarrow X^1\Sigma^+$ and $E^1\Pi \rightarrow X^1\Sigma^+$ states of CO at 100eV impact energy using electron energy-loss spectroscopy.

1. Introduction

Electron collision cross sections for CO are needed for modeling of various discharge, plasma and laser systems [1], planetary atmospheres and interstellar clouds [2,3]. Electron collision cross section data available for CO have been summarized by Trajmar et al. [4] up to 1983. Electron-impact induced optical emission cross sections were reported by Aarts and de Heer [5] for the $A^1\Pi \rightarrow X^1\Sigma^+$, $B^1\Sigma^+ \rightarrow X^1\Sigma^+$ and $C^1\Sigma^+ \rightarrow X^1\Sigma^+$ processes. Mumma et al. [6] and Ajello [7] have determined absolute emission cross sections for the $A^1\Pi \rightarrow X^1\Sigma^+$ system. Cross sections for excitation of high-lying metastable states were measured by Wells et al. [8] and more recently by Mason and Newell [9]. Zetner et al. [10] presented preliminary results for the angular distributions for excitation of some valence states at electron impact energies of 12.5 and 15 eV. Recently, James et al. [11] reported the extreme ultraviolet emission cross sections for CO produced by electron impact at 20 and 200 eV. Total electronic excitation cross sections by electron impact, in the energy range of 1-1000 eV, for CO have been recommended by Kanik et al. [12]. On the other hand, there has been a limited number of theoretical studies of this corresponding problem . Chung and Lin [13] calculated integral cross sections for excitation of the three states investigated here (at impact energies from threshold to 1000 eV) using Born and Born-Ochkur-Rudge type approximations as did Lee and McKoy [14] using distorted-wave approximation. These theories are not in good agreement with each other nor with experiment at low and intermediate impact energies. Most recently, the cross sections for electron impact excitation of the valence states of CO have been reported by Sun et al. [15]. It is evident from these works that the available data for excitation cross sections are very fragmentary.

Here we describe the application of our absolute cross section measurement techniques [16] to CO and report differential cross sections (DCS) for the electron impact excitation of the $B\ ^1\Sigma^+$, $C\ ^1\Sigma^+$ and $E\ ^1\Pi$ states. The impact enery in these measurements was 100 eV and the scattering angles ranged from 5 to 120°. Integral cross sections have also been obtained from these DCS. No previous experimental or theoretical DCS results are available for these states to which our results could be compared.

2. Experimental Procedures

The apparatus used in the present measurements has been described in detail elsewhere [17]. Cylindrical electrostatic optics and double hemispherical energy selectors were used both in the electron gun and detector. Energy-loss spectra including both the elastic peak and the inelastic region of interest, were obtained by pulse-counting, multichannel scaling techniques at fixed impact energies (E_o) and scattering angles (θ). The target CO beam was formed by effusing the gas through a capillary array (with collimation = $l/2r = 100$) at low (~ few Torr) back pressure.

The procedures for obtaining energy-loss spectra with the target beam ON and OFF, the background subtraction, the calibration of the instrument response function, the unfolding of the overlapping vibrational band structures and normalization of the measurements to the absolute scale have been described in detail by Nickel et al. [16]. To obtain energy-loss spectra which represents the true relative scattering intensities associated with elastic scattering and various excitation processes, the background scattering and the response function of the apparatus were determined (the former by chopping the CO beam and the latter by calibration to He n=2 excitation). The corrected energy-loss spectra were then unfolded into contributions from various electronic transitions utilizing a least-squares fitting procedure [16,18]. The energy-loss values and the Franck-Condon factors for the individual bands and the band shapes were the input into the computer code for unfolding. Normalization of the relative scattering intensities (cross sections) to the absolute scale was achieved by utilizing the absolute elastic DCS for CO at 100 eV. These elastic DCS were measured by Nickel et al. [19].

The integral cross sections were obtained by extrapolating the DCS to 0° and to 180° and integrating them over all angles. In the extrapolations we relied on the general trend.

The experimental errors associated with the present measurements are estimated as follows: a) 10% error from background subtraction and response function calibration, b) 15% from unfolding procedure, c) 11% from the elastic DCS. Thus the overall error in the DCS is 21% (square root of the sum of the squares of the contributing errors). For the integral cross sections an additional error of about 5% is added due to extrapolations to 0° and to 180° scattering angles.

3. Results and Discussion

There are three electronic transitions with their vibrational band structures which are the subject of this study. The features ($B^1\Sigma^+ \rightarrow X^1\Sigma^+$, $C^1\Sigma^+ \rightarrow X^1\Sigma^+$ and $E\ ^1\Pi \rightarrow X^1\Sigma^+$) fall into the 10.5 to 12 eV energy-loss region. Figure 1 shows a typical energy-loss spectrum and designations of features of interest. The absolute DCS for the $B^1\Sigma^+$, $C^1\Sigma^+$ and $E\ ^1\Pi$ states are given in Table I. Each one of these absolute cross sections is obtained (a) by summing over individual vibrational level intensities for that particular electronic state and then (b) by normalizing the relative (relative to elastic) intensity for that particular electronic state to the absolute elastic DCS [19] for each angle at 100eV impact energy. Figures 2, 3 and 4 show that the DCS for the $B^1\Sigma^+$, $C^1\Sigma^+$ and $E\ ^1\Pi$ states respectively. All three states exhibit foreward peaking. There are no experimental data or theoretical calculation to which these DCS results can directly be compared.

Table II summarizes the integral cross sections (Q) for the $B^1\Sigma^+$, $C^1\Sigma^+$ and $E\ ^1\Pi$ states at 100eV electron impact energy along with the other available experimental and theoretical data. The emission cross section measurement results of Aarts and deHeer [5] are about 50% lower for the $B^1\Sigma^+$ state and about 9% larger for the $C^1\Sigma^+$ state than our results. More recent emission cross section results of James et al. [11] are 27% lower for the $B^1\Sigma^+$ state and 38% lower for the $C^1\Sigma^+$ state than our results. This may be due to the fact that these states are subject to small amount of predissociation. Predissociation of the $B^1\Sigma^+$, $C^1\Sigma^+$ and $E\ ^1\Pi$ states has recently been under investigation and some light will be shed on this subject [20]. The theoretical value of Chung and Lin [13] is about 15% higher that our results for the $B^1\Sigma^+$ state. Their result for $C^1\Sigma^+$ state is about 40% and higher than ours. While the disagreement (in our results) for the $E\ ^1\Pi$ states reaches almost a factor of three.

It is clear that more experimental and theoretical works are needed in order to improve present situation.

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TABLE I

Differential Cross Sections of CO at 100 eV Impact Energy[a]

Angle (deg)	DCS(10^{-18} cm^2/sr) $B^1\Sigma^+$	$C^1\Sigma^+$	$E^1\Pi$	Elastic[b]
0	(120.1)	(626.0)	(180.8)	(2080.0)
5	19.34	141.5	62.5	(1368.0)
10	3.41	15.5	6.50	(850.9)
15	1.04	3.6	1.56	(495.9)
20	0.54	1.38	0.72	270.0
30	0.49	0.62	0.28	74.2
40	0.28	0.24	0.088	27.2
50	0.16	0.12	0.042	15.0
60	0.12	0.077	0.028	10.8
70	0.084	0.048	0.015	8.4
75	0.073	0.050	0.015	7.9
80	0.064	0.043	0.012	7.7
90	0.065	0.041	0.011	7.3
100	0.065	0.046	0.012	7.2
110	0.072	0.051	0.012	8.2
120	0.093	0.057	0.013	9.6
130	(0.14)	(0.063)	(0.014)	(11.1)
140	(0.21)	(0.070)	(0.015)	(12.5)
150	(0.33)	(0.079)	(0.016)	(13.9)
160	(0.49)	(0.090)	(0.018)	(15.0)
170	(0.71)	(0.105)	(0.021)	(15.7)
180	(1.01)	(0.124)	(0.024)	(16.0)

(a) Numbers in paranthesis are extrapolated values.
(b) Elastic DCS used to normalize the inelastic DCS were obtained from Nickel et al. [19].

TABLE II

Summary of Integral Cross Sections of CO at 100 eV Impact Energy

	$Q(10^{-18}\ cm^2)$		
$B^1\Sigma^+$	$C^1\Sigma^+$	$E^1\Pi$	Reference
3.83	12.34	4.43	Present Results
2.79	7.58	-	James et al. [11]
1.96	13.4	-	Aarts and deHeer [5]
4.47	16.79	11.20	Chung and Lin [13]*

* Theory

Figure Captions

Figure 1. CO energy-loss spectrum at 100 eV electron impact energy and 20° scattering angle.

Figure 2. Absolute differential electron-impact excitation cross sections for the B $^1\Sigma^+$ state of CO at 100 eV. Values are in 10^{-18} cm^2/sr units.

Figure 3. Absolute differential electron-impact excitation cross sections for the C $^1\Sigma^+$ state of CO at 100 eV. Values are in 10^{-18} cm^2/sr units.

Figure 4. Absolute differential electron-impact excitation cross sections for the E $^1\Pi$ state of CO at 100 eV. Values are in 10^{-18} cm^2/sr units.

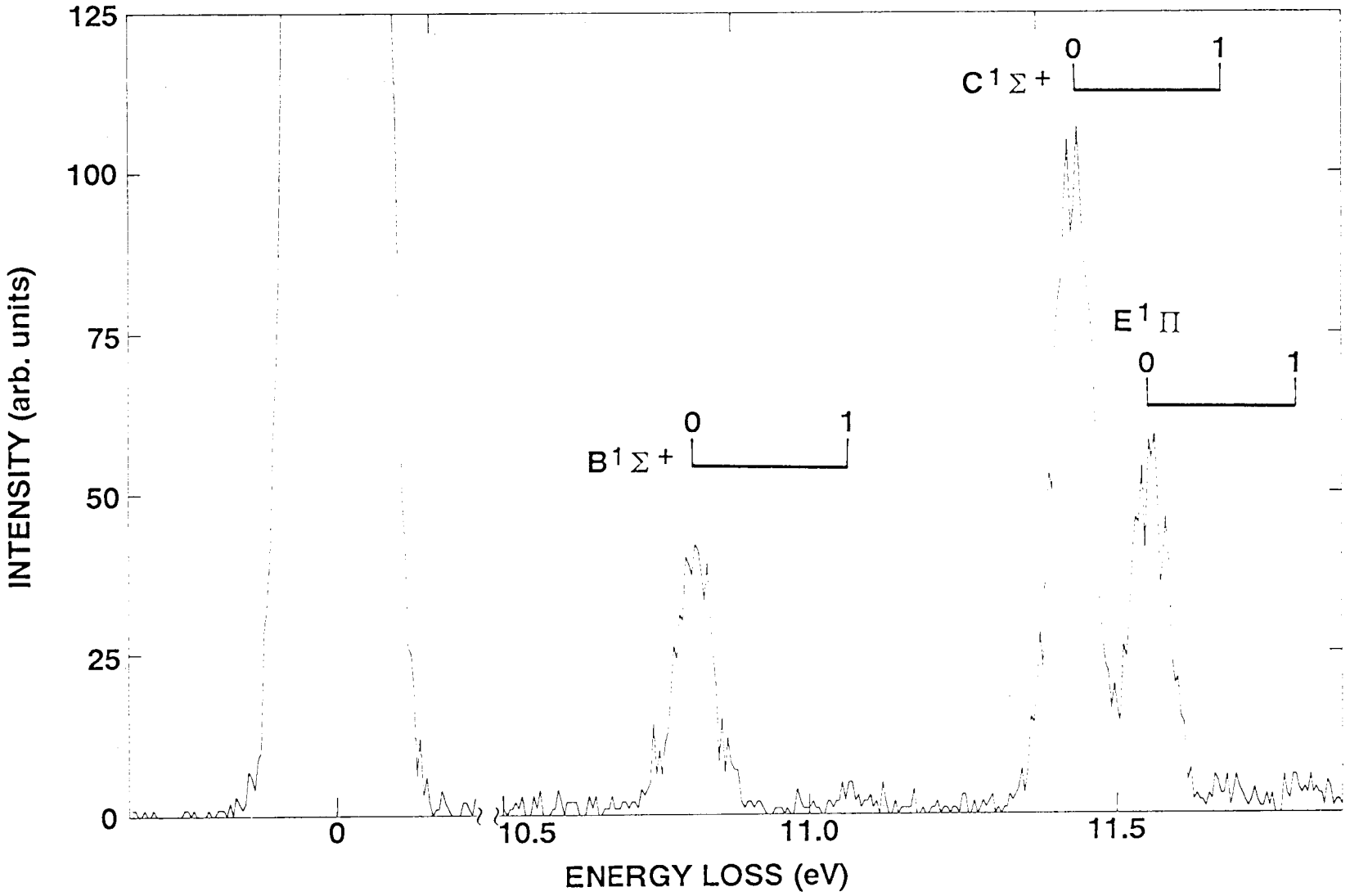

125
100
75
50
25
0
INTENSITY (arb. units)
0
10.5
11.0
11.5
ENERGY LOSS (eV)
C 1 Σ +
0
1
B 1 Σ +
0
1
E 1 Π
0
1

Figure 1

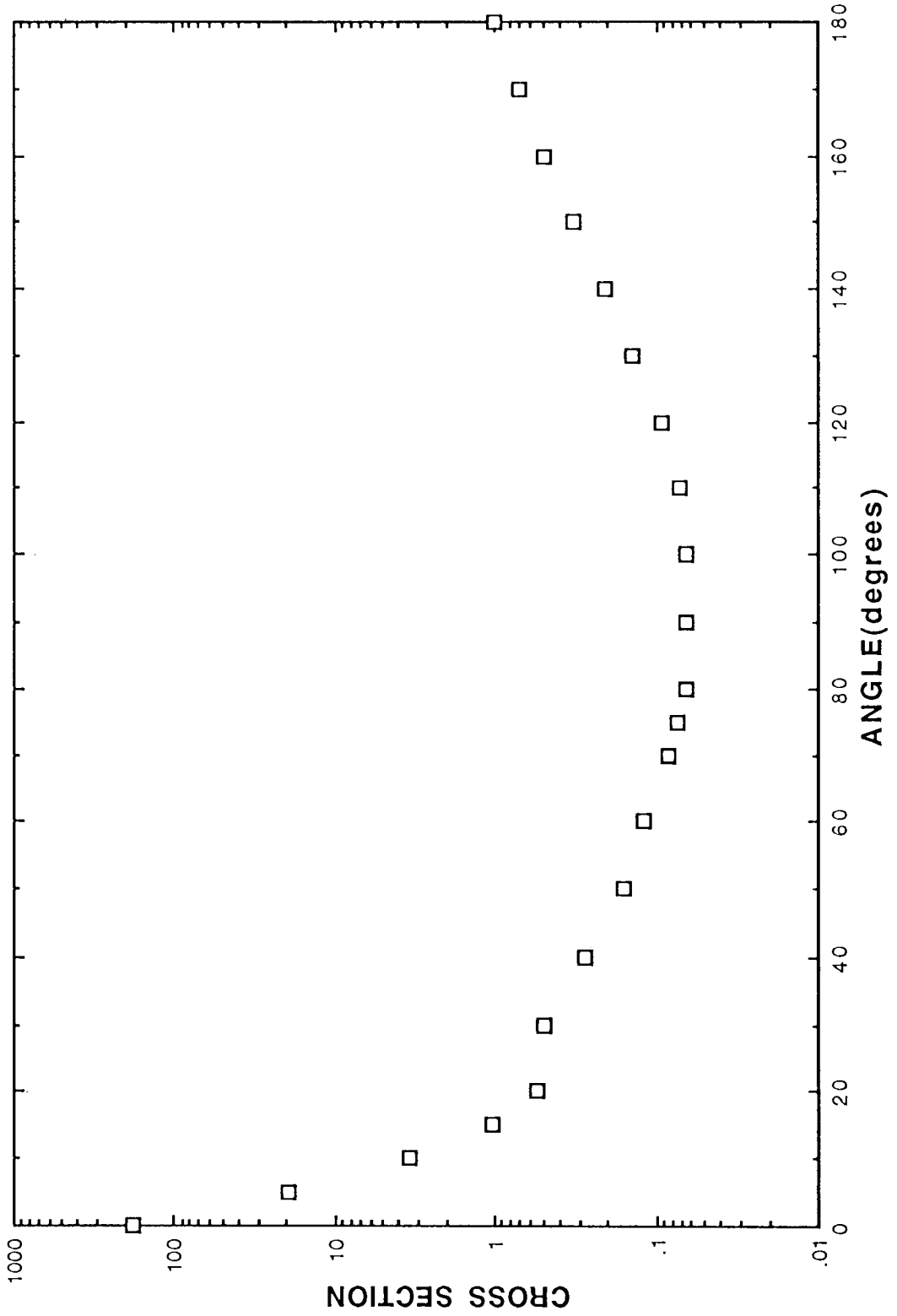
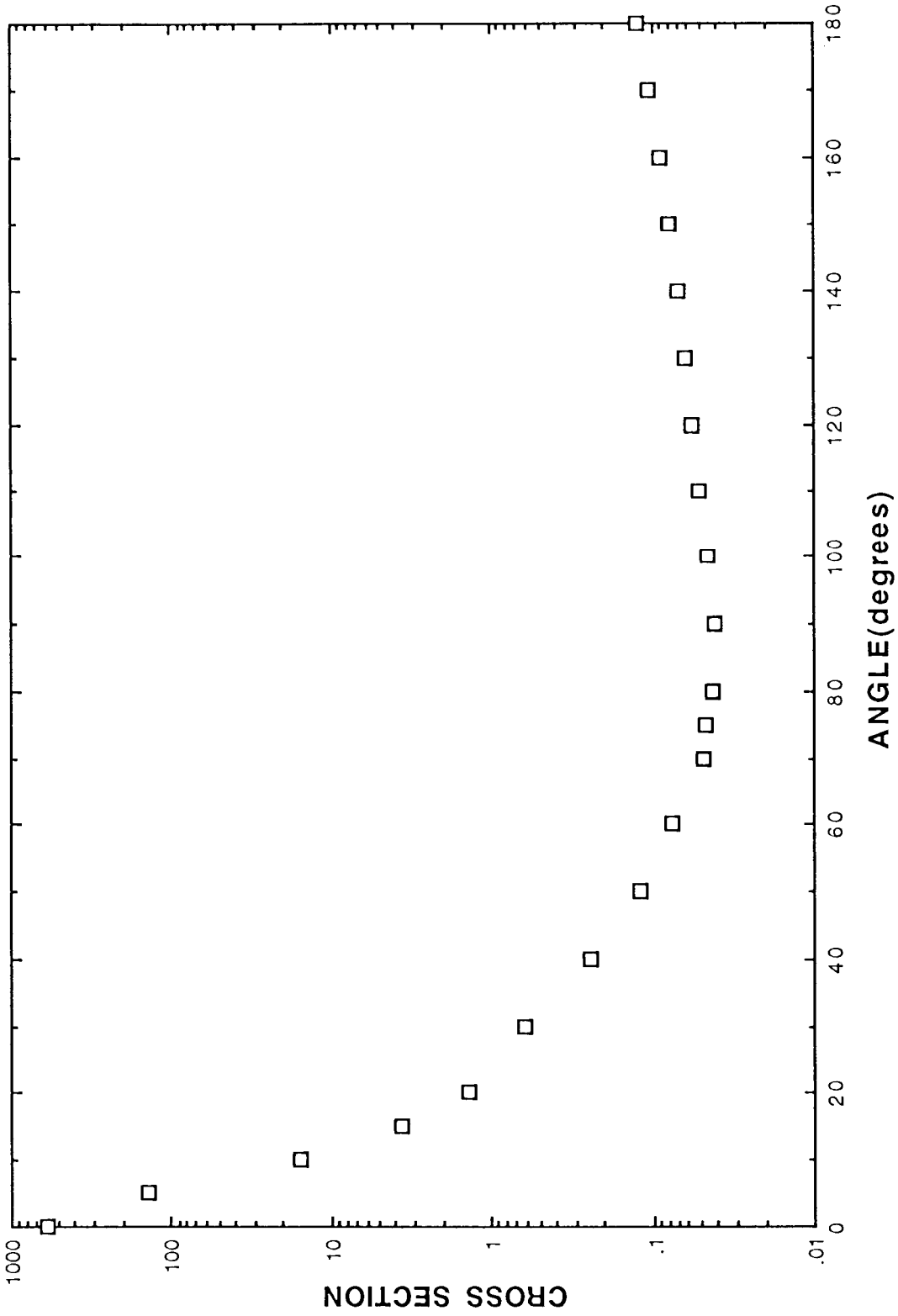

CROSS SECTION
1000
100
10
1
.1
.01
0
20
40
60
80
100
120
140
160
180
ANGLE(degrees)

Figure 2


CROSS SECTION
1000
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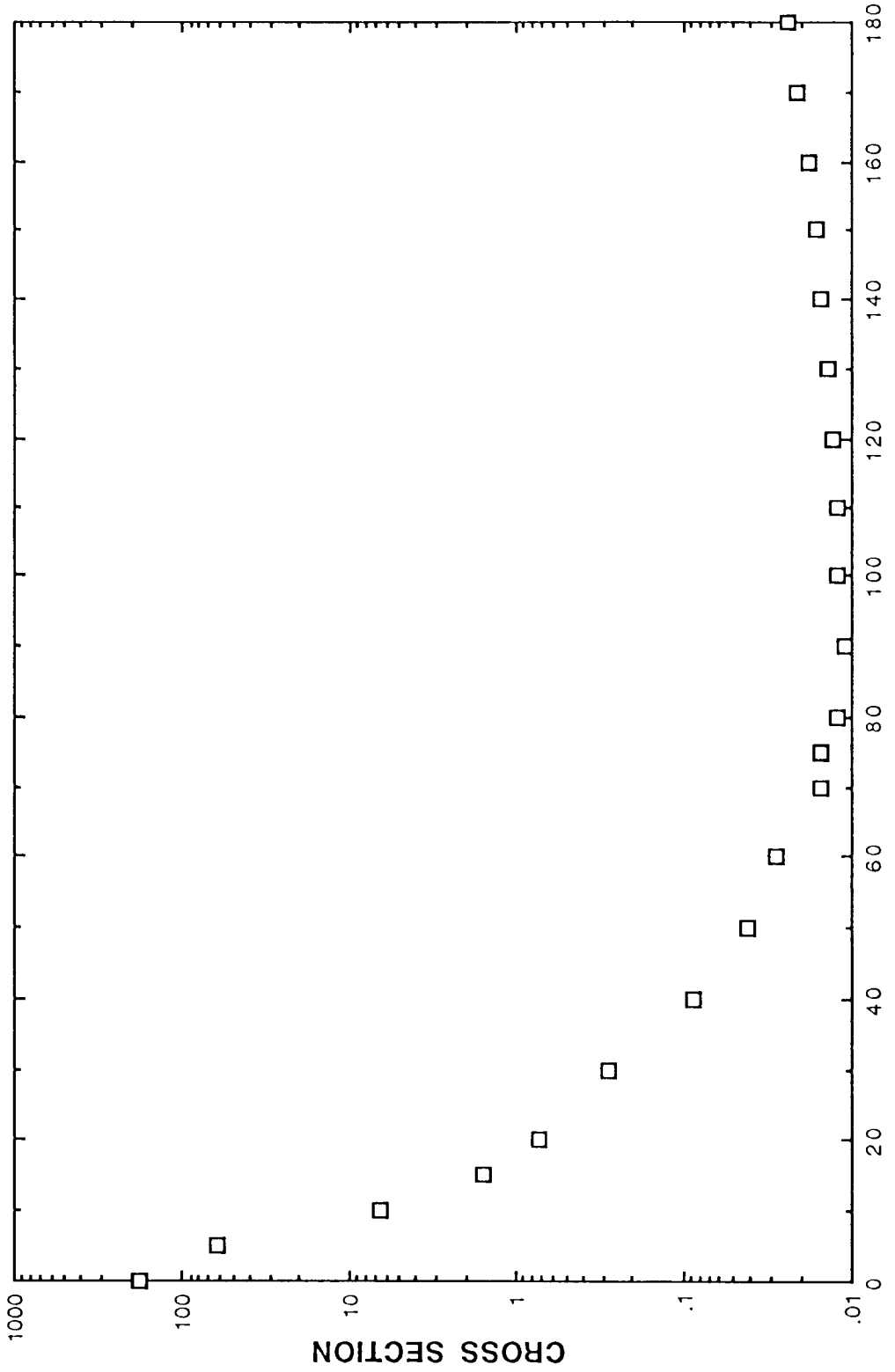
ANGLE(degrees)

Figure 3


CROSS SECTION
1000
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.1
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40
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180
ANGLE(degrees)

Figure 4