

Electron Impact Ionization Cross-
Sections and Ionization Rate Co-
efficients for Atoms and Ions from
Hydrogen to Calcium

Wolfgang Lotz

IPP 1/62

May 1967

MAX-PLANCK-INSTITUT FÜR PLASMAPHYSIK
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Die nachstehende Arbeit wurde im Rahmen des Vertrages zwischen dem Institut für Plasmaphysik GmbH und der Europäischen Atomgemeinschaft über die Zusammenarbeit auf dem Gebiete der Plasmaphysik durchgeführt.

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W. Lotz

Electron Impact Ionization Cross-
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from Hydrogen to Calcium.

(in English)

Abstract:

Using the empirical formula recently proposed, electron impact ionization cross-sections for single ionization from the ground state are given for free atoms and for all ionization stages from hydrogen to calcium ($Z = 20$). For these species ionization rate coefficients are given under the assumption of a Maxwellian distribution of the impacting electrons. Lowering of ionization potential, collision limit, or multiple ionization are not taken into account.

Introduction

In a recent paper¹ the author attempted to predict ionization cross-sections hitherto unknown in the triangle H I - Na I and Na XI on an empirical basis after certain regularities had been discovered.

In the meantime an empirical formula has been proposed² with the help of which experimentally determined cross-section curves have been approximated within experimental error. The question then arose if this formula could be used for predictions of yet unknown cross-sections.

The Formula used

For predictions Formula 4 of Reference 2 seems to be the most versatile and is used here:

$$\sigma = \sum_{i=1}^N a_i \zeta_i \frac{\ln E/\chi_i}{E \cdot \chi_i} \left\{ 1 - b_i \exp \left[-c_i (E/\chi_i - 1) \right] \right\}. \quad (1)$$

\uparrow cm^2 \uparrow $\text{cm}^2 (\text{eV})^2$ \uparrow eV \uparrow eV

E is the energy of the impacting electron; χ_i is the binding energy of electrons in the i-th subshell; ζ_i is the number of equivalent electrons in this subshell; a_i , b_i , and c_i are individual constants, which have to be determined by a reasonable guess. In the cases under consideration the two outermost subshells only need to be considered, N can be set equal to 2.

In Table 1 all quantities needed for the above formula are tabulated for the first few ionization stages of hydrogen through calcium; as far as experimentally known cross-sections are concerned, the above Formula agrees with them within experimental error, in most cases even within 10 %. For the species not mentioned (four times and higher ionized ions) I assumed that $a_i = 4.5 \times 10^{-14} \text{ cm}^2 (\text{eV})^2$, $b_i = 0$, and $c_i = 0$; this assumption agrees with the theoretical calculations of Rudge and Schwartz³ for a hydrogen-like ion with high Z-number, its validity for ions not hydrogen-like might be questioned but no better approximation is known.

In Table 2 the ionization potential for electrons in the outermost subshell⁴ is given, in Table 3 the binding energy of electrons in the next inner subshell^{5,6}.

Cross-Sections and Rate Coefficients

With the data of Table 1 cross-section curves for free atoms and for singly charged ions have been drawn (Fig. 1 through 24). I estimate the error of these cross-sections to be not higher than $\begin{matrix} +40 \\ -30 \end{matrix}$ % (two times probable error). For cross-sections of atoms and ions known experimentally the respective curves can be found in References 1 or 2 and are not reproduced here. Hitherto unknown cross-sections of Reference 1 have been recalculated and are repeated here as they are more or less different.

Formula 1 can be folded with a Maxwellian electron distribution

$f(u) 4\pi u^2 du = \frac{dn}{n} = \frac{2}{kT} \left(\frac{E}{\pi kT} \right)^{1/2} \exp(-E/kT) dE$ (2) *u = relat. Geschw.*

and yields the following rate coefficient (in cm³/s):

$\langle \sigma u \rangle = S = 6.7 \times 10^7 \sum_{i=1}^N \frac{a_i \zeta_i}{T^{3/2}} \left\{ \frac{1}{X_i/T} \int_{X_i/T}^{\infty} \frac{\exp(-x)}{x} dx - \frac{b_i \exp c_i}{X_i/T + c_i} \int_{X_i/T + c_i}^{\infty} \frac{\exp(-y)}{y} dy \right\}$ (3) cm³/sec

$d^3u = 4\pi u^2 du = 2\pi \left(\frac{2}{m} \right)^{3/2} \sqrt{E} dE$ (Becker p. 73) mit $E = \frac{1}{2} m u^2$ $\int d^3u = \frac{2}{hT} \left(\frac{E}{\pi kT} \right)^{1/2} e^{-E/kT} dE$ (OK)

Check: $\langle E \rangle := \int_0^{\infty} E f^N d^3u = \frac{3}{2} kT$ mit Benutzung von ! (Becker p. 73)

Beweis: $\int_0^{\infty} E f^N d^3u = \frac{2}{(\pi (hT)^{3/2})} \int_0^{\infty} E^{3/2} e^{-E/kT} dE = 2C \int_0^{\infty} u^4 e^{-u^2/kT} du = 2C \cdot \frac{3\sqrt{\pi}}{8} = 2 \cdot \frac{2}{\sqrt{\pi} (hT)^{3/2}} \cdot \frac{3\sqrt{\pi}}{8} = \frac{3}{2} hT$ (OK)

This rate coefficient has been computed with the data of Table 1 through 3 for a number of discrete electron temperatures between 1 and 10^4 eV. The results are given in Table 4 numerically and in Fig. 25 through 44 graphically.

These rate coefficients give a lower limit to the true value, the rate might be increased by the following effects:

1. Multiple ionization,
2. Lowering of ionization potential⁷, or
3. A "collision limit" lower than the ionization potential⁸ (ionization from excited levels).

In cases 2 and 3 the ionization potential of Table 2 is to be replaced by the lowered ionization potential or by the value of the collision limit. It should still be possible then to use Formula 1 and 3 after these corrections to the ionization potential have been applied, though it is not known whether the form of the cross section curve is changed drastically or not.

As the lowering of the ionization potential and the collision limit depend on electron density, no general conclusions can be drawn, but for electron temperatures small compared to the ionization potential the deviations to be expected may be as large as an order of magnitude.

References

- 1 W. Lotz, Astrophys. J. Suppl. 14, No. 128 (1967).
- 2 W. Lotz, Report IPP 1/50, to be published in Astrophys. J. (1967).
- 3 M. R. H. Rudge and S. E. Schwartz, Proc. Phys. Soc. 88, 563 (1966).
- 4 W. Lotz, Report IPP 1/49, J. Opt. Soc. Am., in press (1967).
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- 8 H. R. Griem, in Plasma Spectroscopy, McGraw-Hill Book Company, New York 1964, p. 159.

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$Z.P. IV \equiv 2^{+} 16. Z = 2$
feeding model

Table 1: Relevant data for the first few ionization stages of the elements under consideration. a_1 and a_2 are given in $10^{-14} \text{ cm}^2(\text{eV})^2$.

Con-fig.	ζ_1	ζ_2	Spe-cies	a_1	a_2	b_1	b_2	c_1	c_2	Spe-cies	a_1	a_2	b_1	b_2	c_1	c_2
1s	1	0	H I	4.0	-	0.60	-	0.56	-	He II	4.4	-	0.38	-	0.60	-
1s ²	2	0	He I	4.0	-	0.75	-	0.46	-	Li II	4.0	-	0.48	-	0.60	-
2s	1	2	Li I	4.0	4.4	0.70	0.6	2.4	0.6	Be II	4.4	4.5	0	0.4	0	0.6
2s ²	2	2	Be I	4.0	4.4	0.7	0.6	0.5	0.6	B II	4.4	4.5	0.4	0.4	0.6	0.6
2p	1	2	B I	3.8	4.0	0.7	0.7	0.4	0.5	C II	4.2	4.4	0.4	0.4	0.6	0.6
2p ²	2	2	C I	3.5	4.0	0.7	0.7	0.4	0.5	N II	3.9	4.4	0.46	0.4	0.62	0.6
2p ³	3	2	N I	3.2	4.0	0.83	0.7	0.22	0.5	O II	3.7	4.4	0.6	0.4	0.5	0.6
2p ⁴	4	2	O I	2.8	4.0	0.74	0.7	0.24	0.5	F II	3.5	4.4	0.6	0.4	0.5	0.6
2p ⁵	5	2	F I	2.7	4.0	0.90	0.7	0.20	0.5	Ne II	3.2	4.4	0.83	0.4	0.48	0.6
2p ⁶	6	2	Ne I	2.6	4.0	0.92	0.7	0.19	0.5	Na II	3.4	4.4	0.84	0.4	0.32	0.6
3s	1	6	Na I	4.0	3.4	0	0.84	0	0.32	Mg II	4.4	4.0	0	0.6	0	0.5
3s ²	2	6	Mg I	4.0	3.4	0.4	0.84	0.6	0.32	Al II	4.4	4.0	0.2	0.6	0.6	0.5
3p	1	2	Al I	4.0	4.0	0.3	0.4	0.6	0.6	Si II	4.4	4.4	0.2	0.2	0.6	0.6
3p ²	2	2	Si I	4.0	4.0	0.3	0.4	0.6	0.6	P II	4.4	4.4	0.2	0.2	0.6	0.6
3p ³	3	2	P I	4.0	4.0	0.4	0.4	0.6	0.6	S II	4.4	4.4	0.3	0.2	0.6	0.6
3p ⁴	4	2	S I	4.0	4.0	0.4	0.4	0.6	0.6	Cl II	4.4	4.4	0.3	0.2	0.6	0.6
3p ⁵	5	2	Cl I	4.0	4.0	0.6	0.4	0.5	0.6	A II	4.2	4.4	0.3	0.2	0.6	0.6
3p ⁶	6	2	A I	4.0	4.0	0.62	0.4	0.40	0.6	K II	4.0	4.4	0.3	0.2	0.6	0.6
4s	1	6	K I	4.0	4.0	0	0.5	0	0.6	Ca II	4.4	4.4	0	0.3	0	0.6
4s ²	2	6	Ca I	4.0	4.0	0.4	0.5	0.6	0.6	-	-	-	-	-	-	-

Table 2: Binding energy X_1 (ionization potential) of electrons in the outermost shell in eV.

Z	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX
1 H	13.6																			
2 He	24.6	54.4																		
3 Li	5.39	75.6	122																	
4 Be	9.32	18.2	154	218																
5 B	8.30	25.2	37.9	259	340															
6 C	11.3	24.4	47.9	64.5	392	490														
7 N	14.5	29.6	47.4	77.5	97.9	552	667													
8 O	13.6	35.1	54.9	77.4	114	138	739	871												
9 F	17.4	35.0	62.7	87.1	114	157	185	954	1103											
10 Ne	21.6	41.1	63.5	97.1	126	158	207	239	1196	1362										
11 Na	5.14	47.3	71.7	98.9	138	172	208	264	300	1465	1649									
12 Mg	7.65	15.0	80.1	109	141	187	225	266	328	367	1762	1963								
13 Al	5.99	18.8	28.4	120	154	190	241	285	330	399	442	2086	2304							
14 Si	8.15	16.3	33.5	45.1	167	205	246	303	351	401	476	523	2438	2673						
15 P	10.5	19.7	30.2	51.5	65.0	220	263	309	372	424	480	561	612	2817	3070					
16 S	10.4	23.4	35.0	47.3	72.7	88.1	281	328	379	447	505	564	652	707	3224	3493				
17 Cl	13.0	23.8	39.9	53.5	67.6	97.0	114	348	400	456	529	592	656	750	809	3658	3946			
18 A	15.8	27.6	40.9	59.7	75.2	91.2	125	143	423	479	539	618	686	755	855	918	4121	4426		
19 K	4.34	31.7	45.8	61.1	82.7	100	118	155	176	504	565	629	715	787	861	968	1034	4611	4934	
20 Ca	6.11	11.9	51.2	67.3	84.5	109	128	148	189	211	592	657	727	818	894	974	1087	1157	5129	5470

Table 3: Binding energy X_2 of electrons in the next inner subshell in eV.

Z	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII
3	Li	57																
4	Be	115	125															
5	B	12.9	206	220														
6	C	16.6	30.9	325	343													
7	N	20.3	36.7	55.8	471	493												
8	O	28.5	42.6	63.8	87.6	644	670											
9	F	37.8	53.8	71.9	97.8	126	845											
10	Ne	48.5	66.4	86.2	108	139	172	1107										
11	Na	34	80.1	102	126	151	186	1328	1366									
12	Mg	54	65	119	144	172	201	283	1611	1653								
13	Al	10.6	90	103	164	194	225	302	350	1921	1967							
14	Si	13.5	22.9	133	148	217	250	321	371	423	2259	2309						
15	P	16.2	26.8	38.6	183	199	277	352	392	446	502	2624	2678					
16	S	20.2	30.7	43.8	57.6	239	257	384	426	469	528	589	3017	3075				
17	Cl	24.5	36.0	48.9	64.1	79.8	303	417	461	507	553	617	683	3437	3499			
18	A	29.2	41.7	55.5	70.4	87.6	105	394	498	545	594	644	713	784	3885	3951		
19	K	18.7	47.9	62.4	78.0	95.1	114	450	473	585	636	689	742	815	891	4361	4431	
20	Ca	28	37	70.1	86.4	104	123	165	534	559	680	734	790	847	925	1006	4865	4939

Table 4: Ionization rate coefficients for single ionization from the ground state by electron impact. (Maxwellian distribution, no lowering of ionization potential, no collision limit.)

E-08 = 10⁻⁸ etc.; T_e in eV; S = <GV> in cm³/s; error approx. ⁺⁴⁰/₋₃₀ %.
Hydrogen, Helium, Lithium, Beryllium, Boron, Nitrogen, Oxygen.

Table with columns for ionization rate coefficients (I, H I, He I, He II, Li I, Li II, Li III, Be I, Be II, Be III, Be IV, B I, B II, B III, B IV, B V, C I, C II, C III, C IV, C V, N I, N II, N III, N IV, N V, N VI, N VII, O I, O II) and rows for electron temperature (1.0, 1.5, 2.0, 3.0, 4.0, 5.0, 7.0, 10, 15, 20, 30, 40, 50, 70, 100, 150, 200, 300, 400, 500, 700, 1000, 1500, 2000, 3000, 4000, 5000, 7000, 10000).

Table 4: (Continued) Sulfur, Chlorine.

Table with 11 columns (S I to S X) and 11 rows (1.0 to 10000). Values are in scientific notation representing isotopic data for Sulfur and Chlorine.

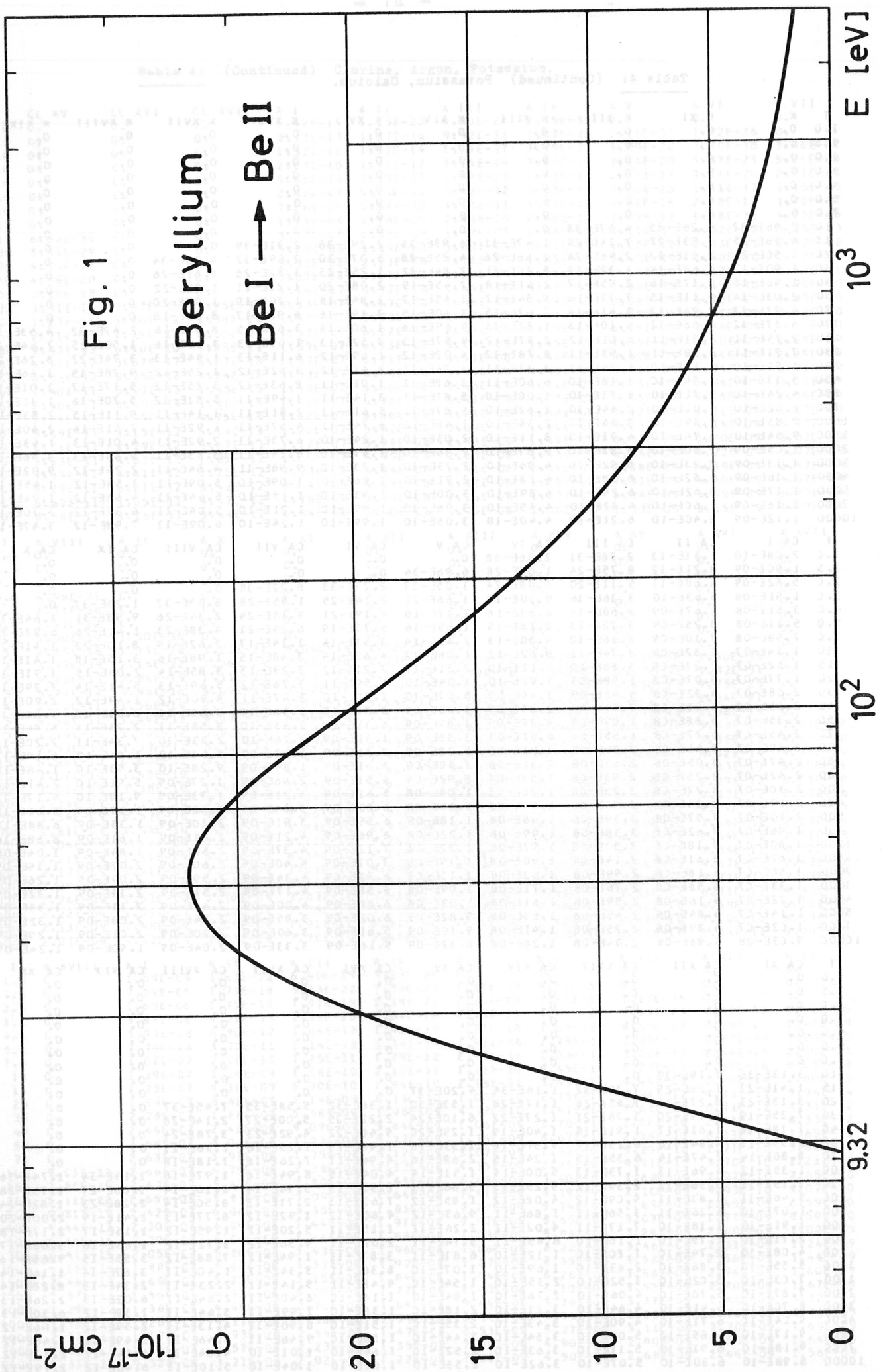
Table with 11 columns (S XI to S XVI and Cl I to Cl IV) and 11 rows (1.0 to 10000). Values are in scientific notation representing isotopic data for Sulfur and Chlorine.

Table with 11 columns (Cl V to Cl XIV) and 11 rows (1.0 to 10000). Values are in scientific notation representing isotopic data for Chlorine.

Fig. 1

Beryllium

Be I \rightarrow Be II



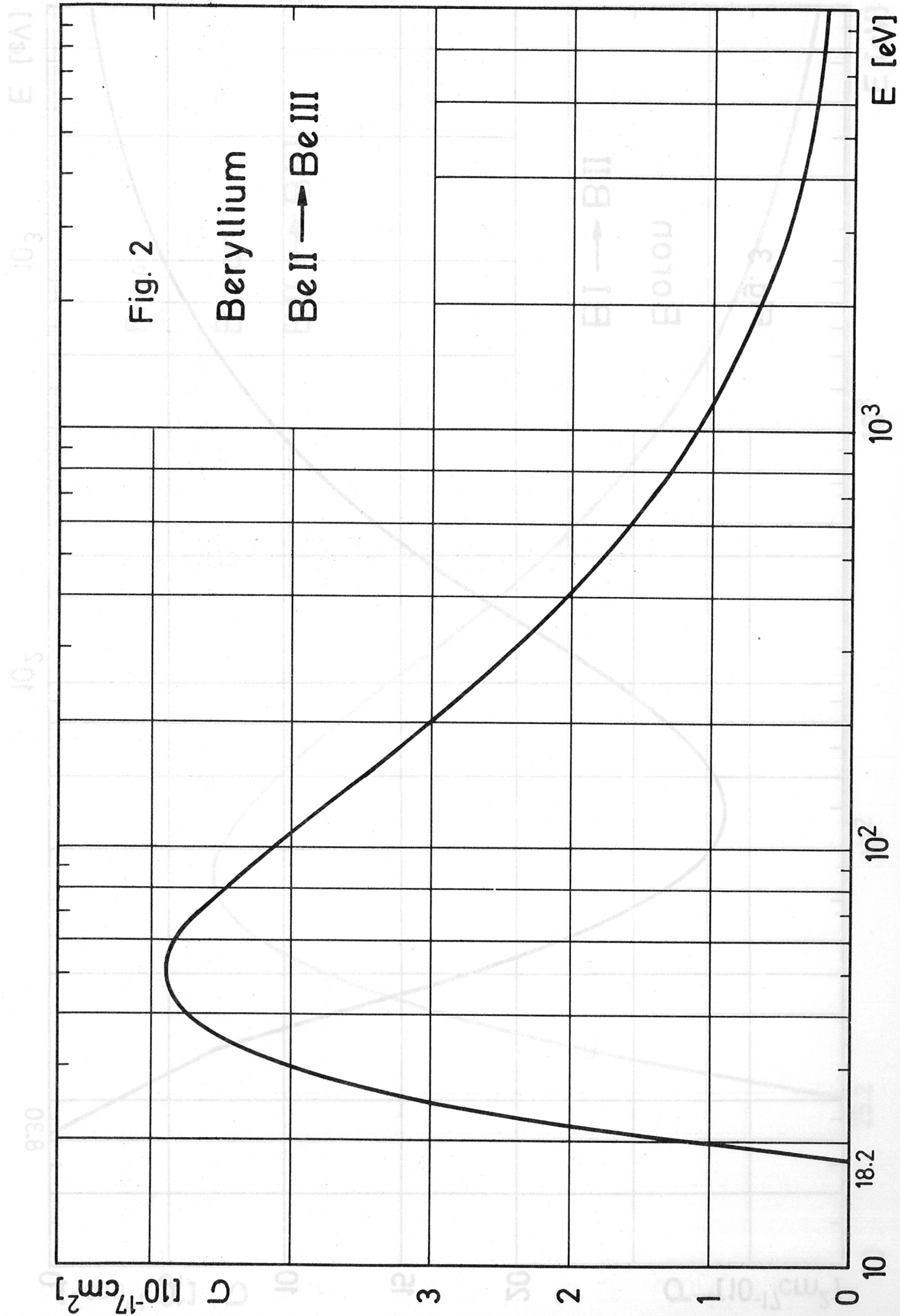
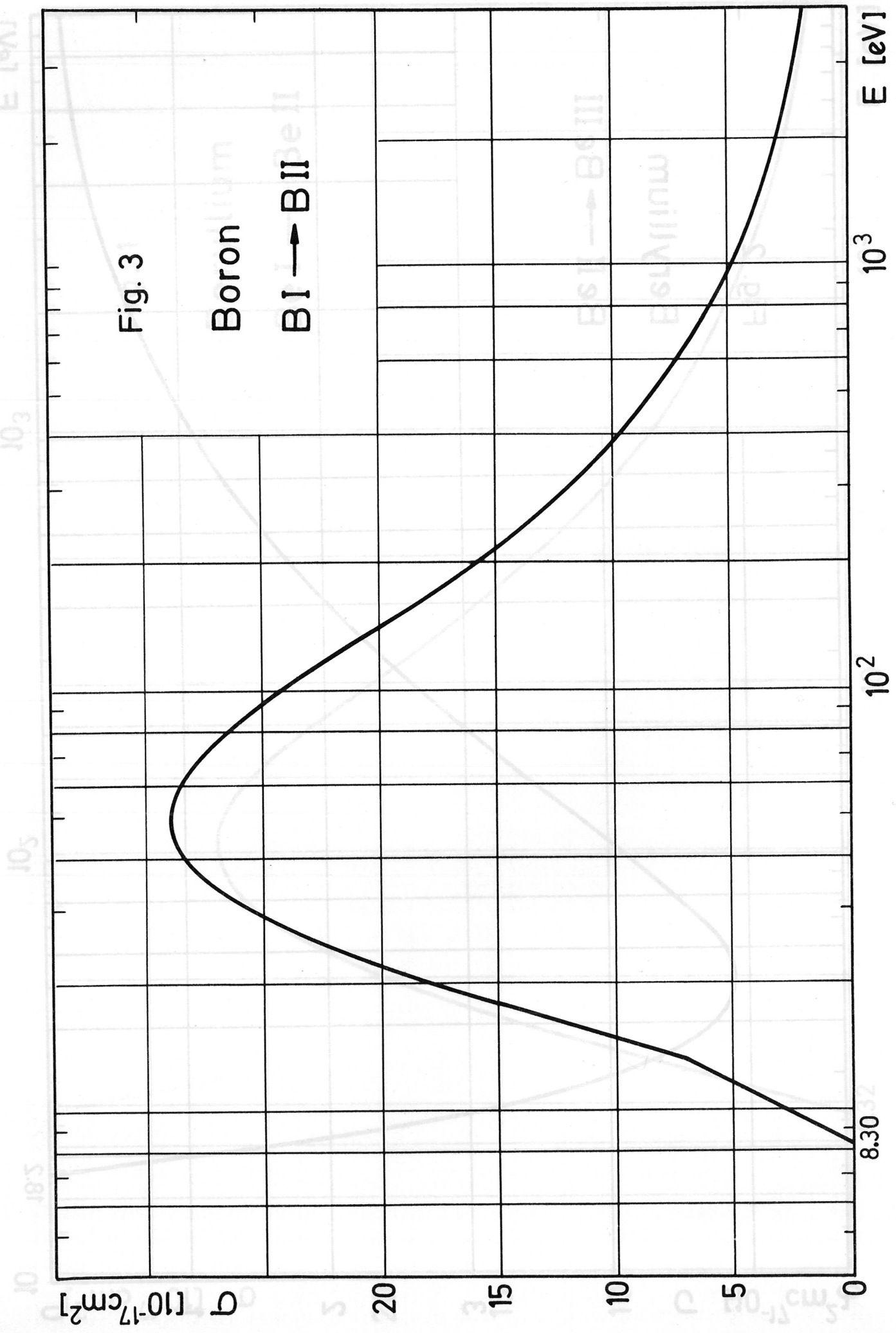


Fig. 3

Boron
BI \rightarrow BII



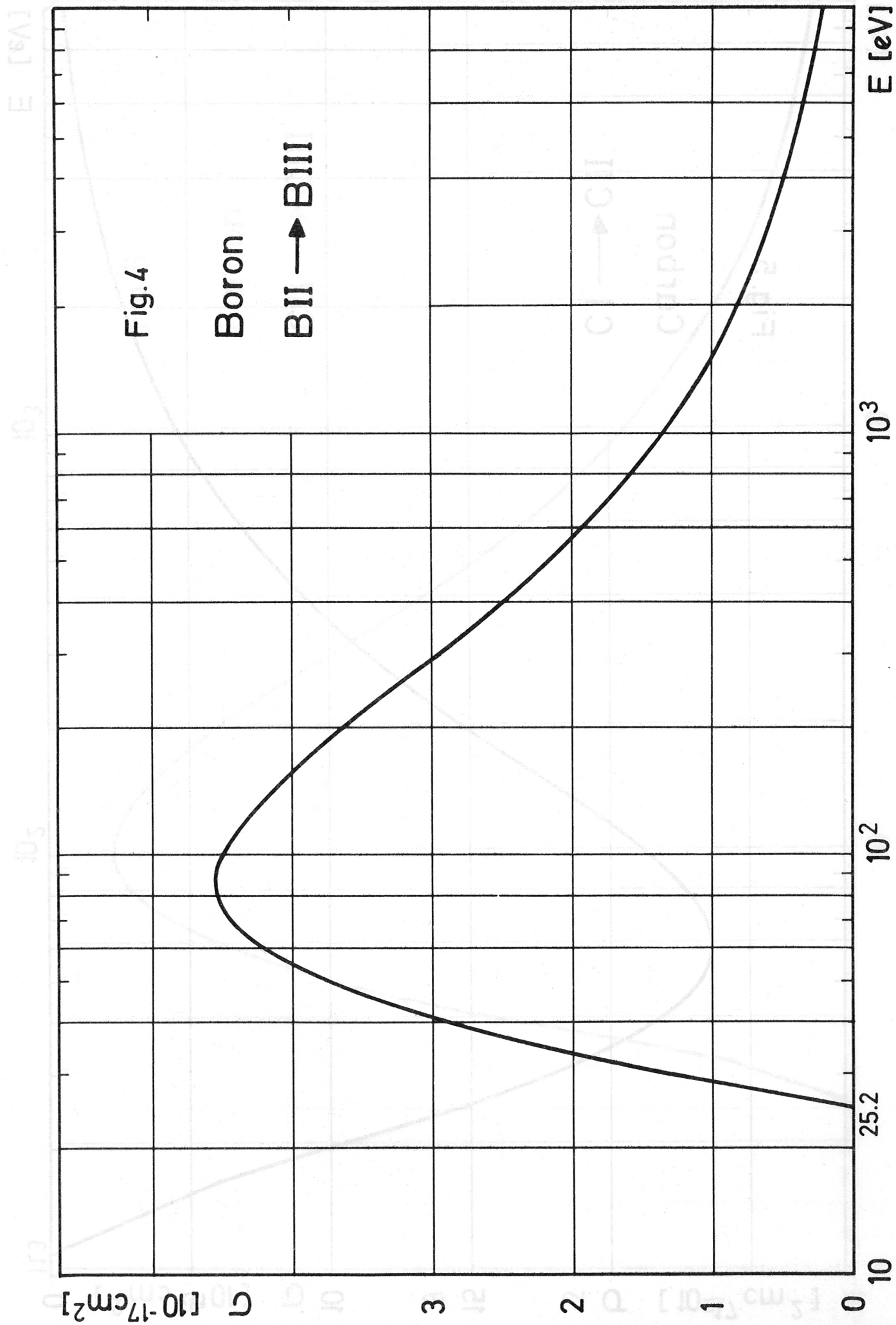
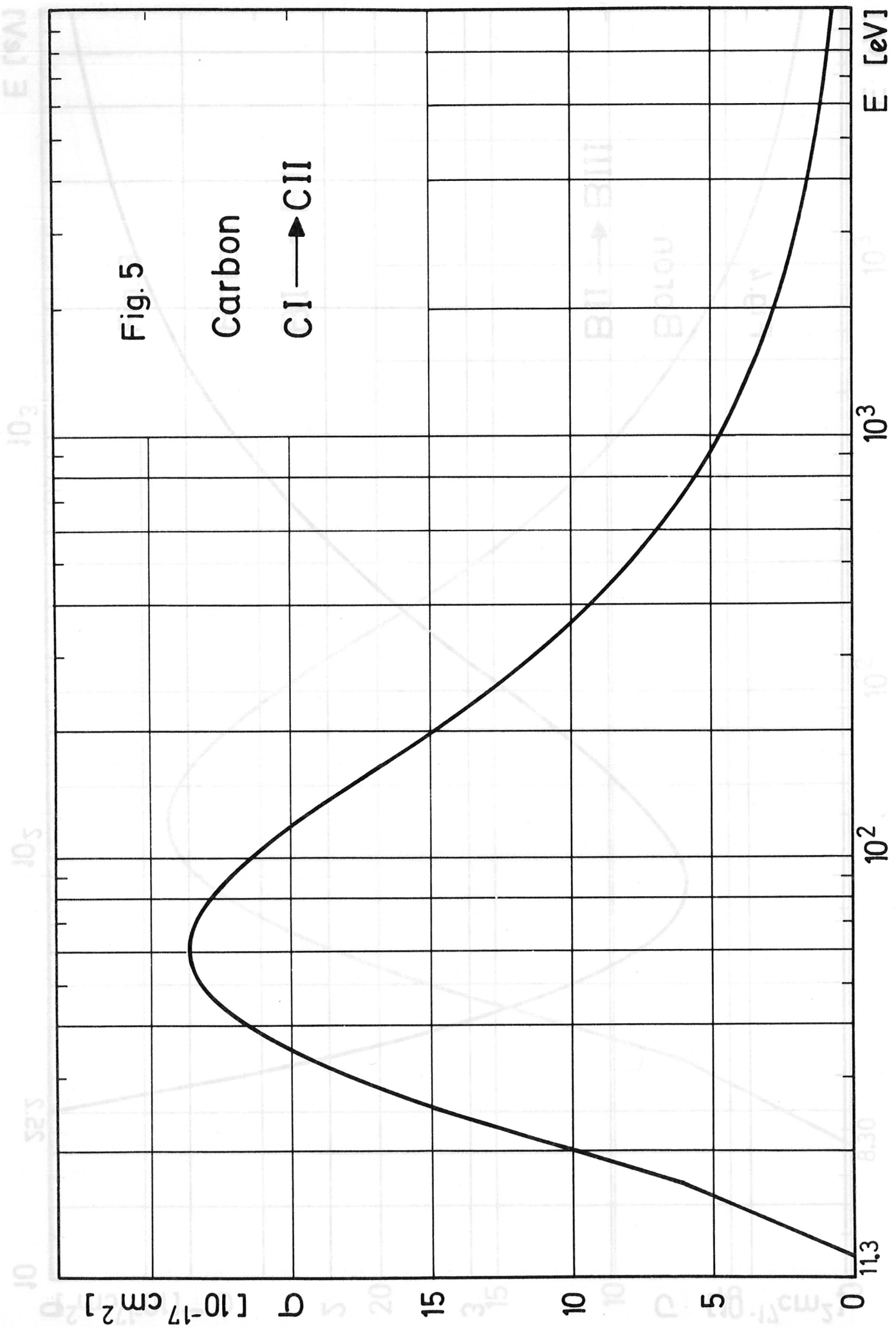


Fig. 5

Carbon

C I \rightarrow C II



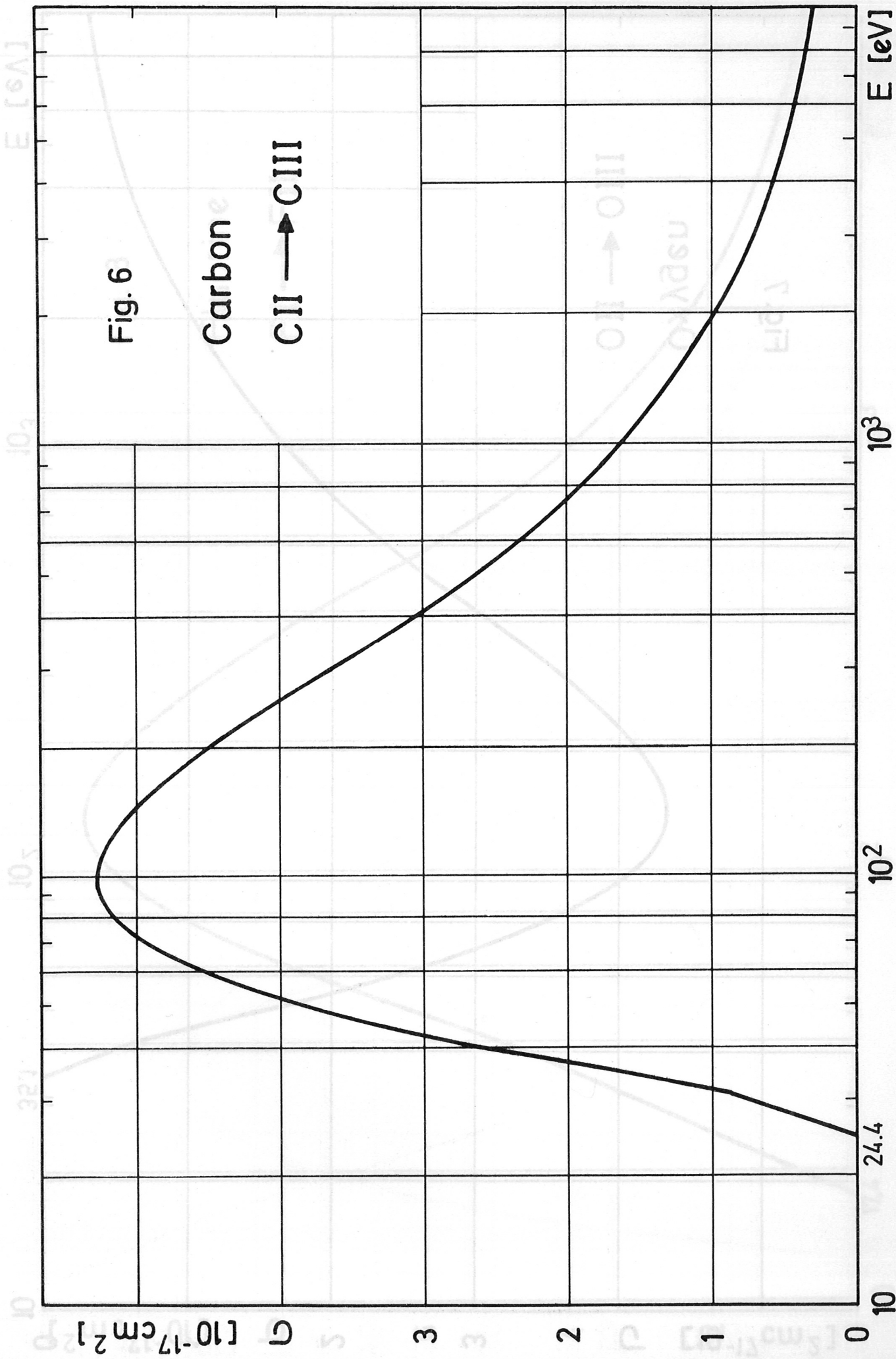
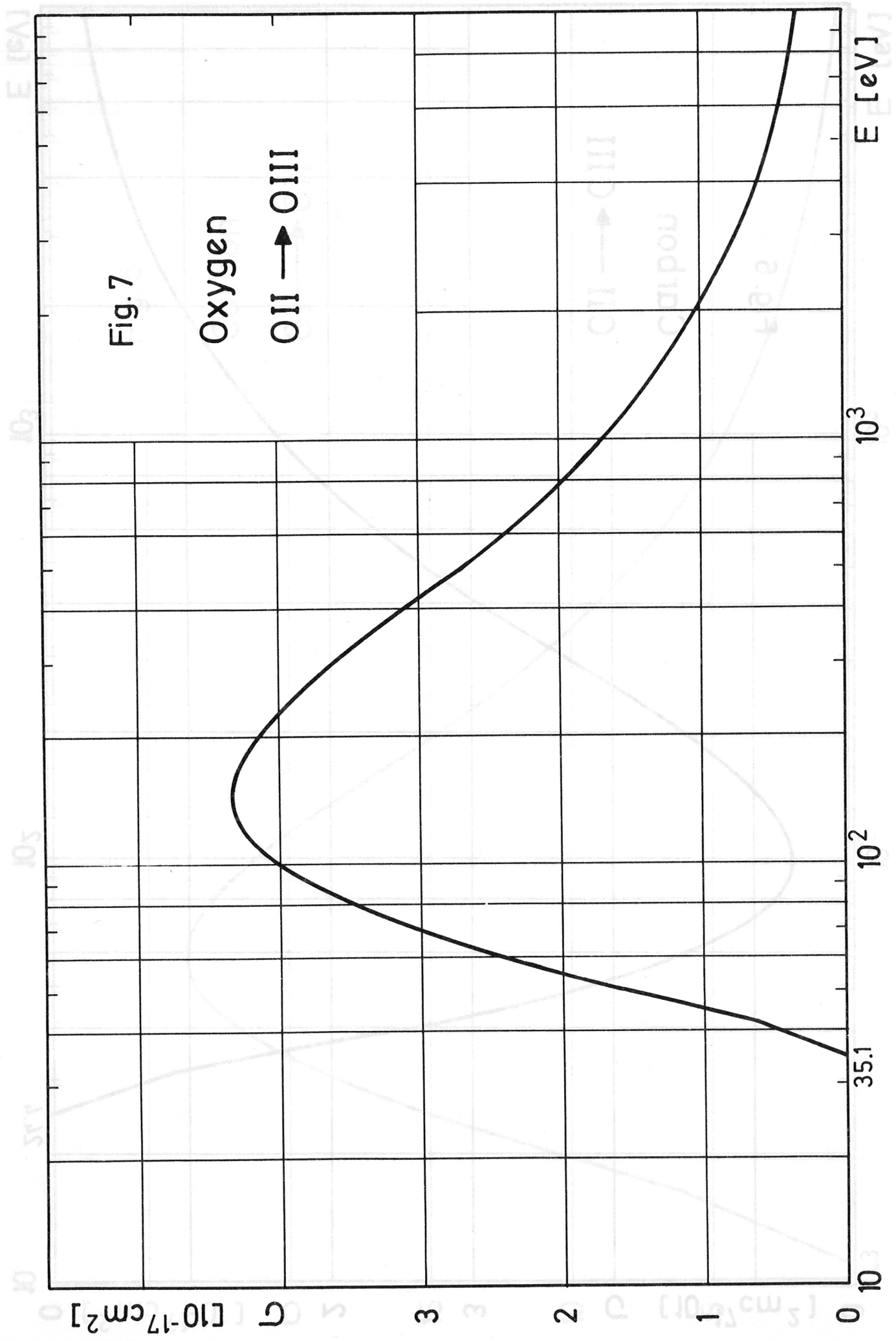


Fig.7

Oxygen
OII → OIII



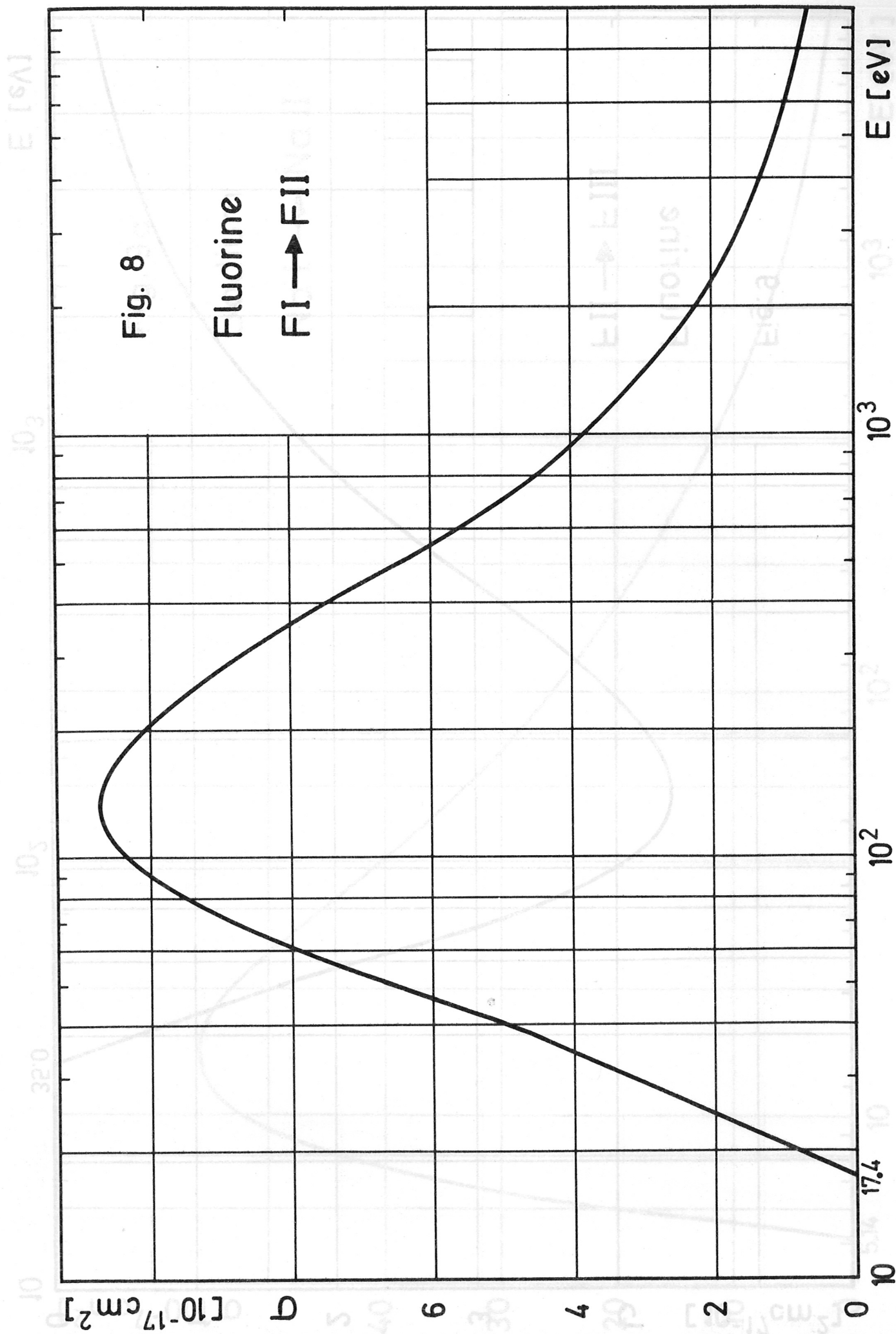
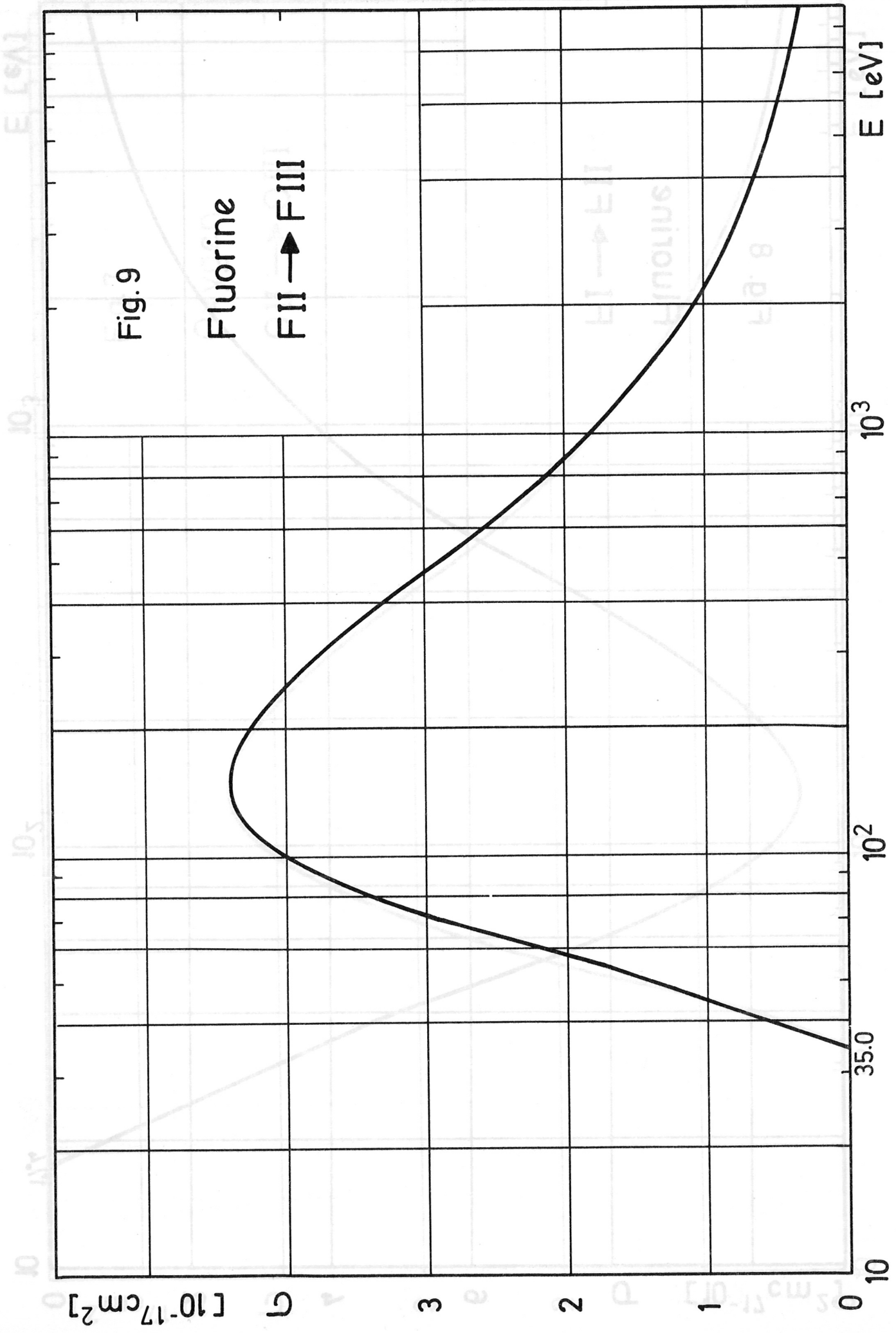


Fig. 9

Fluorine

FII → FIII



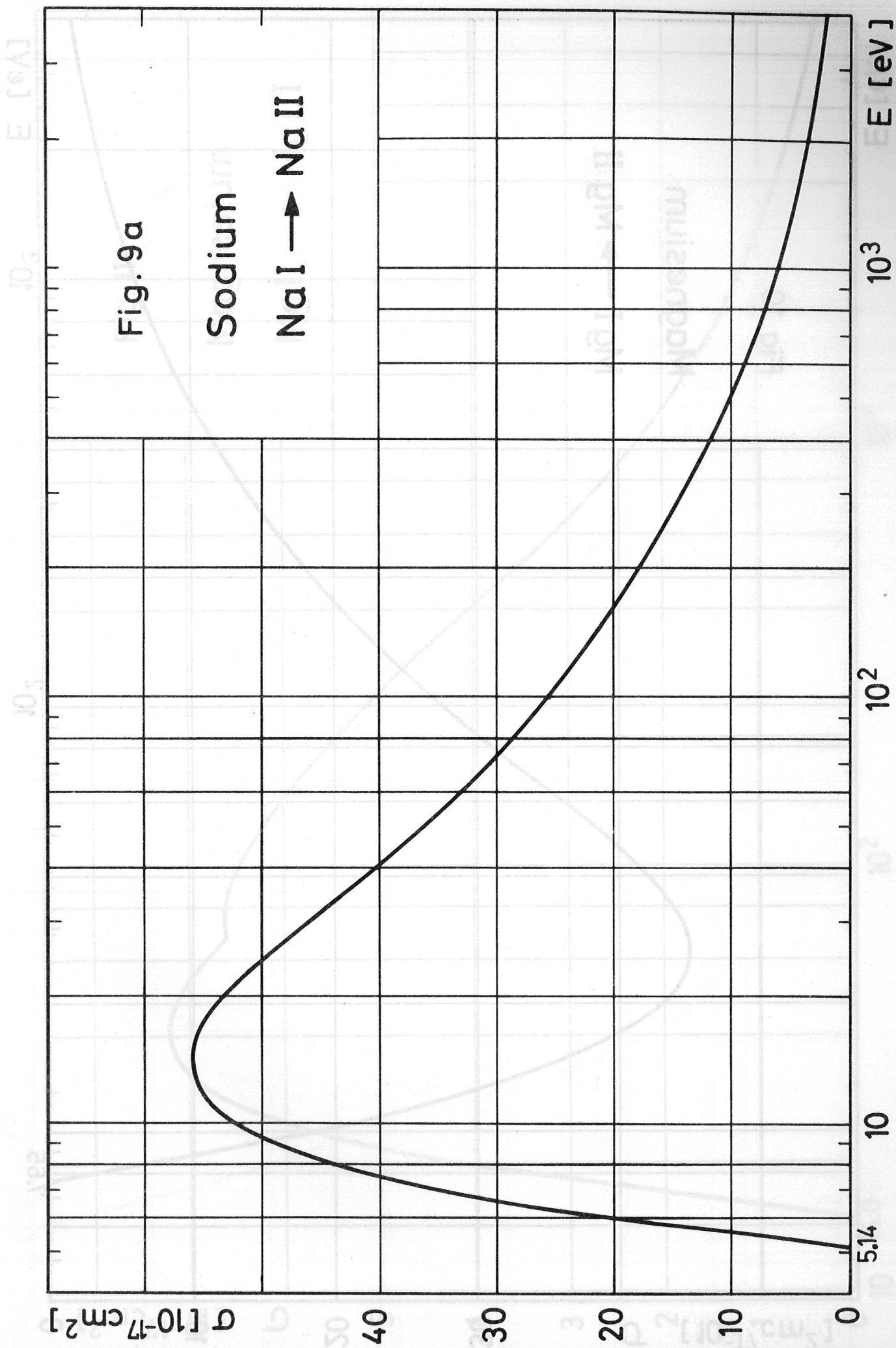
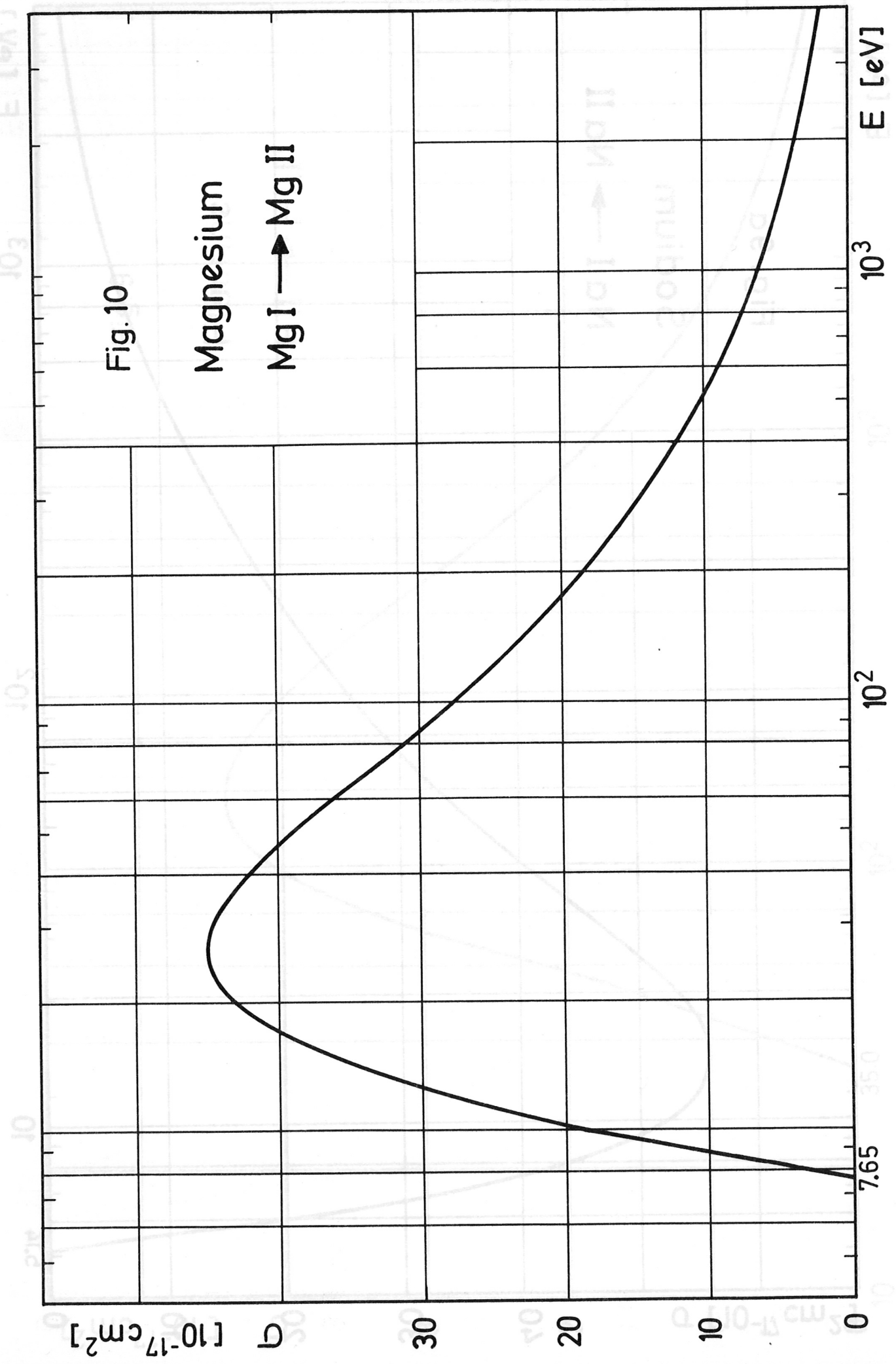


Fig. 10

Magnesium

Mg I \rightarrow Mg II



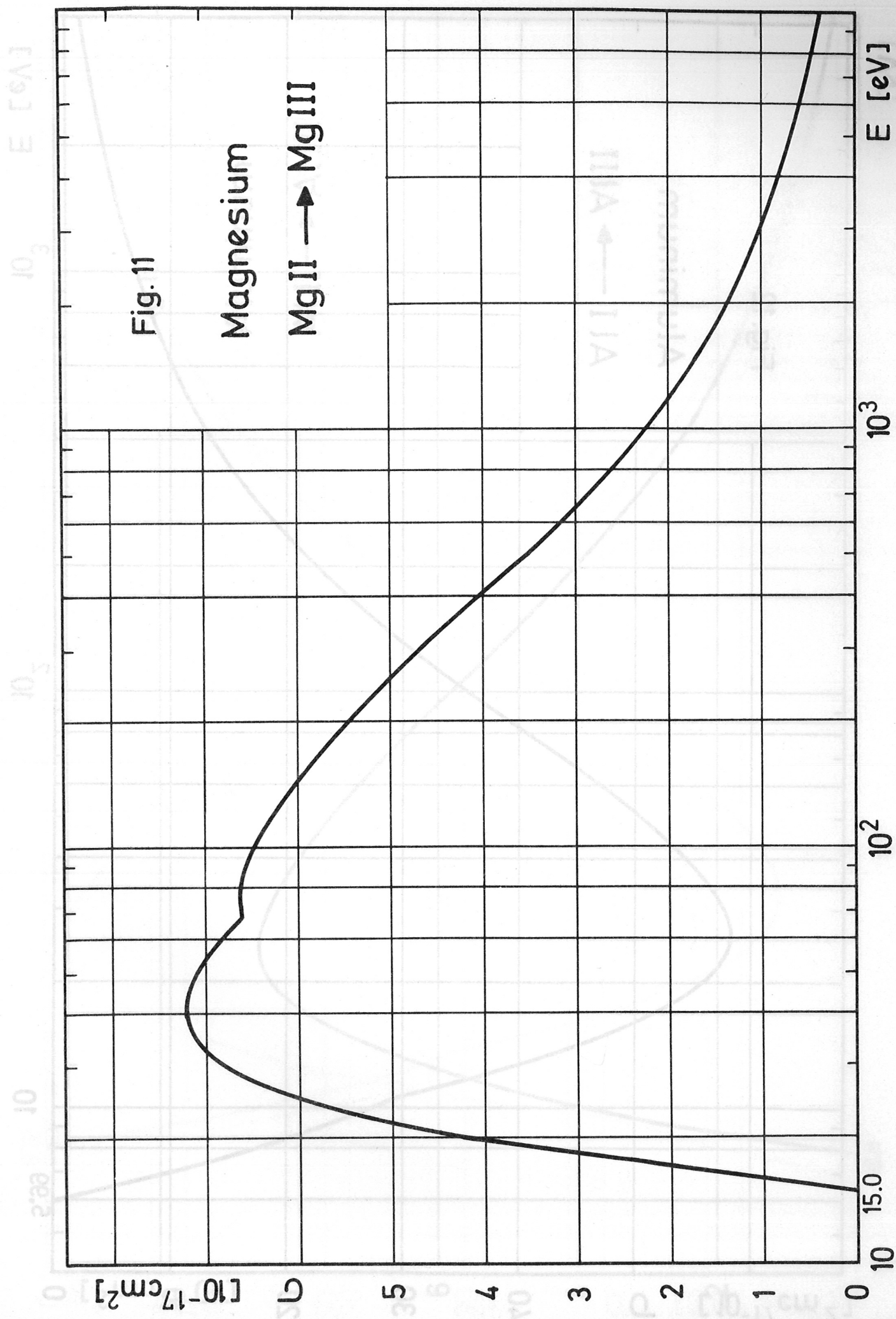
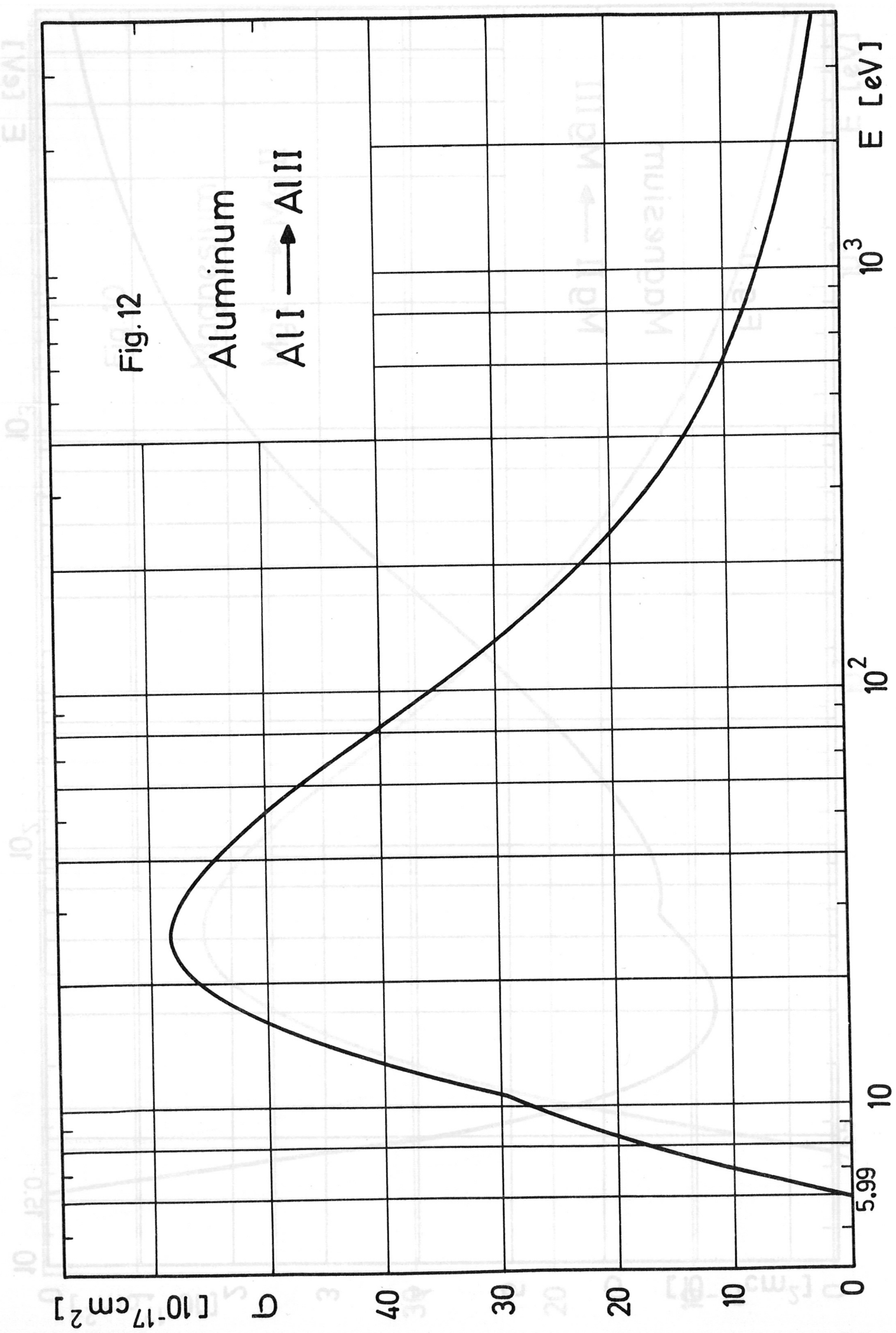
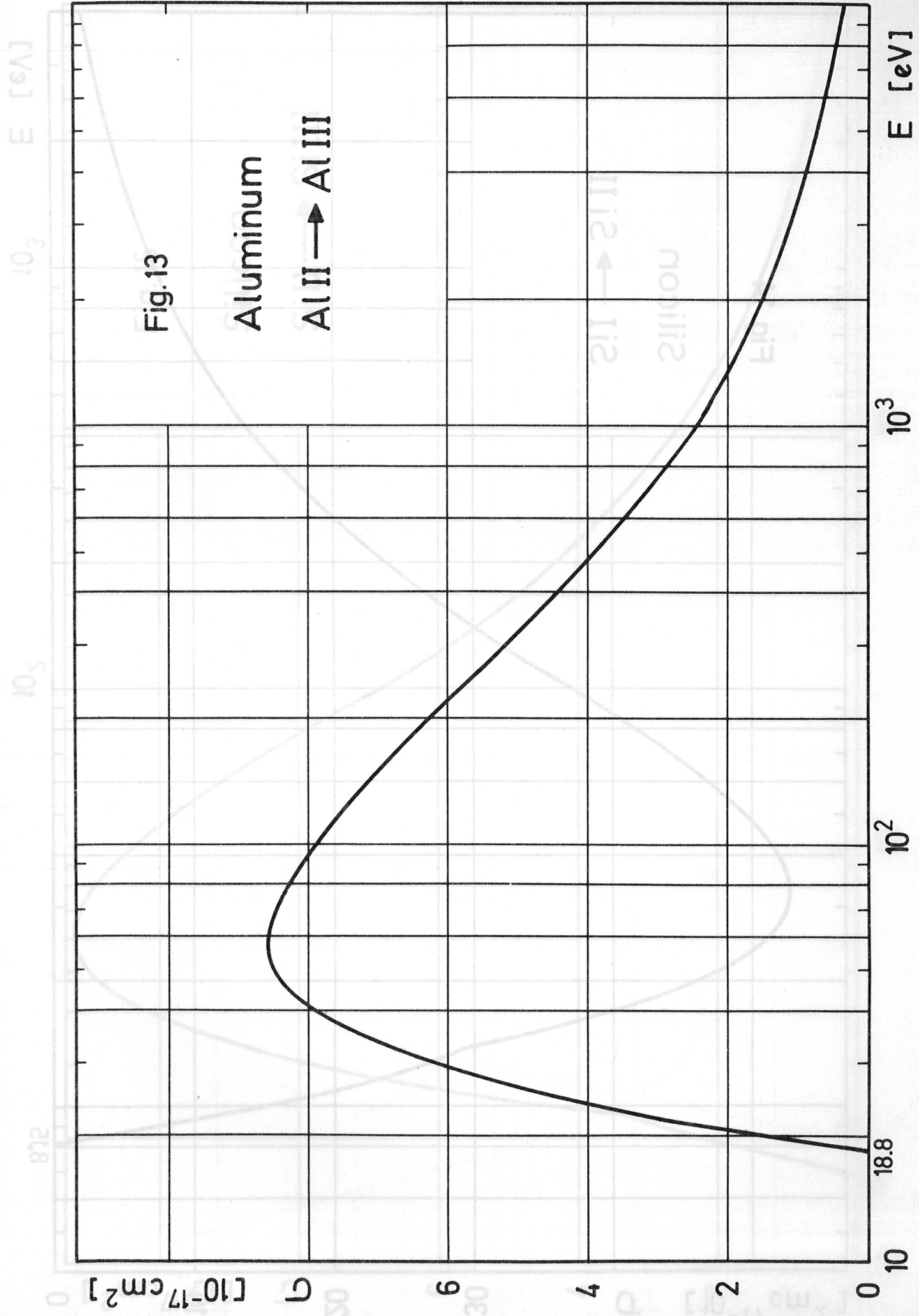


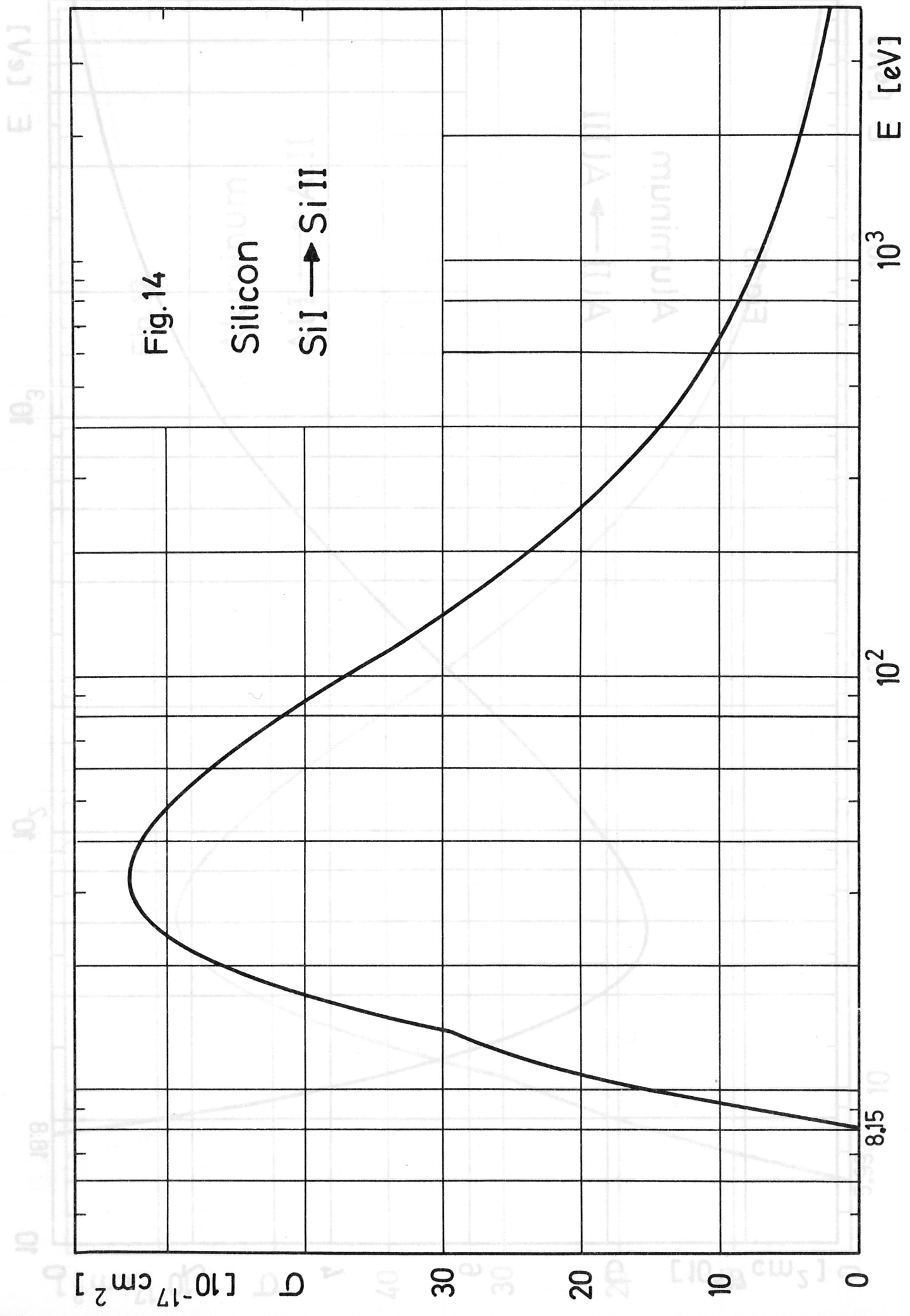
Fig. 12

Aluminum

AlI \rightarrow AlIII







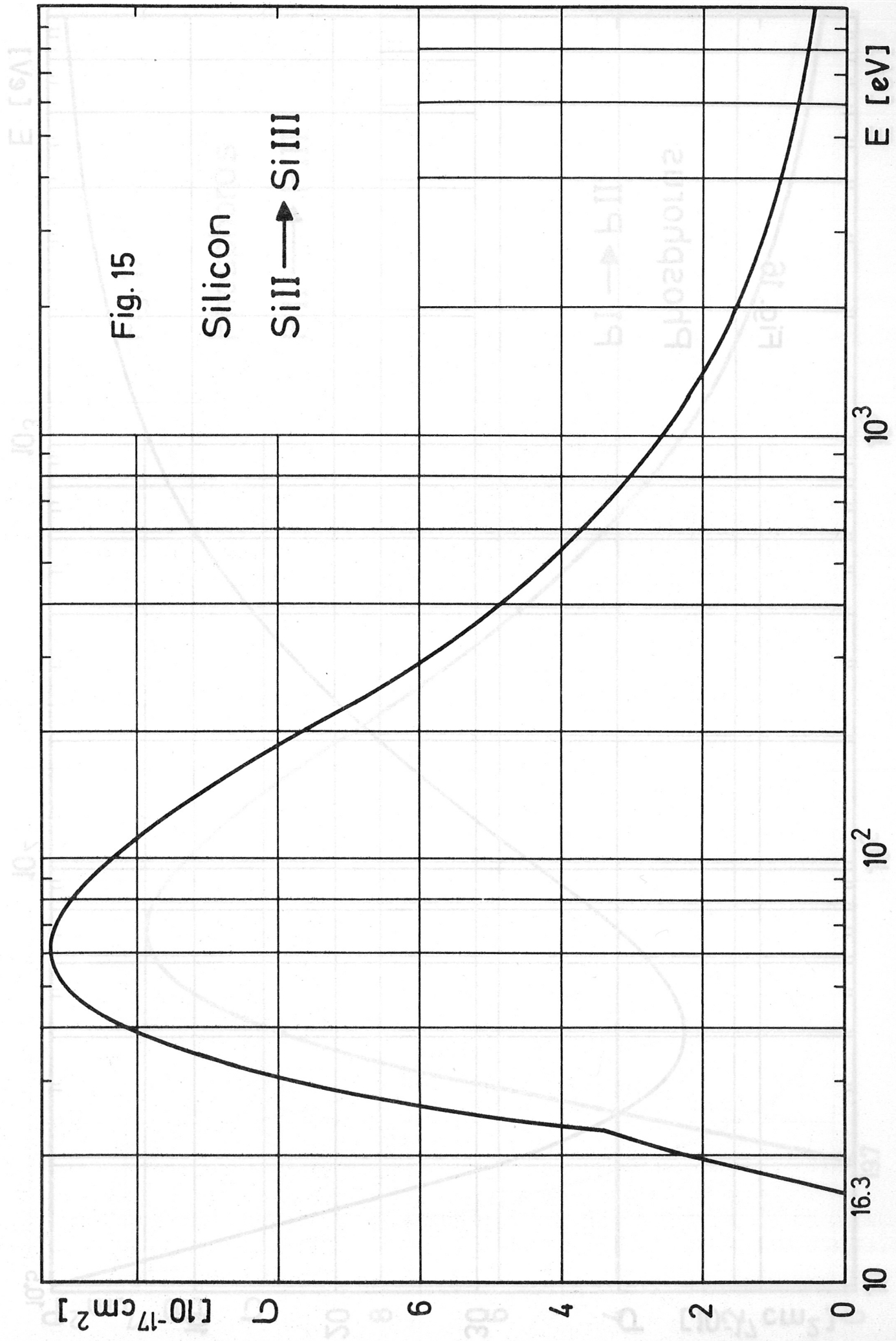
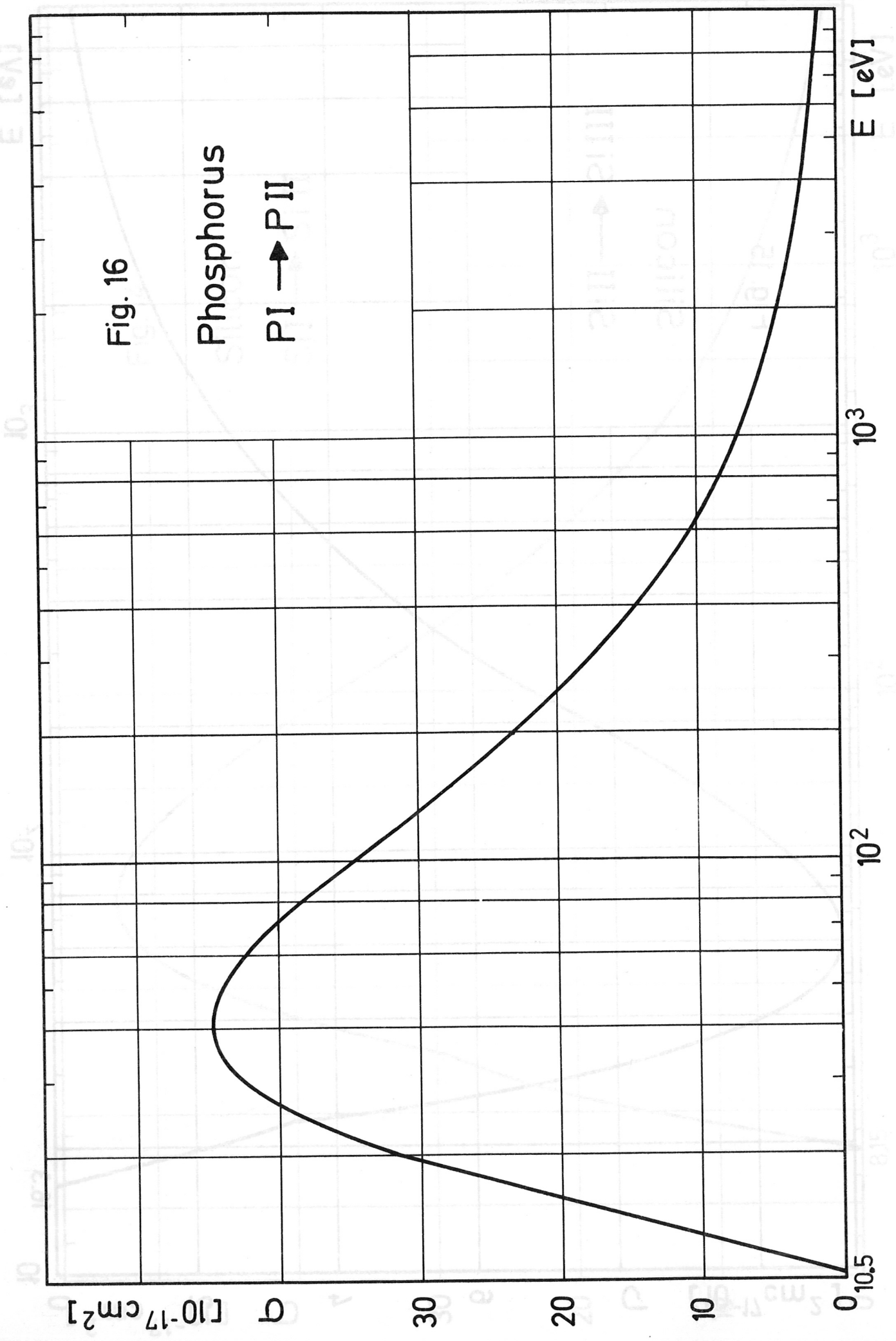


Fig. 16

Phosphorus

PI \rightarrow PII



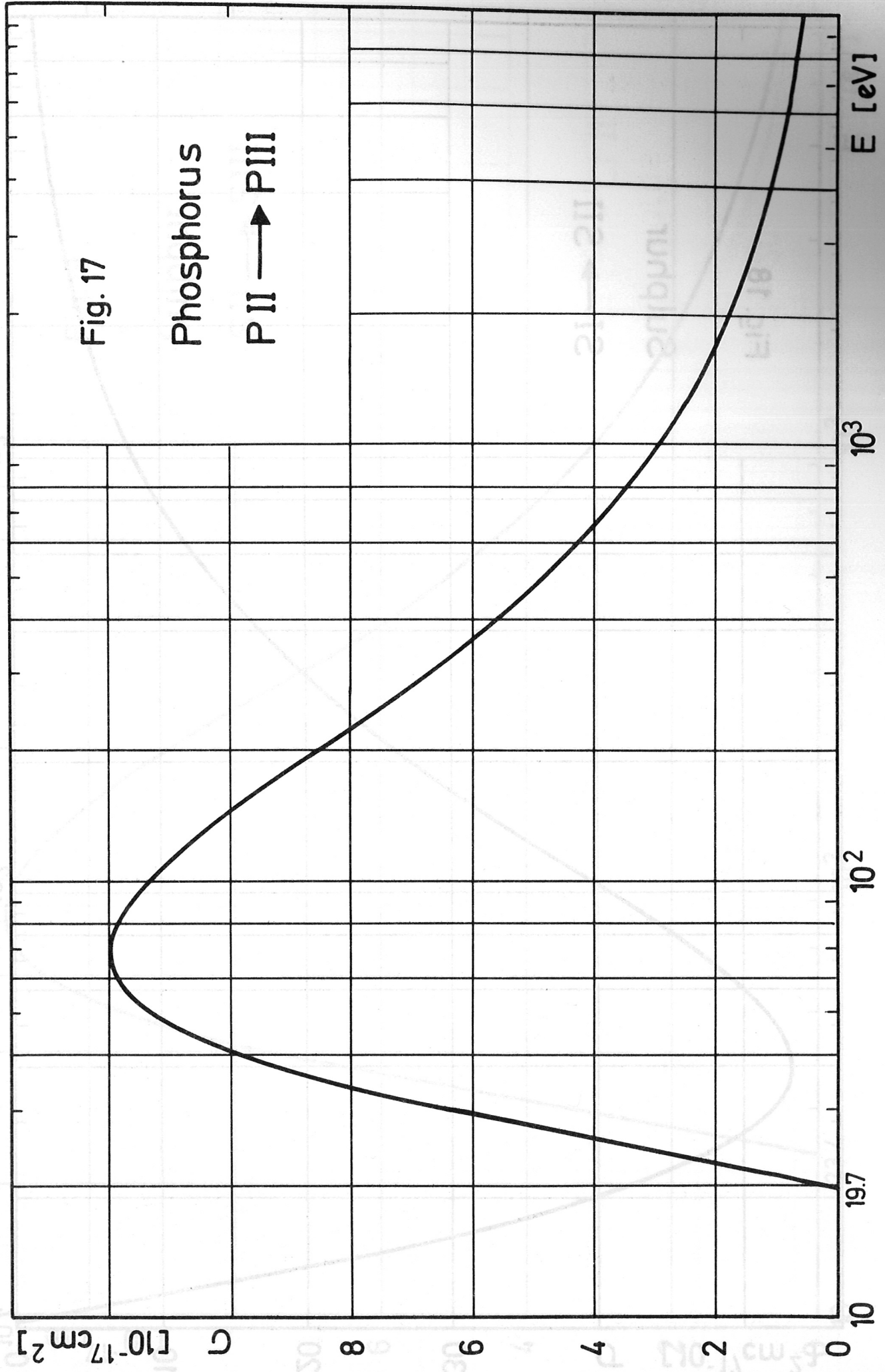


Fig. 17

Phosphorus
P II \rightarrow P III

Fig. 18

Sulphur
SI → SII

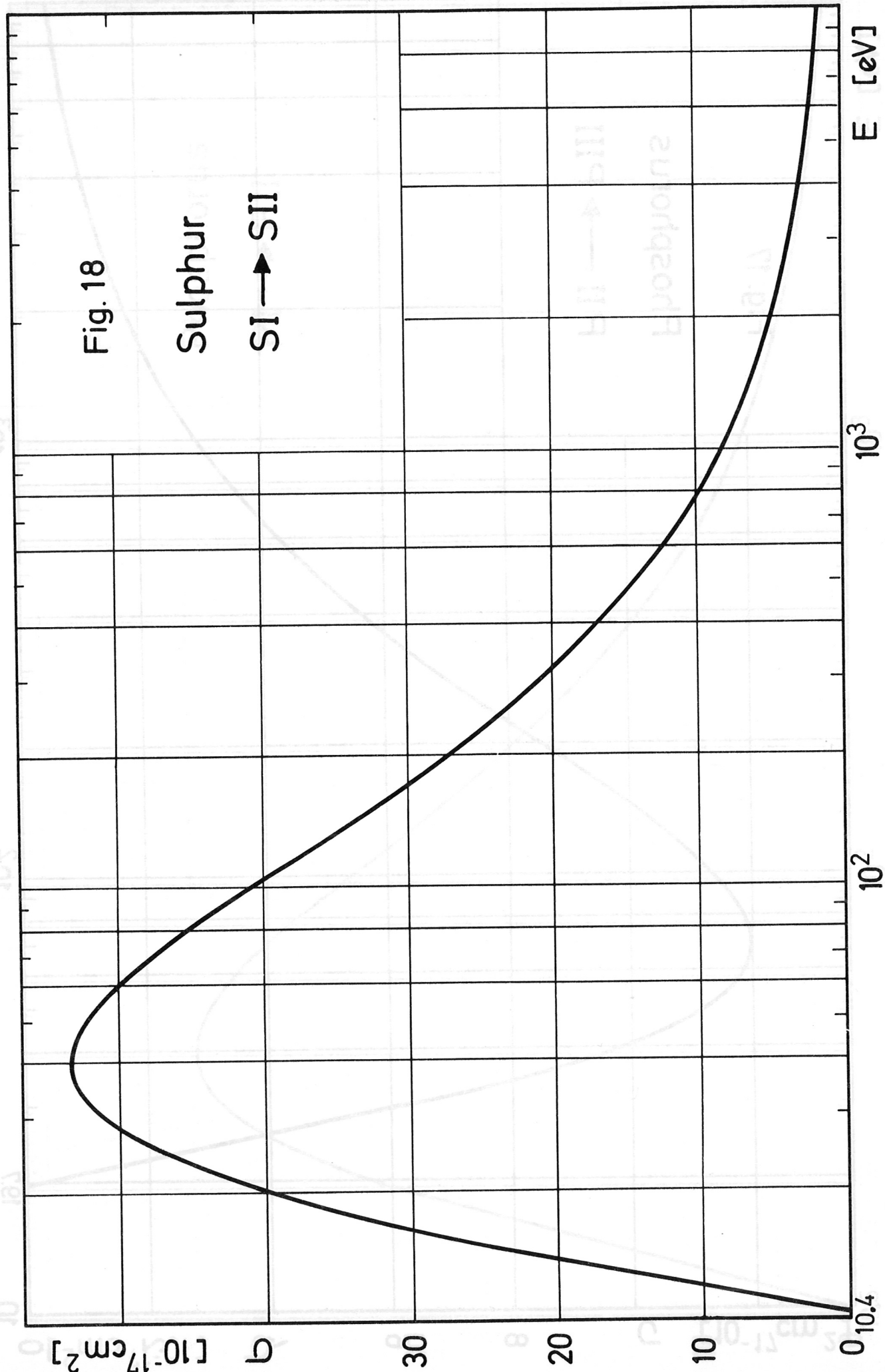


Fig. 19

Sulphur
SII → SIII

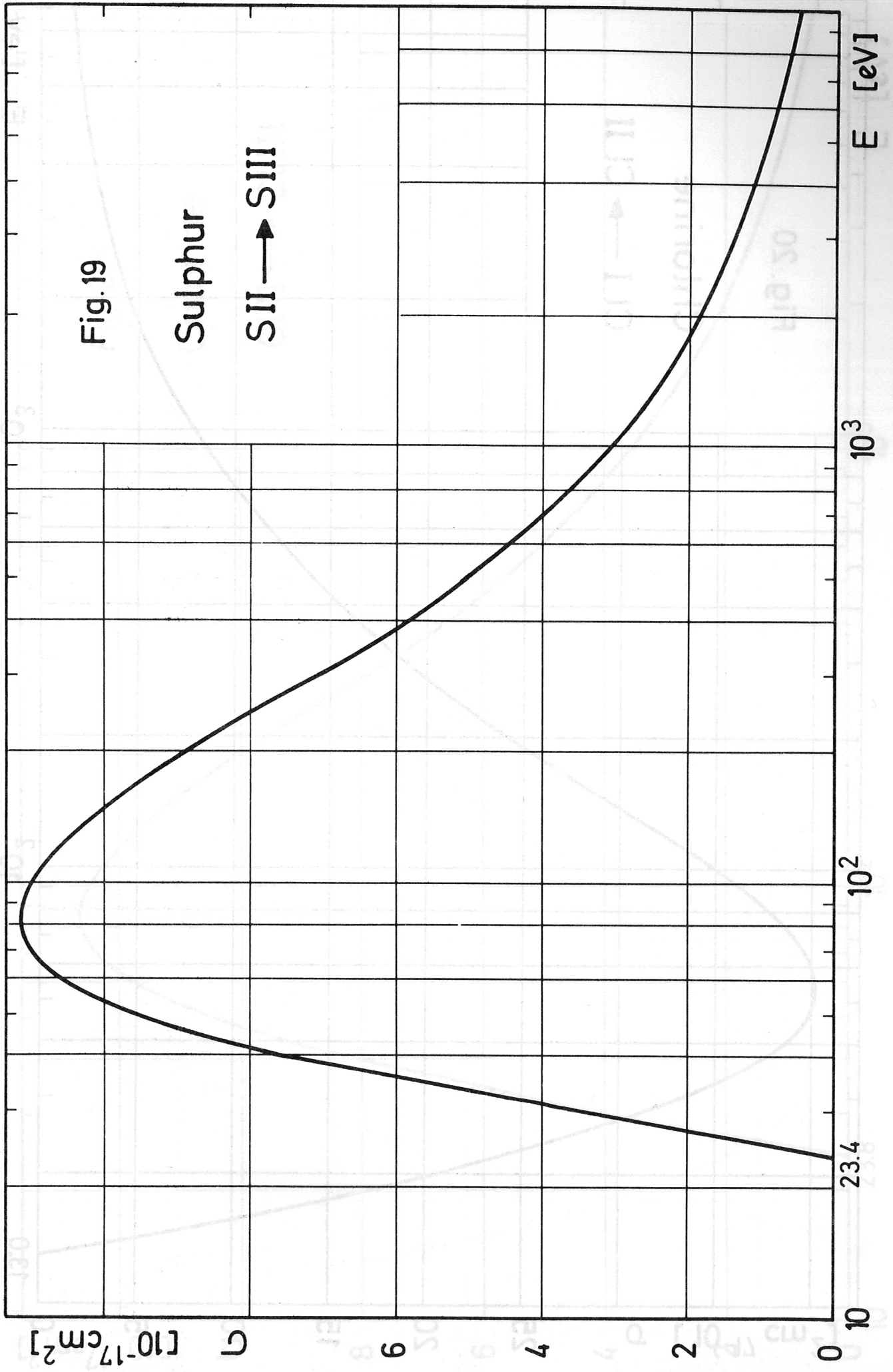
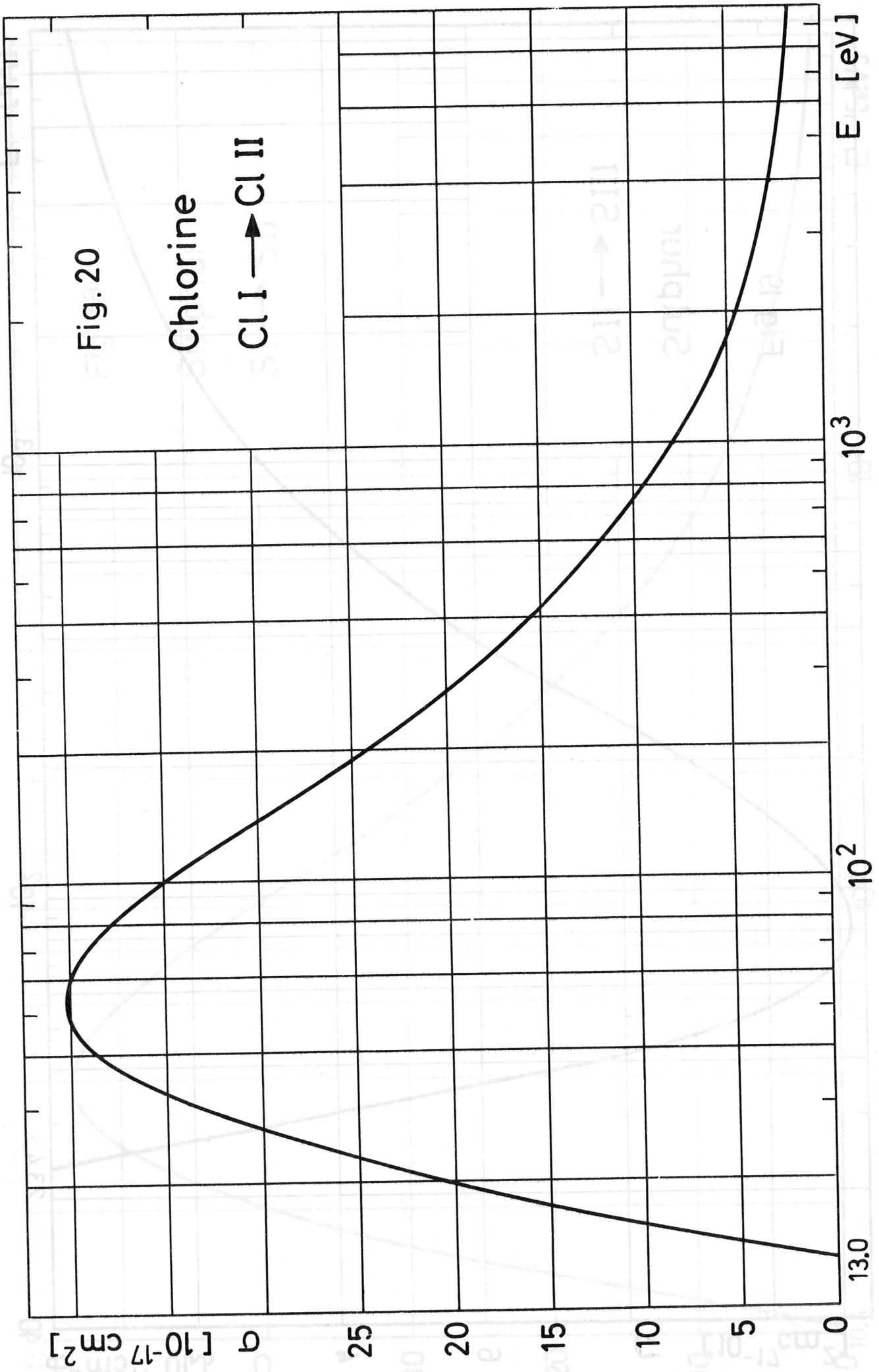


Fig. 20

Chlorine
 $\text{Cl I} \rightarrow \text{Cl II}$



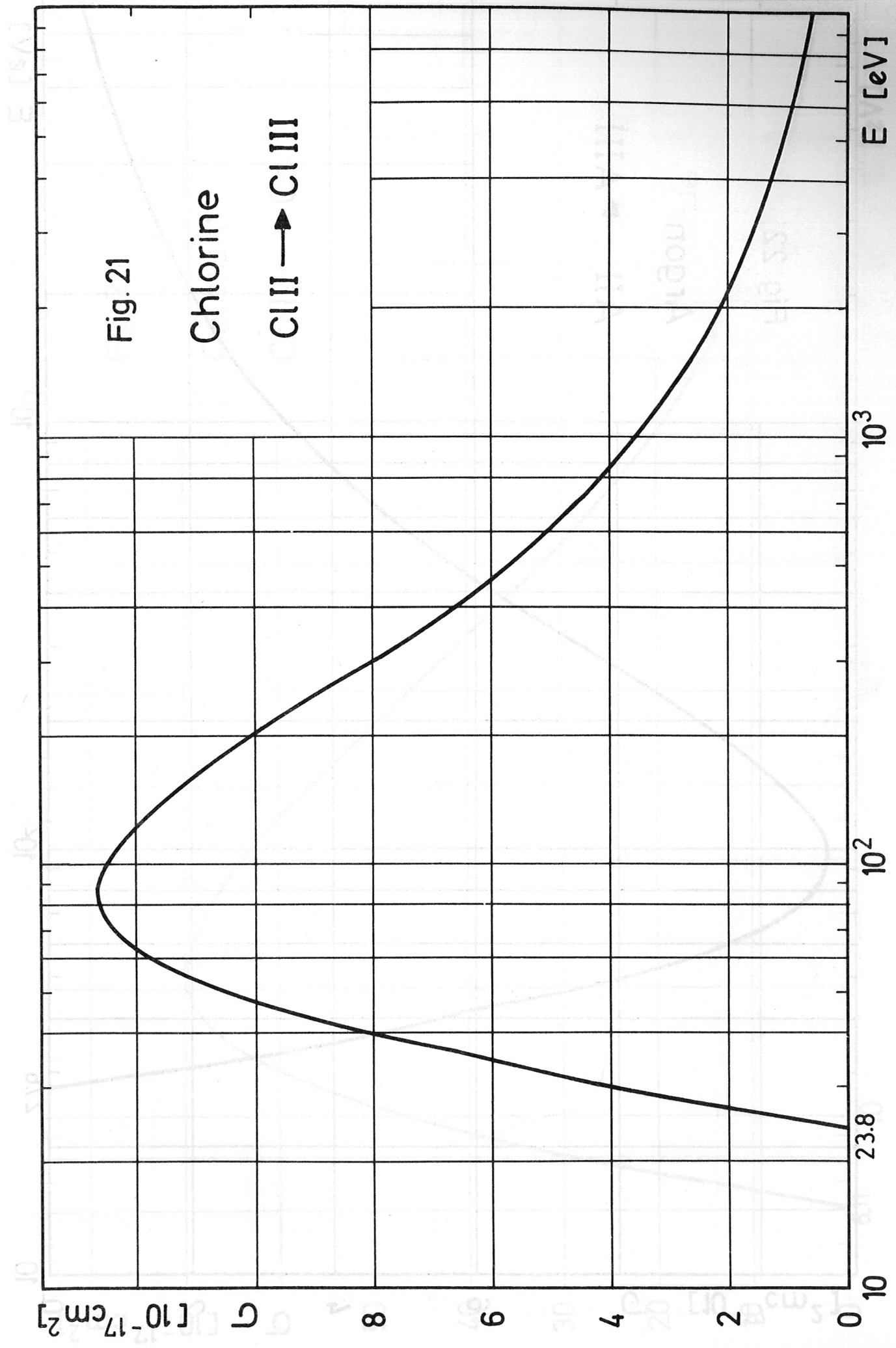


Fig. 22

Argon

AII \rightarrow AIII

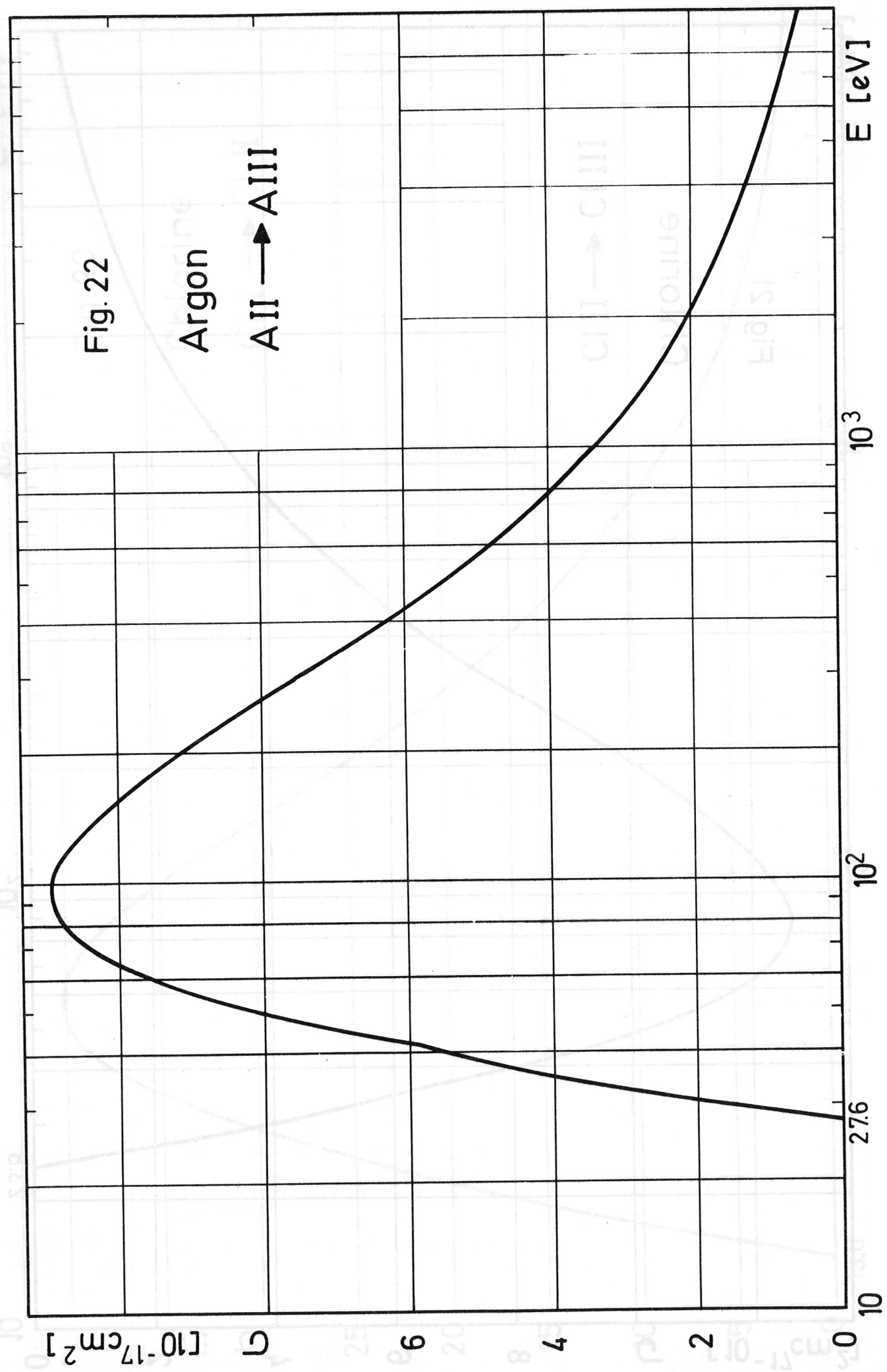


Fig. 23

Calcium

Ca I \rightarrow Ca II

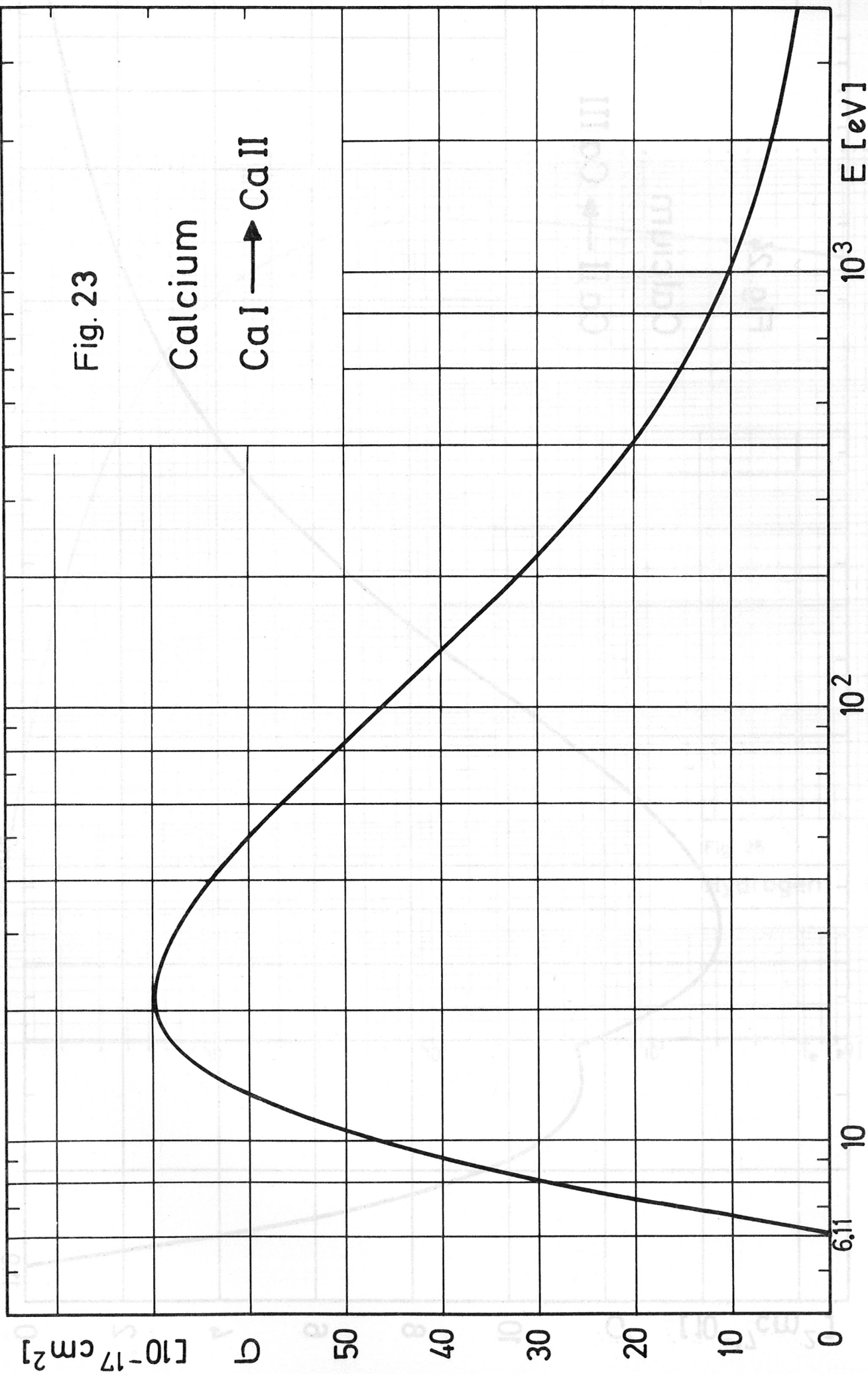
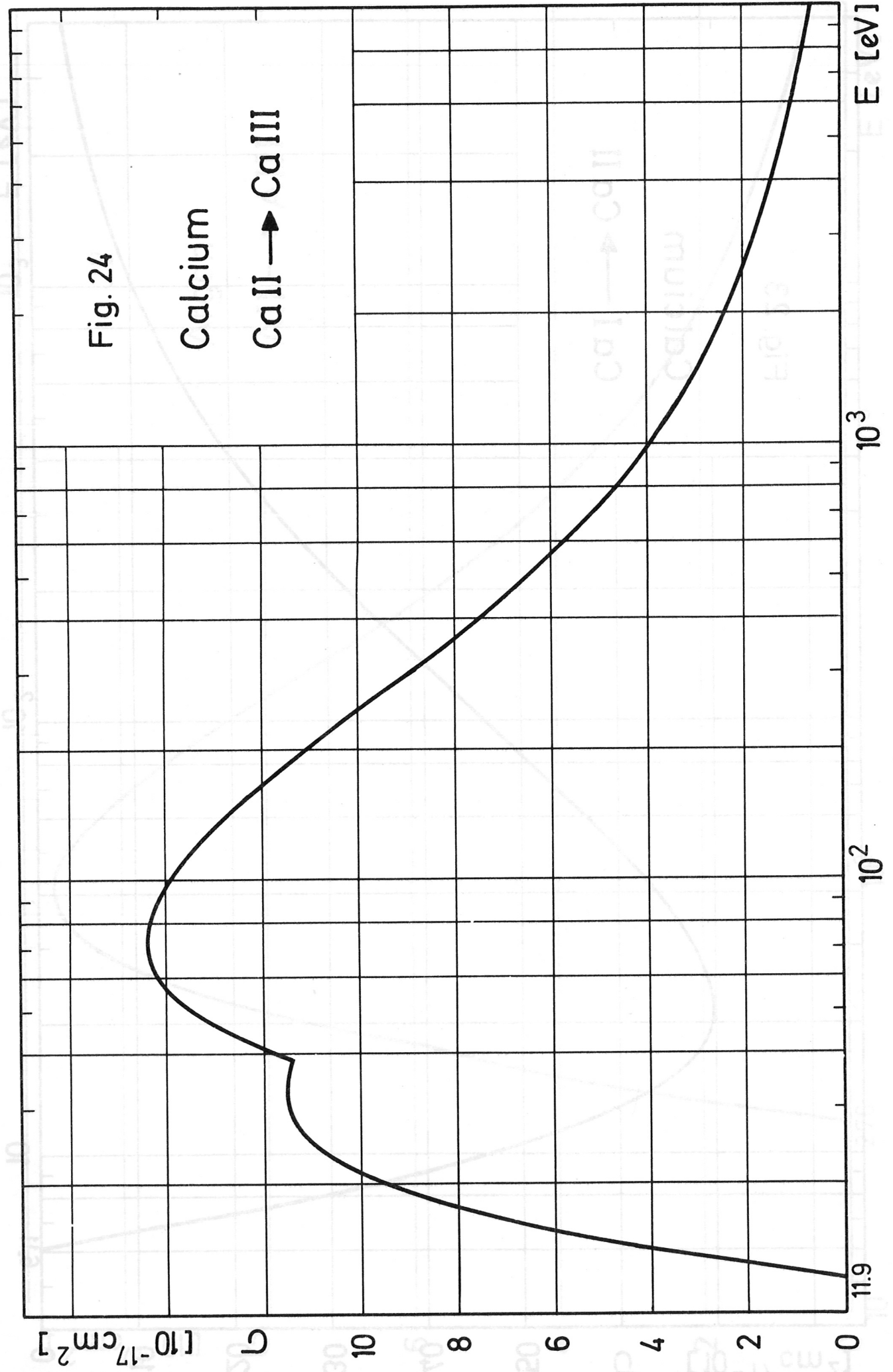


Fig. 24

Calcium

Ca II \rightarrow Ca III



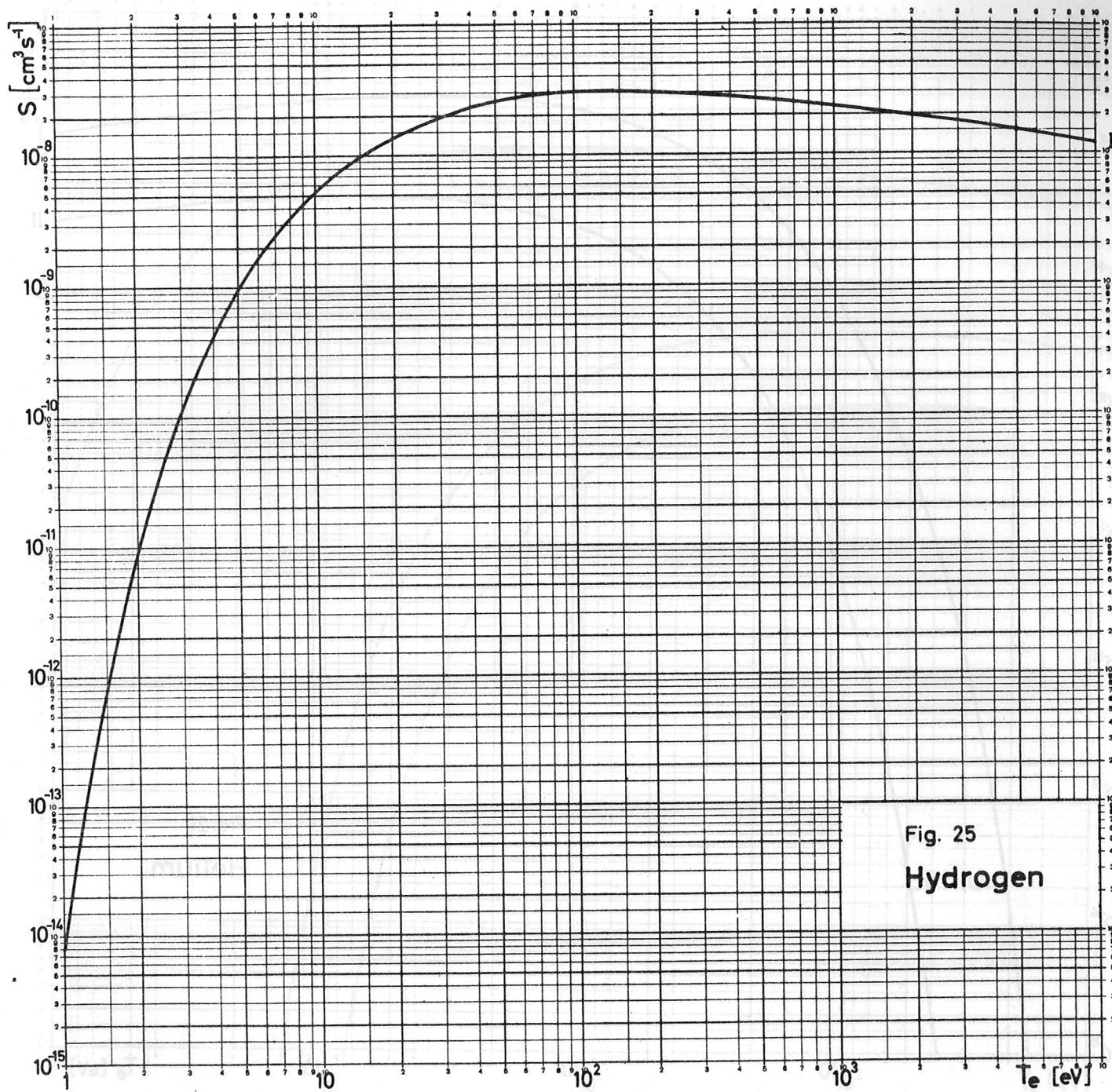


Fig. 25
Hydrogen

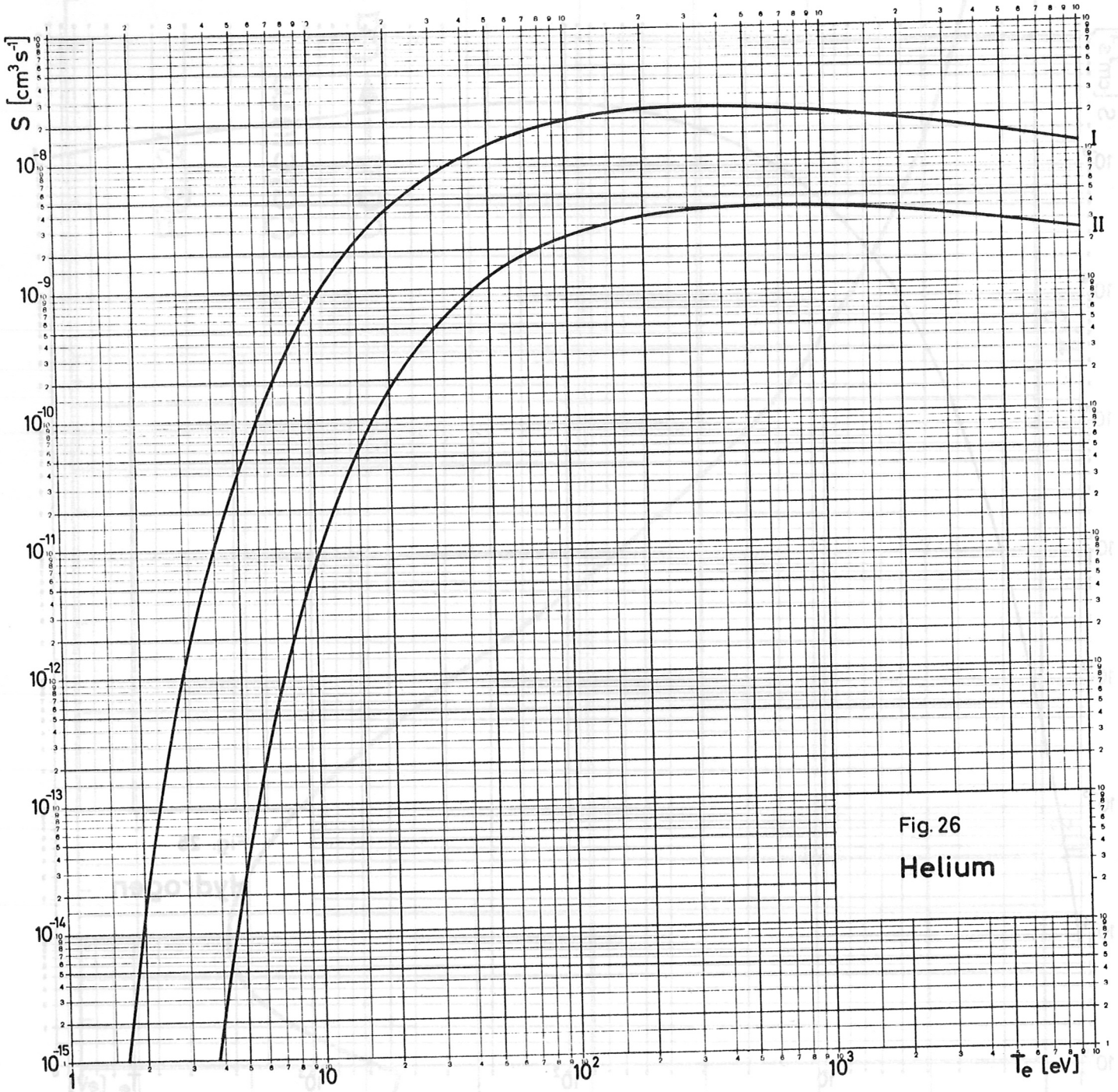


Fig 26
Helium

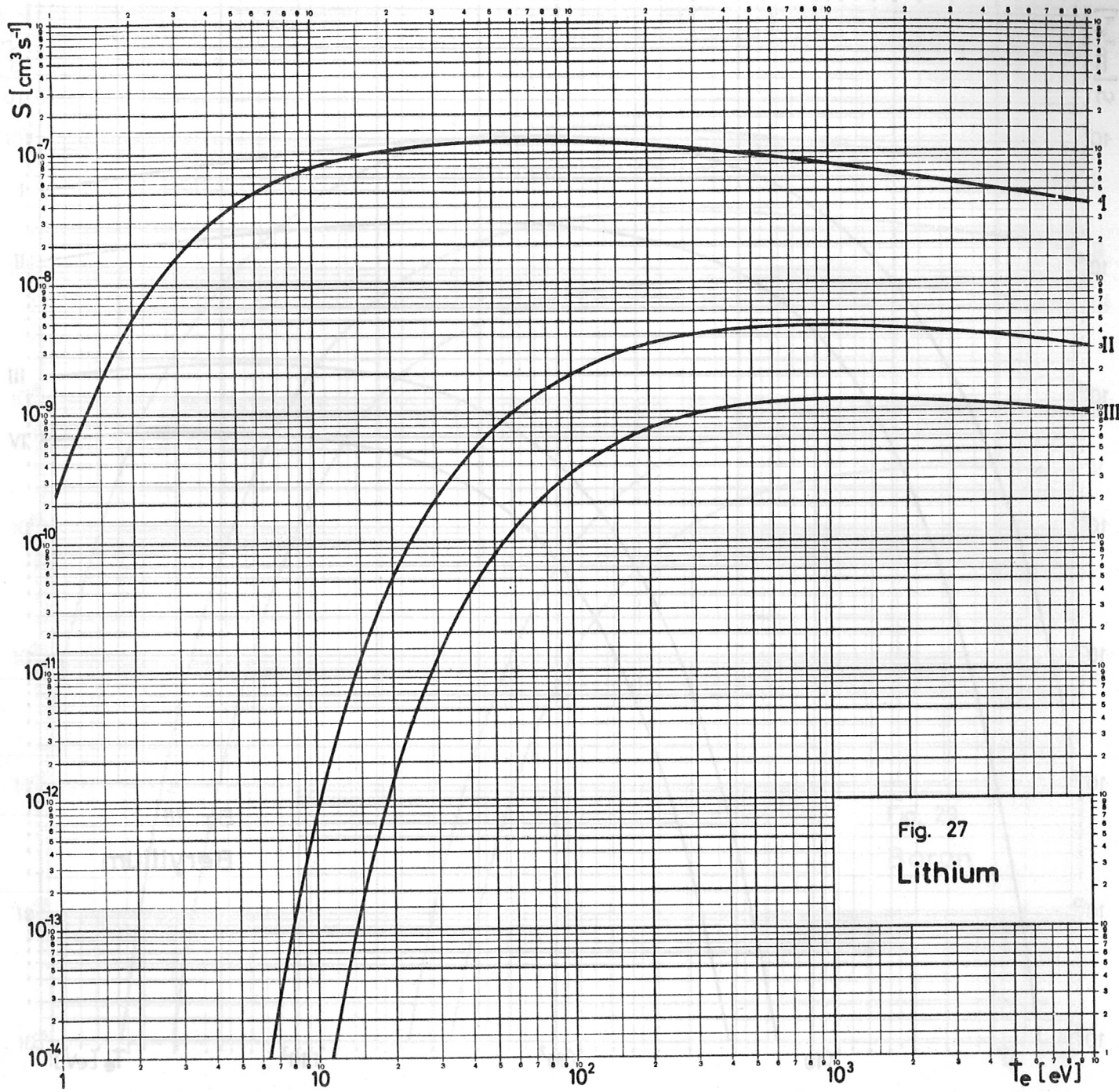


Fig. 27
Lithium

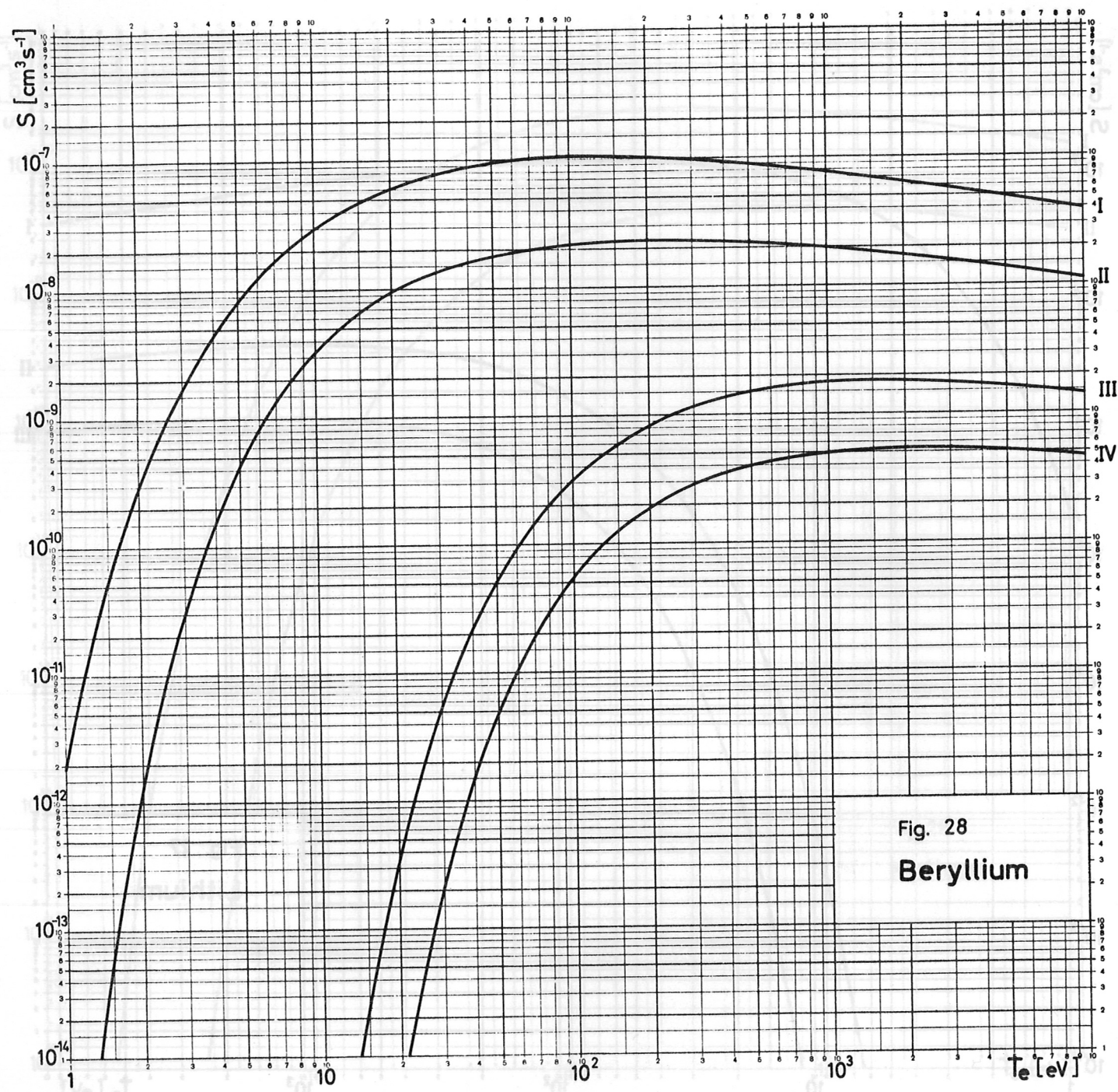


Fig. 28
Beryllium

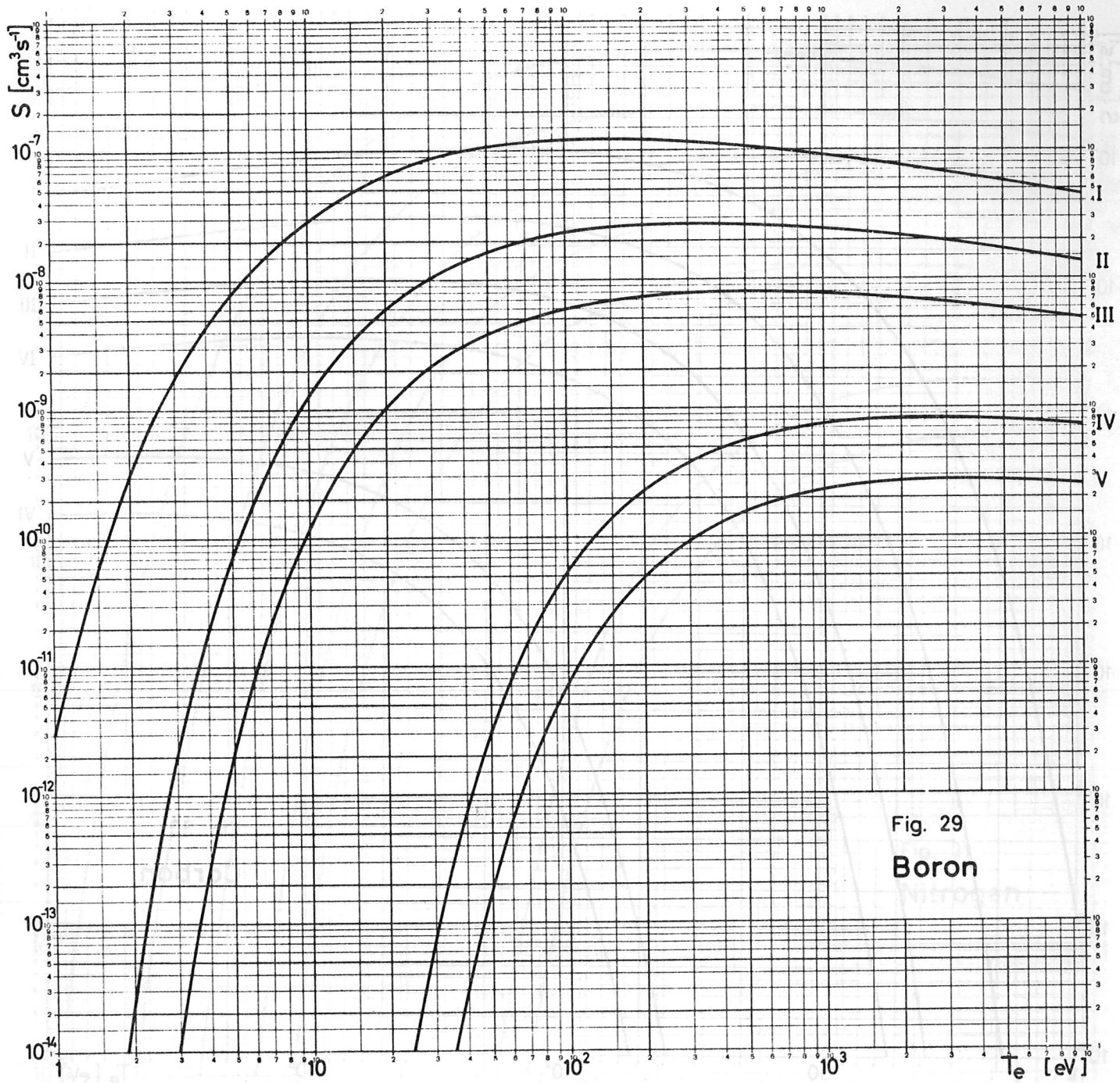


Fig. 29
Boron

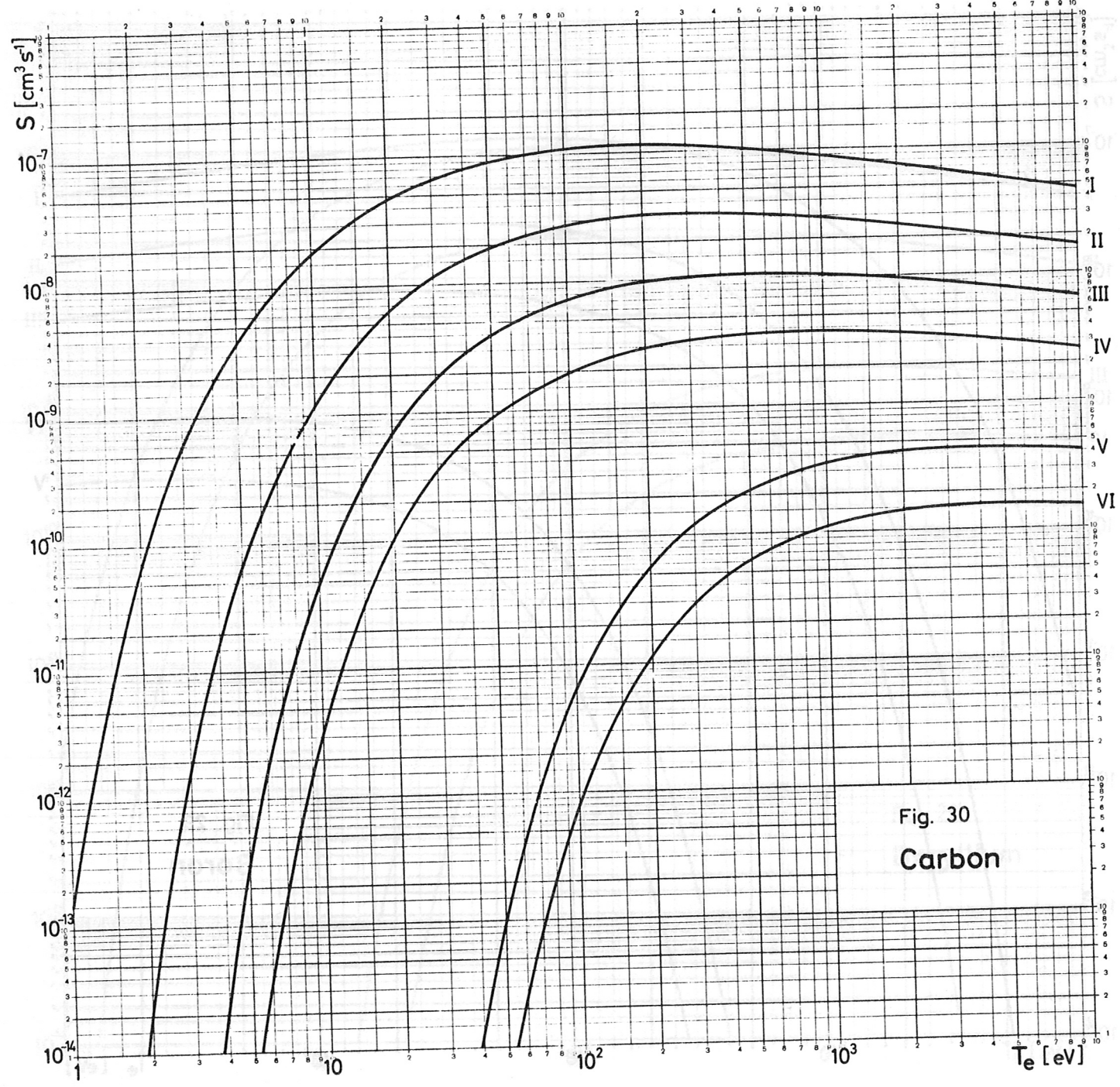


Fig. 30
Carbon

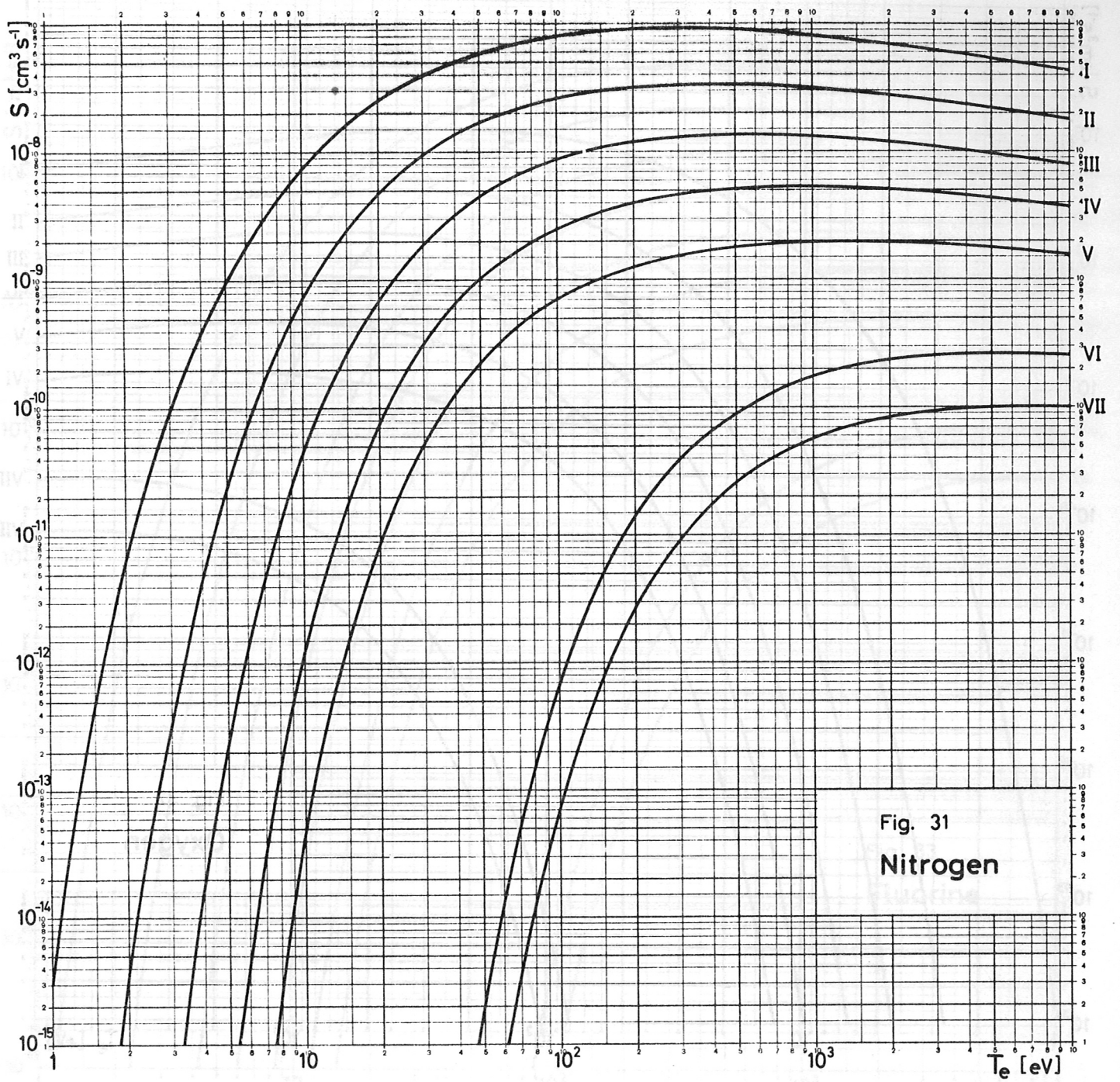


Fig. 31
Nitrogen

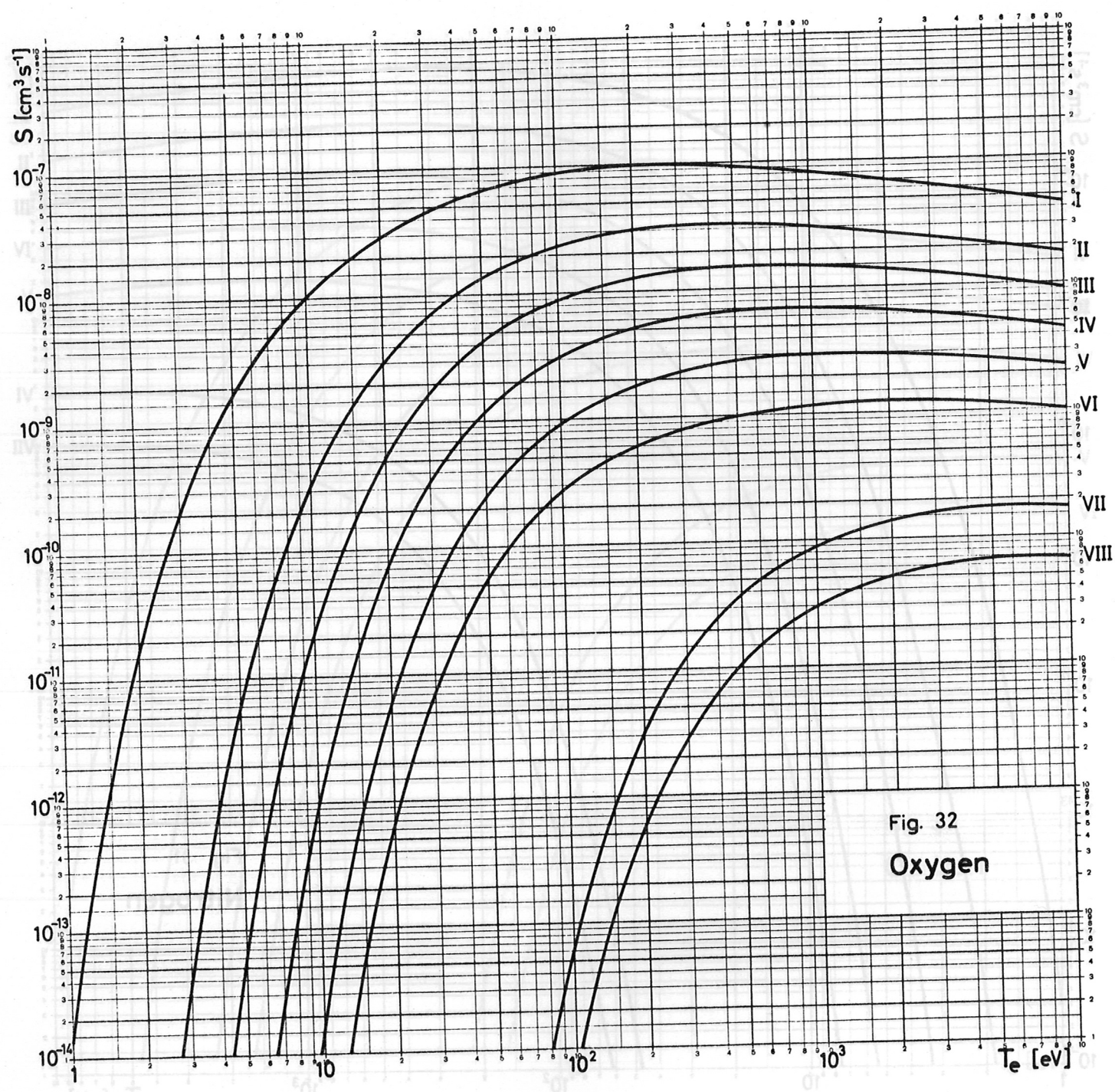


Fig. 32
Oxygen

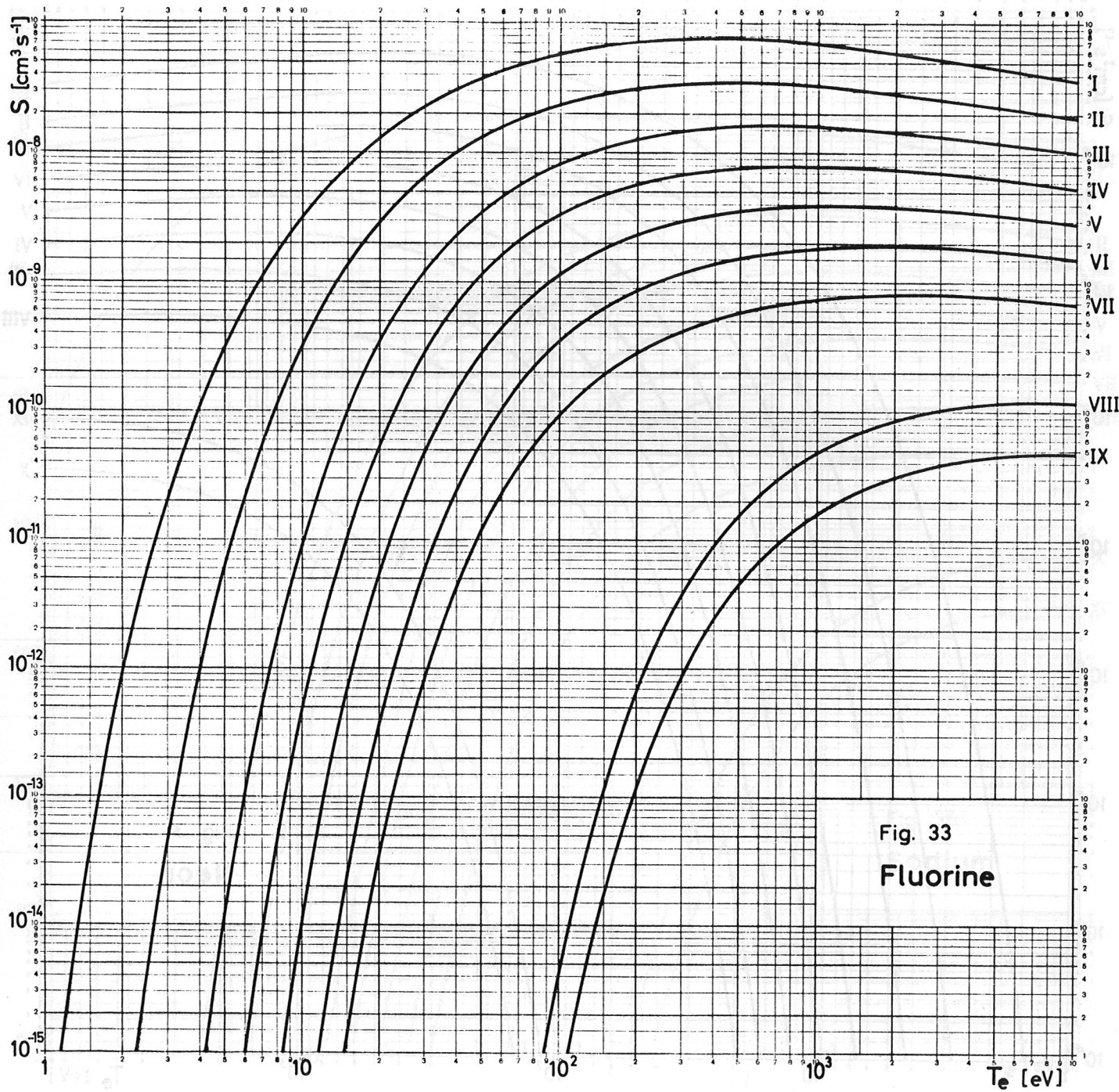


Fig. 33
Fluorine

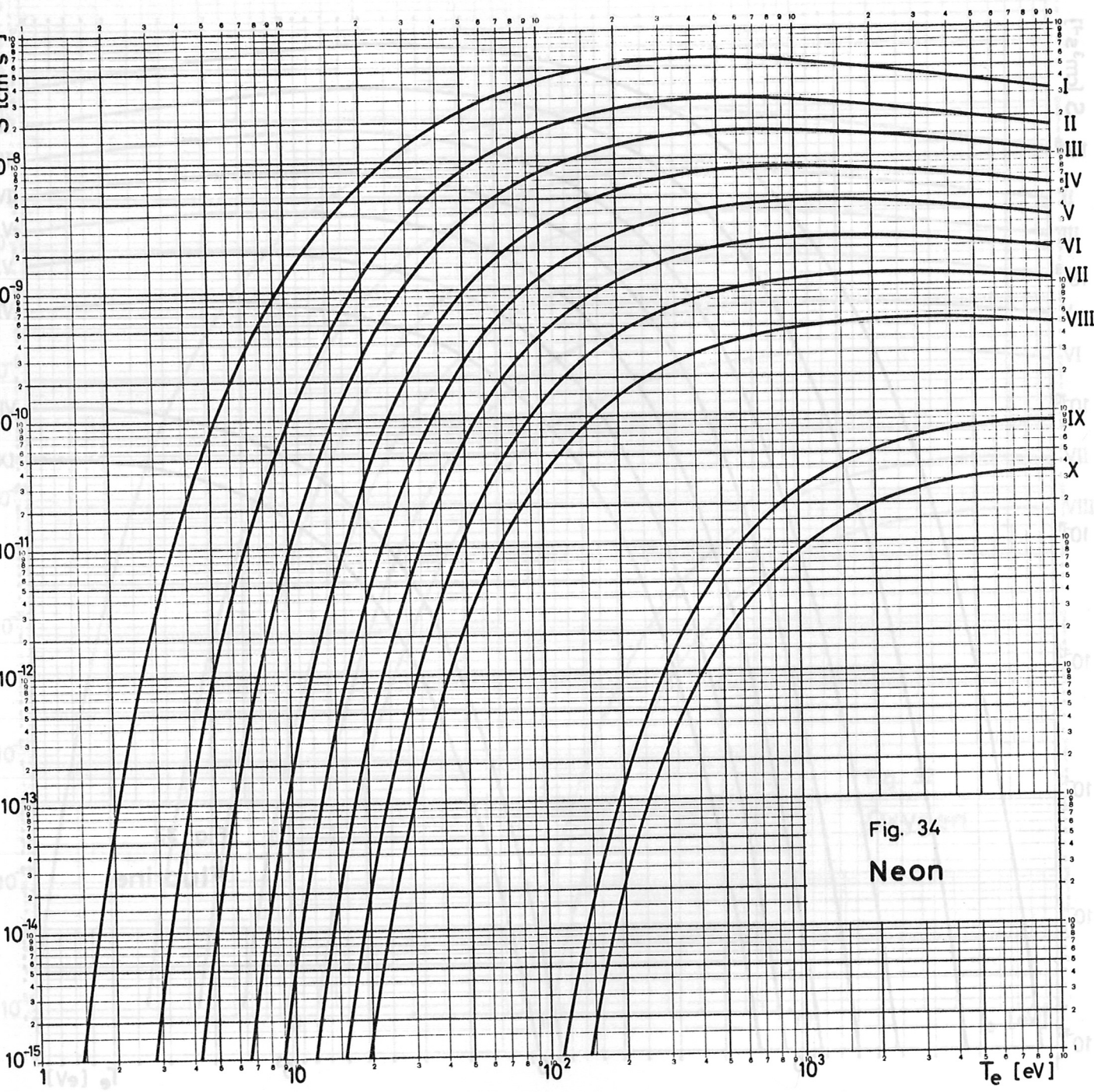


Fig. 34
Neon

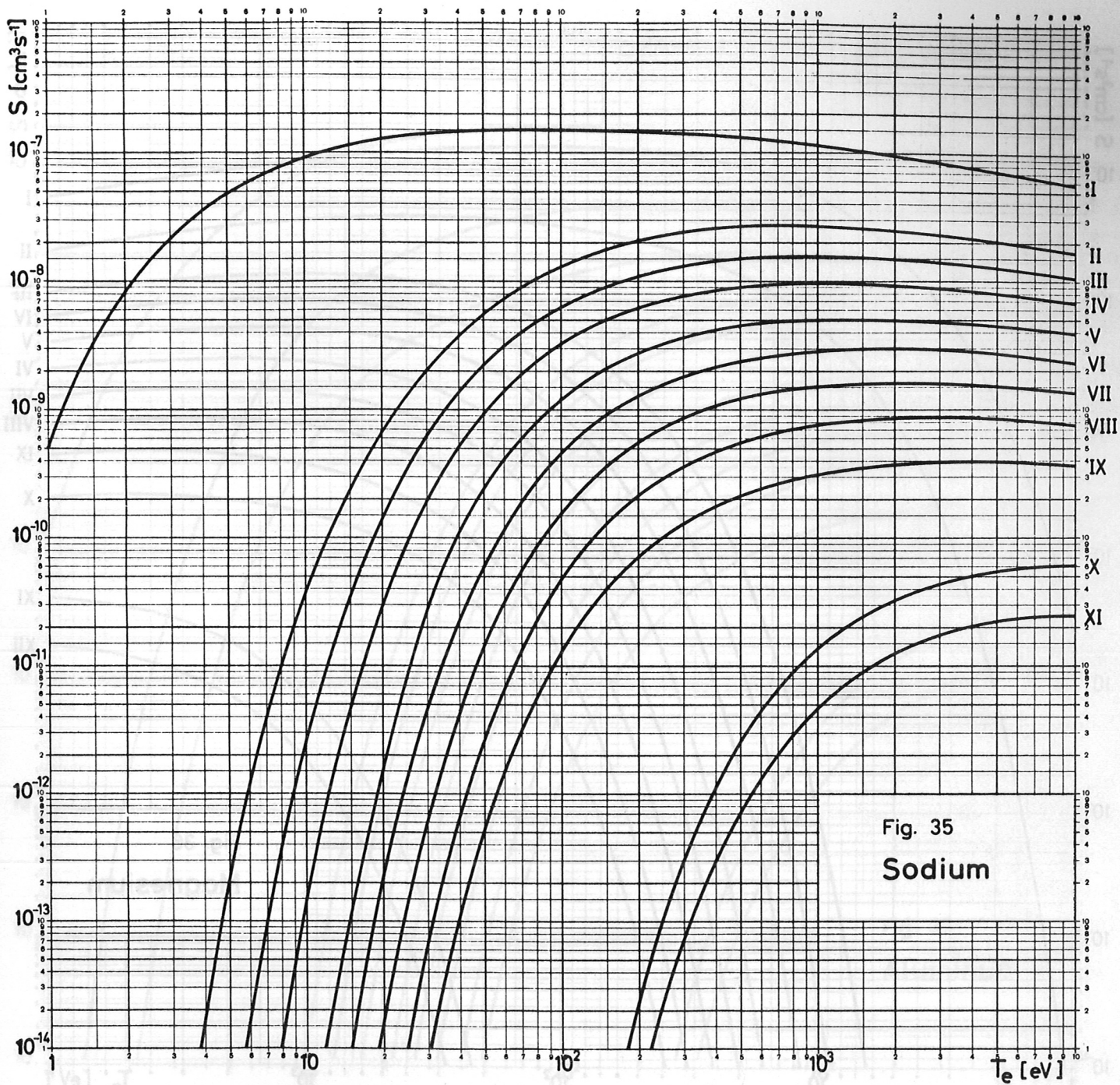


Fig. 35
Sodium

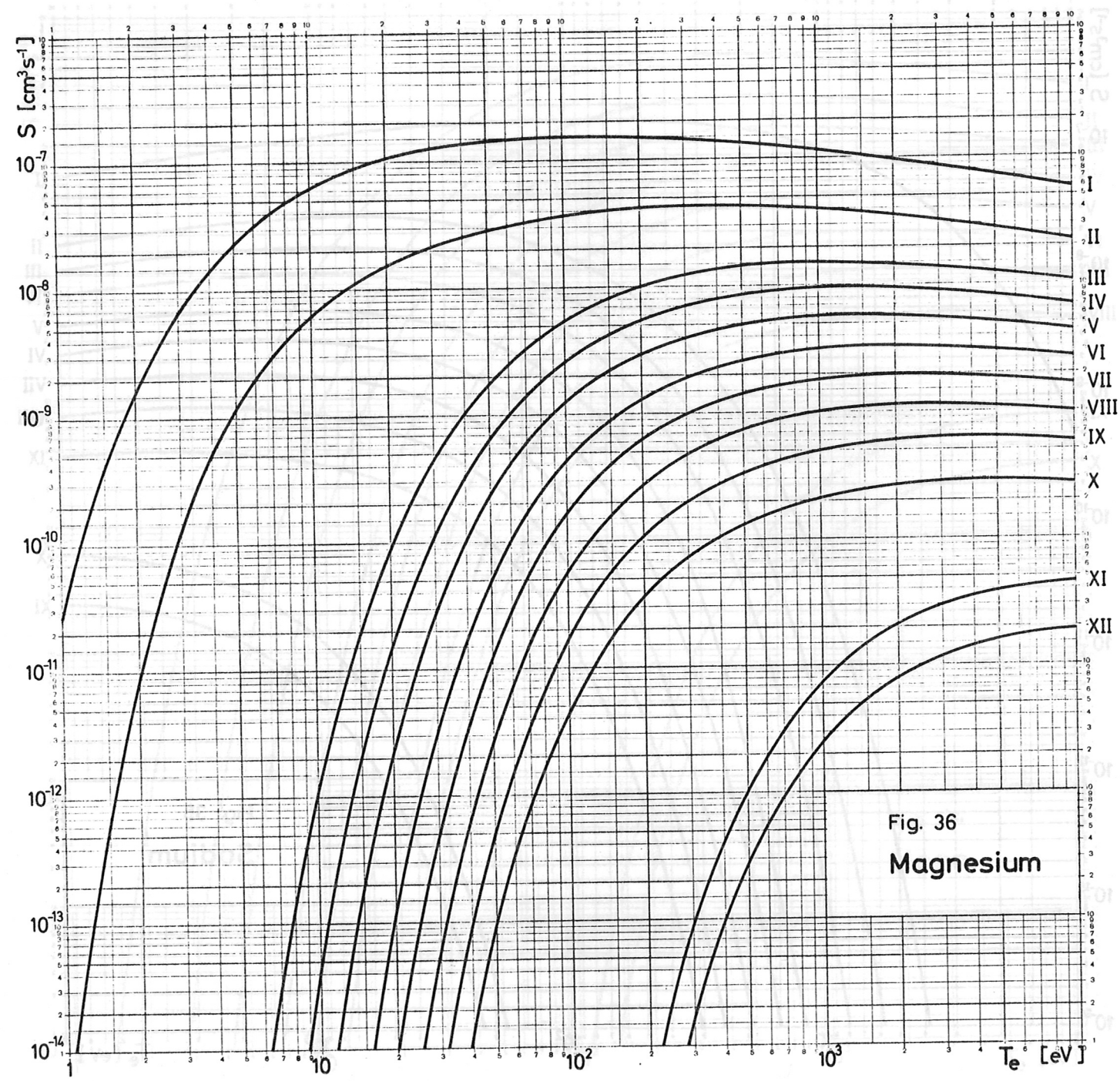


Fig. 36
Magnesium

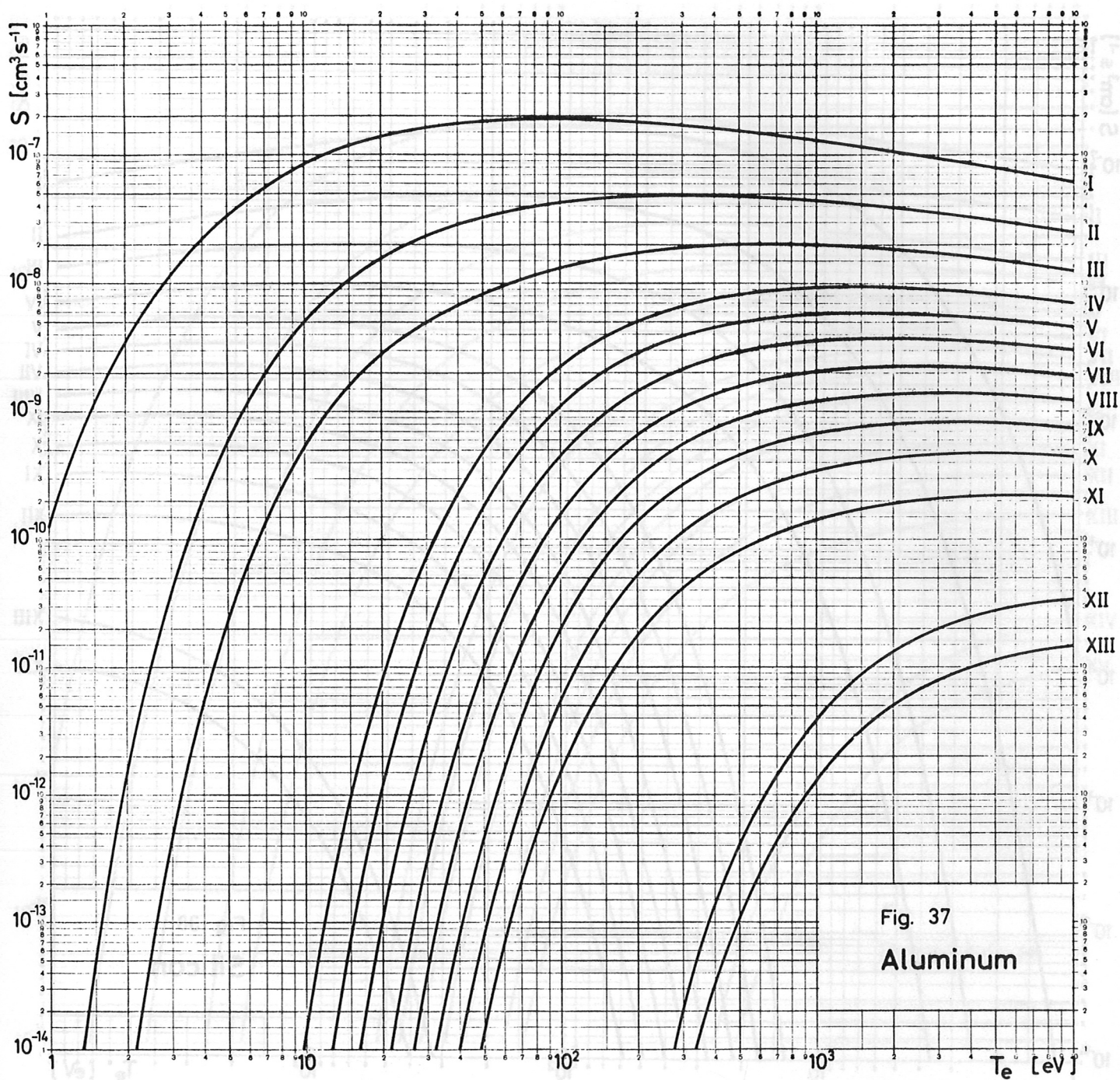


Fig. 37
Aluminum

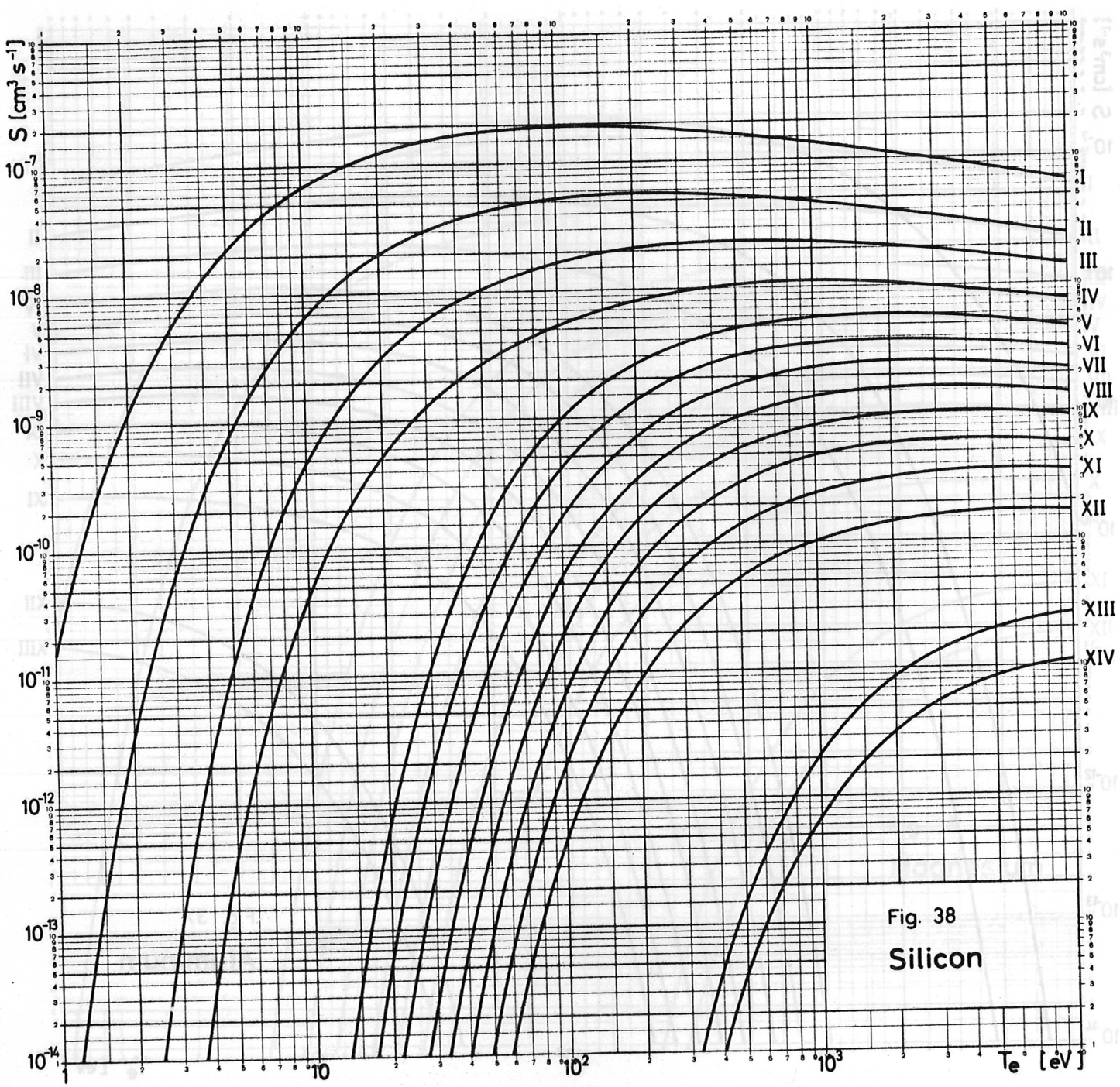


Fig. 38
Silicon

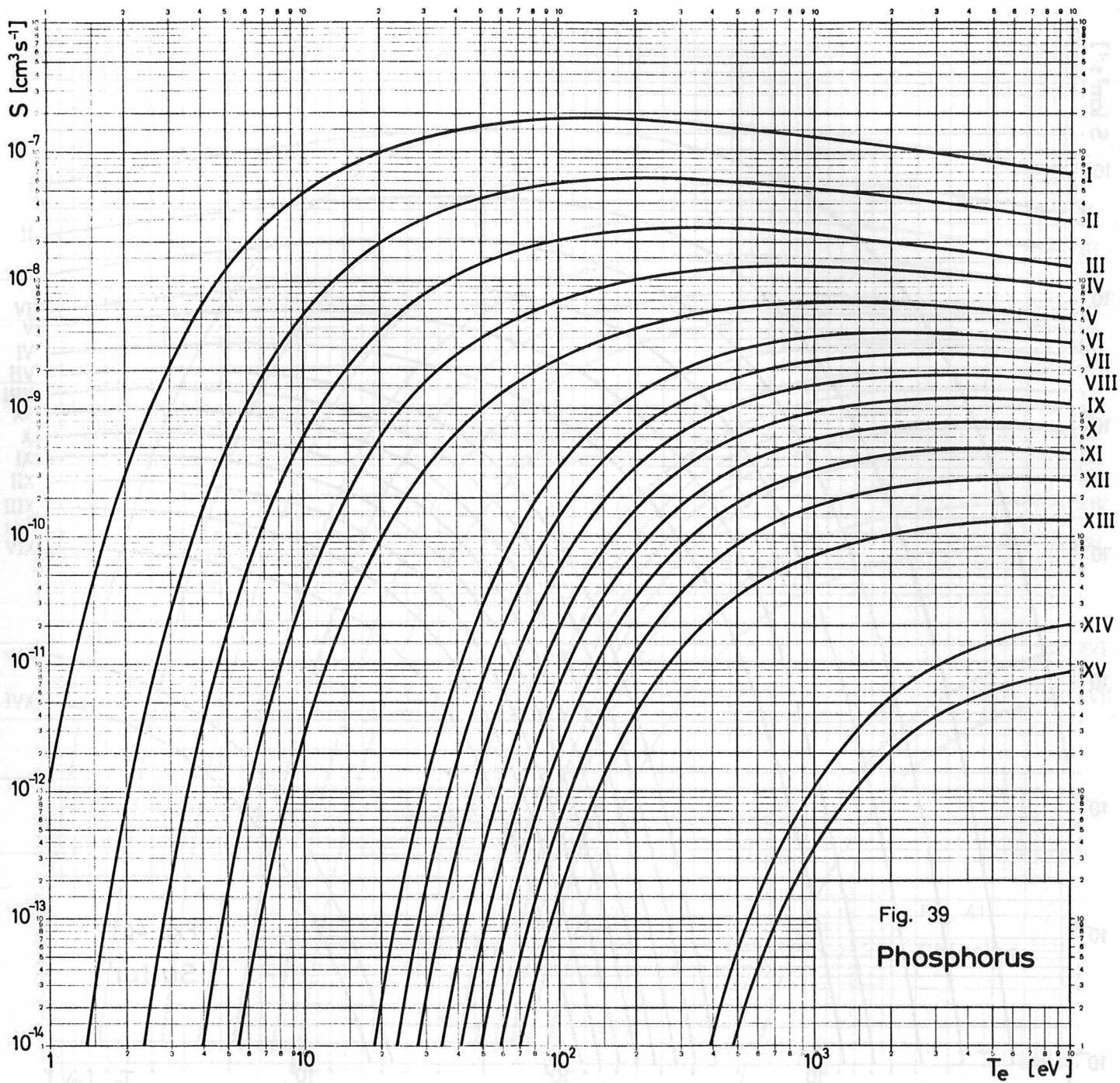


Fig. 39
Phosphorus

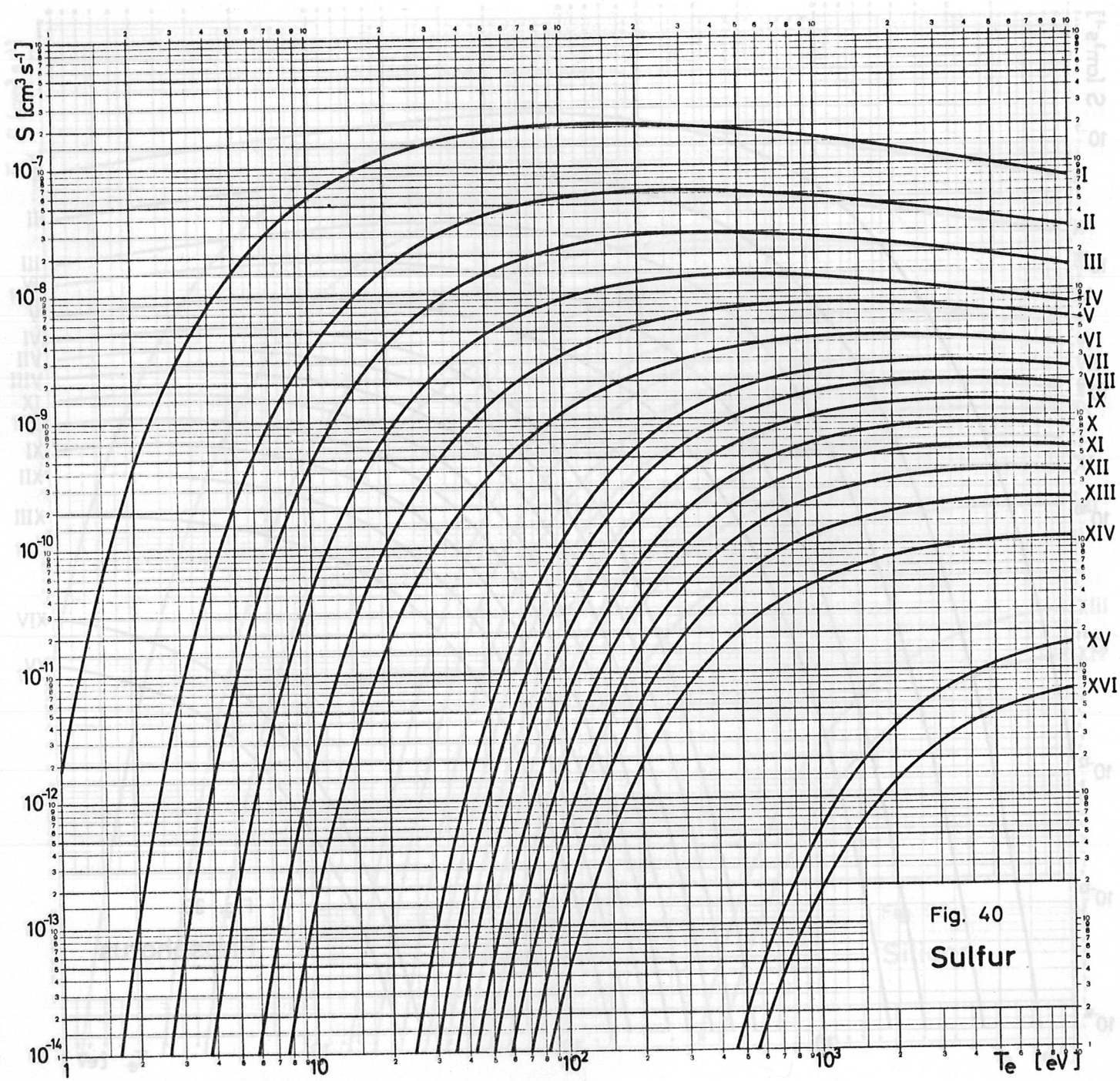


Fig. 40
Sulfur

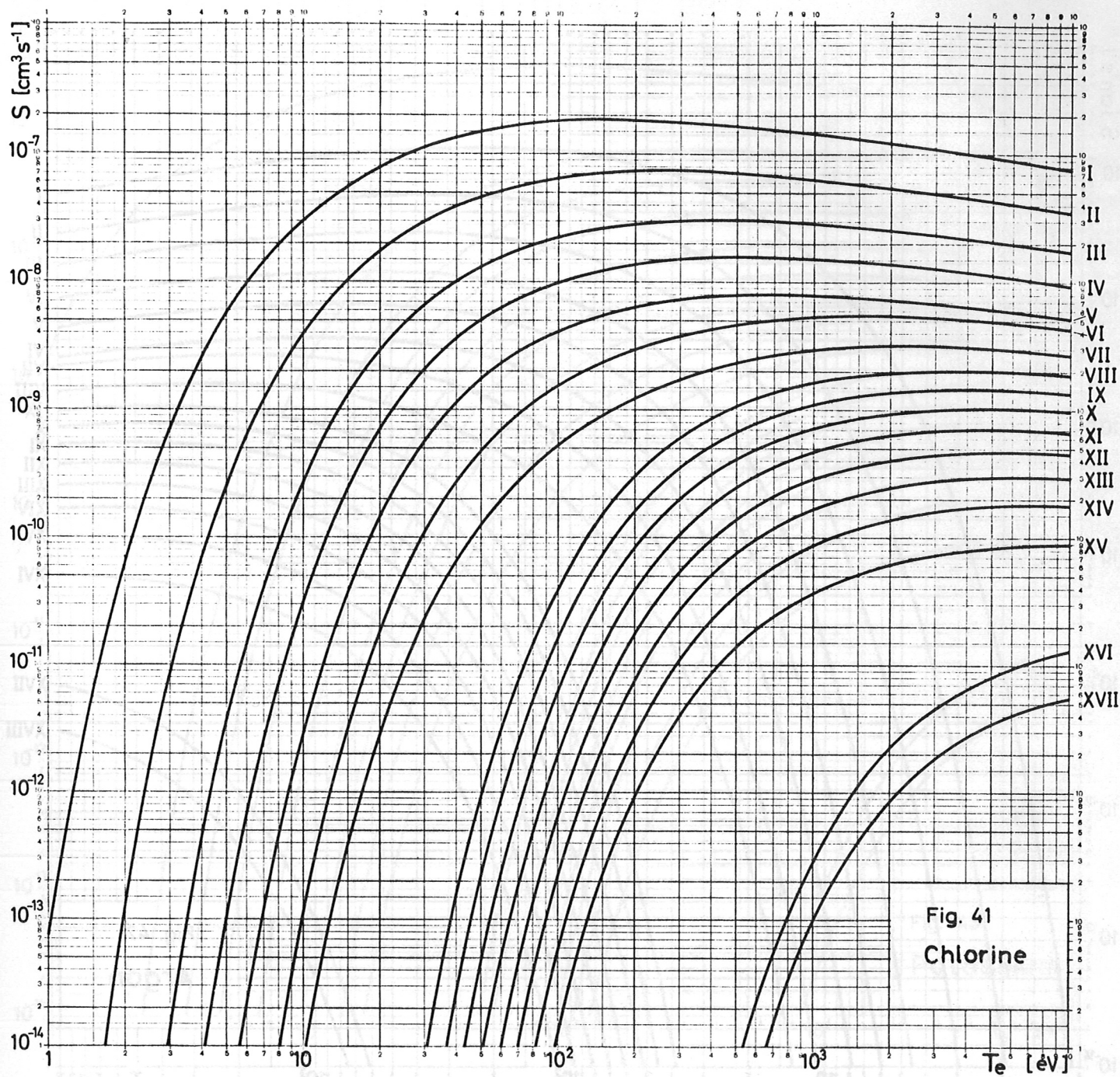


Fig. 41
 Chlorine

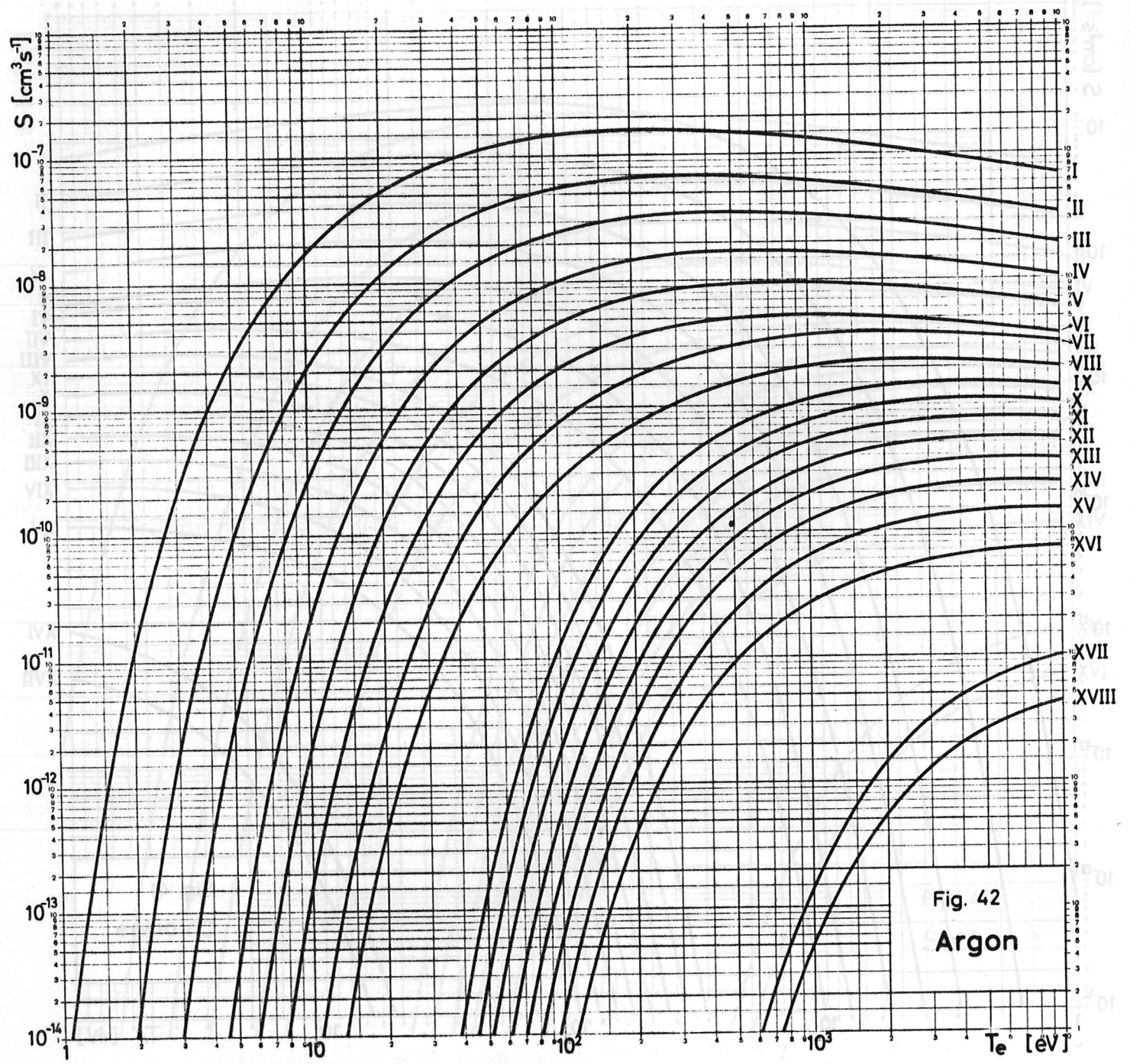


Fig. 42
Argon

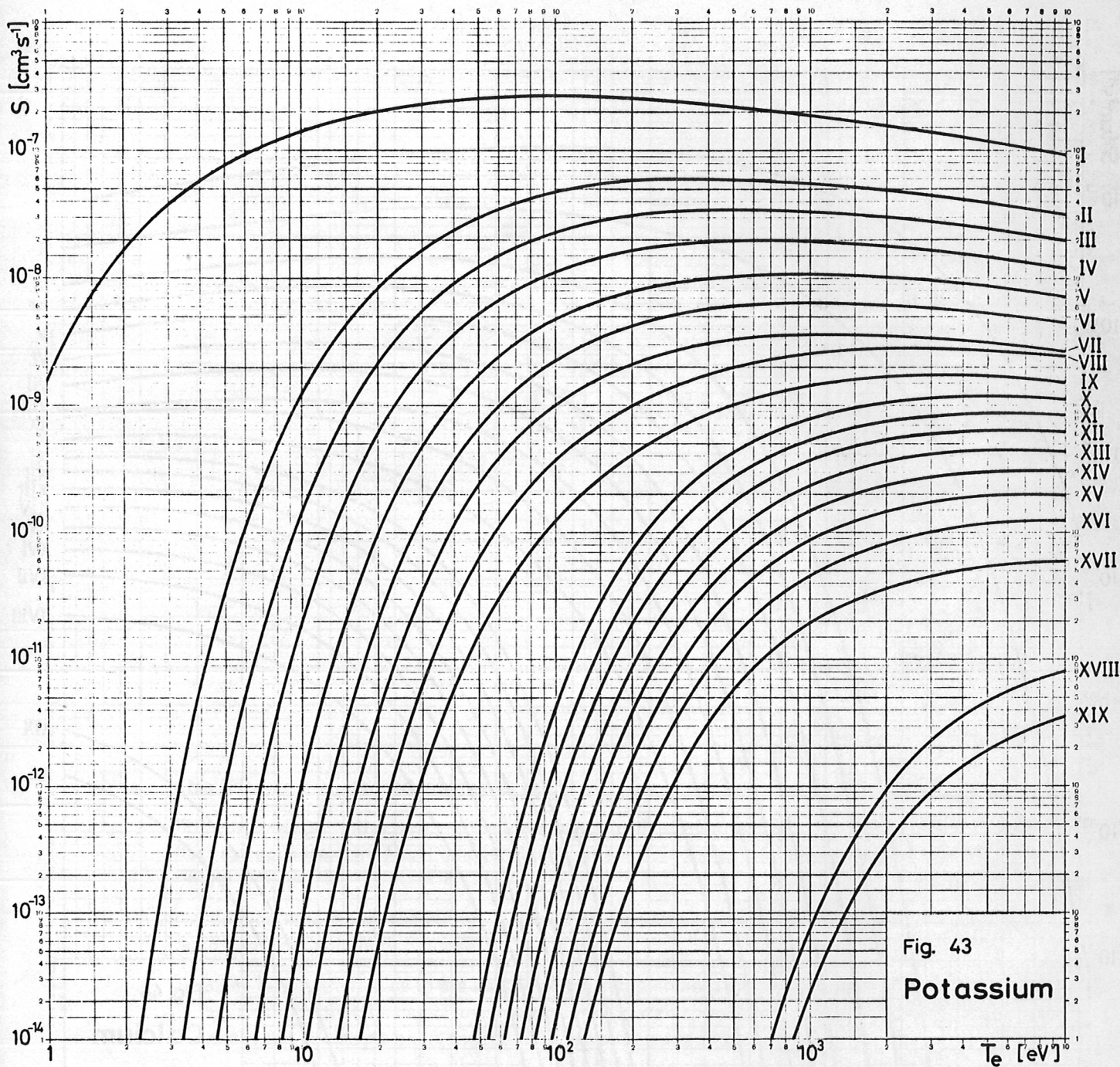


Fig. 43
Potassium

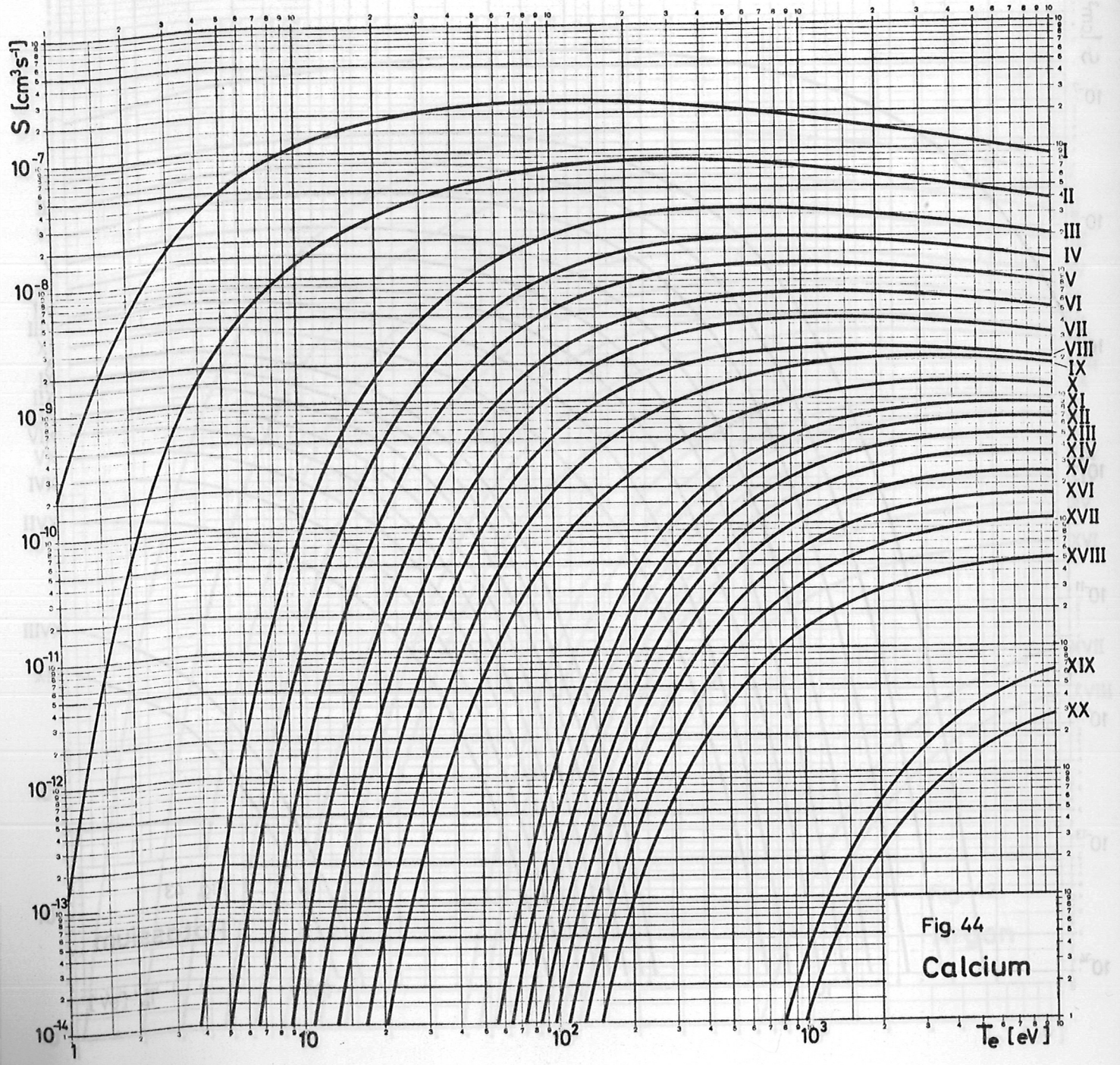


Fig. 44
Calcium