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Photoionization and photoabsorption cross sections for ionospheric calculations

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Abstract—Photoionization and photoabsorption cross sections for N_2, O_2 and O are presented in a form useful for calculation of solar EUV absorption and photoelectron production. The cross sections are based mostly on the data presented in the reviews by Schoen (1969) and Huffman (1969).

1. Introduction

The starting point in all ionospheric calculations must be the interaction of solar ultraviolet radiation with the atmospheric atoms and molecules. This, of course, first requires a knowledge of the solar flux versus wavelength. As of now, the best available data in the EUV region is that of Hinteregger (1970). The next most important information for ionospheric calculations must certainly be the absorption and ionization cross sections which determine how the solar radiation interacts with the atmosphere. This paper presents a proposed set of photo-absorption and photoionization cross sections for N_2, O_2 and O for use in ionospheric calculations.

The cross sections are presented in two forms. First they are presented in tabular form for the wavelength intervals of Hinteregger's (1970) flux table. The absorption cross section values all come from the reviews of Schoen (1969) and Huffman (1969) or are extrapolations of such data. Table 1 shows these results.

The second form of cross section presentation is analytic fits to the smooth portion of the partial photoionization cross section data given in Schoen (1969). The expression used to fit the data is

$$\sigma_i(\lambda) = A_i(1 - {}^{\lambda}/\lambda_{0i})^{m_i}(e^{\lambda/b_i} - 1) \tag{1}$$

where A_i, b_i and m_i are free parameters and λ_{0i} is usually the ionization threshold of the ith state. Table 2 shows the parameters for all of the states of N_2, O_2 and O which were modeled. Note that m_i is always kept integral for ease of integration if this is so desired. These modeled cross sections were used when extrapolations of existing data were necessary.

2. Photoionization and Absorption Cross Sections

N_2

Figures 1 and 2 show some of the analytic fits to the experimental data for N_2. Table 2 gives the parameters for all of the N_2 states modeled. Note that the $C^2\Sigma_u^+$ and $D^2\pi_g$ states were not modeled because the data of Schoen (1969) shows no indication of these states. This is probably to be expected because these states involve double electron excitation. Furthermore the potential curves of Gilmore (1965) indicate that the $D^2\pi_g$ state very likely leads to dissociation. Comes and Lessman (1964) have measured the dissociative ionization cross section for N_2

Table 1. Cross sections for Hinteregger flux table

Desig. no.	Wavelength (Å)	Cross sections (Mb) N_2 Abs.	N_2 Ion.	O_2 Abs.	O_2 Ion.	O Abs. and Ion.
1	1025·7	$<10^{-3}$		1·58	0·98	
2	990 Group	$<10^{-1}$		3·2	2·9	
3	977·0	0·7		4·0	2·5	
4	972·5	370·0		32·0	25·0	
5	949·7	5·2		6·3	3·7	
6	944·5	0·5		18·0	15·0	
7	937·8	10·0		5·0	3·7	
8	933·4	2·0		5·6	3·8	
9	930·7	4·8		26·0	17·0	
10	926·2	4·0		18·5	16·7	
11	1027–911	5·7		4·0	2·8	
12	911–890	6·0		7·4	3·9	0·07
13	904	6·3		11·0	3·9	0·03
14	890–860	8·0		7·4	3·8	0·7
15	860–830	7·5		9·3	4·0	1·8
16	835 Group	13·0		12·2	4·4	2·2
17	830–800	2·2		26·0	9·3	2·8
18	911–800	7·7		11·0	5·0	1·4
19	800–770	27·0	11·2	25·0	12·1	3·6
20	790·2, 790·1	25·0	11·5	28·0	10·0	3·5
21	787·7	9·0	8·0	24·0	13·0	3·6
22	786·5	9·0	8·5	24·0	11·1	3·6
23	780·3	19·0	9·5	28·0	11·0	3·7
24	770·4	15·0	14·4	18·0	11·0	3·9
25	770–740	24·0	14·0	19·0	12·0	4·1
26	765·1	85·0	66·0	23·0	12·0	4·0
27	760	16·0	15·9	19·0	11·0	4·1
28	740–710	18·0	13·5	31·5	27·0	4·4
29	710–680	21·5	21·5	24·0	20·0	8·0
30	703 Group	19·7	19·7	28·0	21·5	7·3
31	800–630	18·0	16·7	25·0	16·8	5·9
32	629·7	24·0	24·0	30·0	29·0	12·3
33	625·3	24·0	23·0	25·0	24·0	12·4
34	609·8	24·0	24·0	27·0	25·0	12·6
35	599·6	23·0	22·0	28·0	27·0	12·6
36	584·3	23·0	23·0	23·0	23·0	12·4
37	554 Group	25·0	24·0	26·0	25·0	11·6
38	521·0	25·0	24·0	24·5	23·9	10·6
39	508 Group	23·0	23·0	23·0	22·5	10·2
40	504	26·8	26·8	23·6	23·6	10·0
41	499·3	26·9	26·9	23·5	23·5	9·9
42	465·2	24·2	24·2	21·3	21·3	9·0
43	630–460	24·0	24·0	23·0	23·0	11·0
44	460–370	19·8	19·8	18·6	18·6	8·3
45	368·1	16·1	16·1	15·8	15·8	8·0
46	364·8	15·8	15·8	15·6	15·6	8·0
47	360·7	15·5	15·5	15·2	15·2	8·0
48	335·4	13·4	13·4	13·3	13·3	7·7
49	303·8	12	12	11·0	11·0	7·3
50	284·1	9·8	9·8	9·7	9·7	7·1

Table 1 (*cont.*)

Desig. no.	Wavelength (Å)	Cross sections (Mb) N_2 Abs.	N_2 Ion.	O_2 Abs.	O_2 Ion.	O Abs. and ion.
51	370–280	12·7	12·7	12·0	12·0	7·5
52	280–231	7·8	7·8	7·6	7·6	6·6
53	231–205	5·8	5·8	5·9	5·9	5·8
54	205–176	4·8	4·8	4·7	4·7	5·0
55	176–153	3·8	3·8	3·8	3·8	4·3
56	153–100	2·6	2·6	2·7	2·7	3·3
57	128–120	2·5	2·5	2·7	2·7	3·2
58	120–110	2·2	2·2	2·4	2·4	3·0
59	103·6, 105·2	1·9	1·9	2·1	2·1	2·7
60	110–100	2·0	2·0	2·1	2·1	2·8
61	94·0, 96·1	1·8	1·8	1·9	1·9	2·5
62	100–90	1·8	1·8	1·9	1·9	2·5
63	80·5, 86·8	1·5	1·5	1·6	1·6	2·2
64	90–80	1·5	1·5	1·6	1·6	2·2
65	76·0	1·3	1·3	1·4	1·4	2·0
66	80–70	1·3	1·3	1·4	1·4	2·0
67	66·3	1·1	1·1	1·2	1·2	1·8
68	70–60	1·1	1·1	1·2	1·2	1·7
69	50·5, 50·7, 55·3	0·85	0·85	0·95	0·95	1·4
70	60–50	0·90	0·90	1·0	1·0	1·5
71	44·1	0·65	0·65	0·80	0·80	1·2
72	50–40	0·70	0·70	0·80	0·80	1·2
73	33·6	0·48	0·48	0·60	0·60	0·9

and found it extremely small, lending further support to the smallness of the $D^2\pi_g$ cross section. A cross section for the $E^2\Sigma$ state of 10 per cent of the extrapolated total was included, but there is no experimental evidence to either confirm or deny this supposition.

Figure 3 shows the sum of the modeled partial cross sections described above in comparison with the total absorption measurements quoted by HUFFMAN (1969). Figure 4 shows the branching ratios derived from the modeled partial cross sections. These branching ratios are tabulated in Table 3 for the Hinteregger wavelength intervals.

O_2

The measured photoionization cross section for the ground state of O_2^+ shown in Fig. 5 is more complicated than any of the other measured partial cross sections for N_2 and O_2. It has been necessary to use the sum of two cross sections of the form of equation (1) to fit the O_2^+ ground state. Because of this the threshold wavelength parameter λ_0 is not the actual threshold for this state but is a pseudo-threshold for each of the two terms. Table 2 lists the parameters for the fits to all of the O_2 partial cross sections. Figures 6 shows the fit to the data for the sum of the $a^4\pi_u$ and $A^2\pi_u$ states which are usually not resolved in experimental data. This lack of resolution is generally not important in ionospheric calculation because the required resolution in a photoelectron production spectrum is usually no greater than that in the laboratory cross section experiments.

Table 2. Parameters for analytic formula

State:		Parameters λ_0	A	b	m
N_2^+	$X^2\Sigma_g^+$	796·0	$3{\cdot}56 \times 10^{-15}$	18·0	2
		796·0	$6{\cdot}52 \times 10^{-1}$	74·0	4
	$A^2\Pi_u^+$	742·7	$3{\cdot}91 \times 10^{-13}$	17·6	3
		742·7	$3{\cdot}29 \times 10^{-1}$	72·6	3
	$B^2\Sigma_u^+$	661·0	$9{\cdot}88 \times 10^{-12}$	21·0	1
		661·0	$1{\cdot}72 \times 10^{-1}$	121·0	1
	$E^2\Sigma_g^+$	355·0	$1{\cdot}51 \times 10^{-6}$	20·0	1
O_2^+	$x^2\Pi_g$	1026·7	$1{\cdot}94 \times 10^{-2}$	121·7	1
		900·0	$3{\cdot}03 \times 10^{-1}$	44·0	10
		850·0	$3{\cdot}10 \times 10^{-20}$	13·7	4
		750·0	$4{\cdot}62 \times 10^{-37}$	10·0	3
	$a^4\Pi_u$	769·8	$1{\cdot}17 \times 10^{-16}$	16·4	2
		769·8	$1{\cdot}44 \times 10^{-1}$	144·8	1
	$A^2\Pi_u$	736·8	$1{\cdot}07 \times 10^{-16}$	16·8	1
		736·8	$7{\cdot}49 \times 10^{-1}$	166·8	1
	$b^4\Sigma_g^+$	682·3	$1{\cdot}39 \times 10^{-1}$	126·9	$\frac{1}{3}$
	$B^2\Sigma_g^-$	613·7	$2{\cdot}01 \times 10^{-10}$	17·9	3
		613·7	$8{\cdot}14 \times 10^{-1}$	223·7	1
	$c^4\Sigma_u^-$	505·4	$2{\cdot}26 \times 10^{-38}$	5·2	2
		505·4	$4{\cdot}12 \times 10^{-3}$	42·7	2
O_2^+	Dissoc.	670·0	$3{\cdot}65 \times 10^{-2}$	67·5	2
O^+	^4S	910·0	$7{\cdot}52 \times 10^{-2}$	100	2
		910·0	$4{\cdot}52 \times 10^{-1}$	50	12
	^2D	725·0	$8{\cdot}41 \times 10^{-2}$	100	1
		725·0	$5{\cdot}40 \times 10^{-1}$	50	9
	^2P	670·0	$7{\cdot}20 \times 10^{-2}$	100	1
		670·0	$3{\cdot}09 \times 10^{-1}$	50	8
	^4P	430·0	$2{\cdot}29 \times 10^{-3}$	40	2
	^2P	310·0	$4{\cdot}07 \times 10^{-2}$	60	1

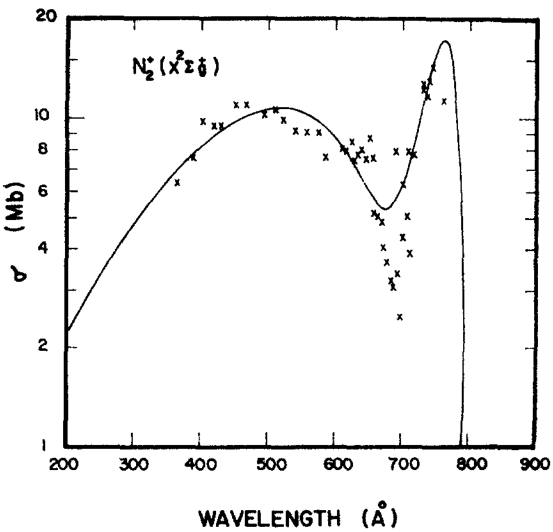

Fig. 1. $N_2^+(X^2\Sigma_g^+)$ partial cross section.

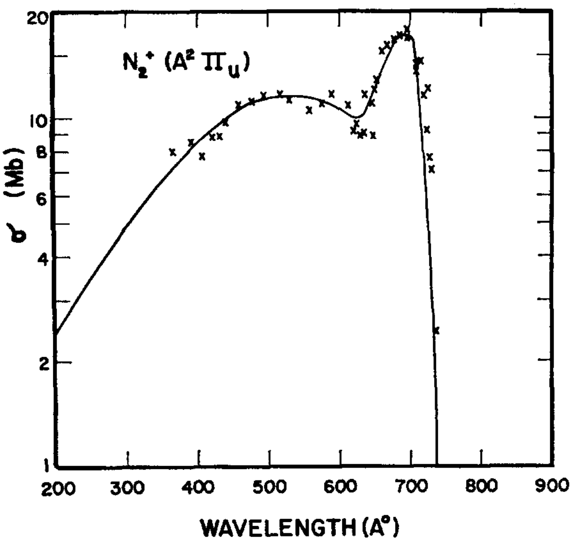

Fig. 2. $N_2^+(A^2\pi_u)$ partial cross section.

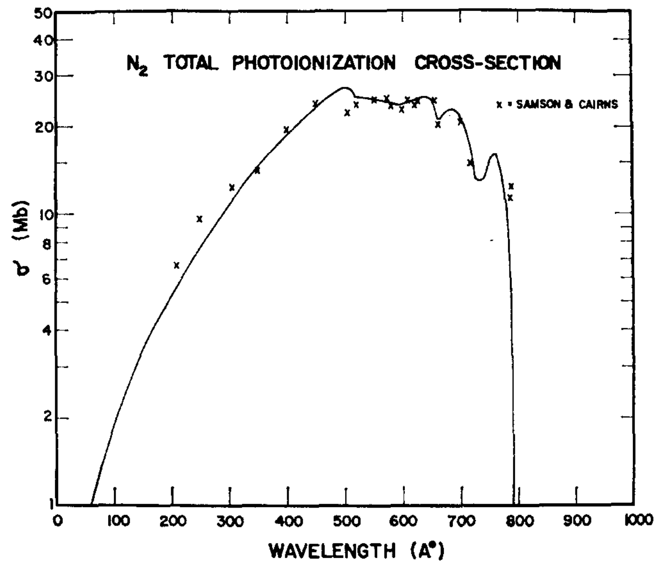

Fig. 3. N_2 total photoionization cross section.

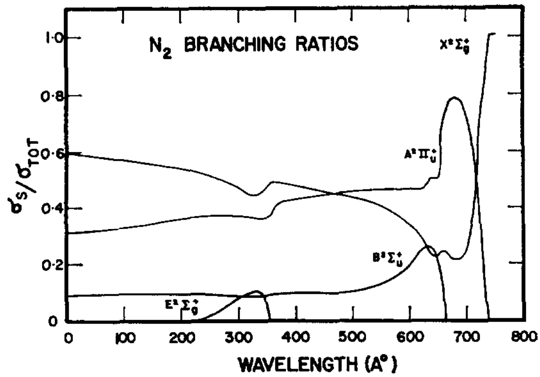

Fig. 4. N_2 branching ratios.

Table 3. N_2 and O branching ratios (first column refers to interval numbers defined in Table 1)

Desig. no	Nitrogen $X^2\Sigma^+g$	$A^2\Pi u$	$B^2\Sigma^+u$	$E^2\Sigma^+g$	^4S	^2D	^2P	^4P	^2P
25	0·999	0·001			1·00	0·0	0·0	0·0	0·0
28	0·68	0·32			1·00	0·0	0·0	0·0	0·0
29	0·24	0·76			0·55	0·45	0·0	0·0	0·0
30	0·26	0·73			0·60	0·40	0·0	0·0	0·0
31	0·56	0·39	0·05		0·75	0·25	0·0	0·0	0·0
32	0·26	0·48	0·26		0·32	0·49	0·19	0·0	0·0
33	0·27	0·48	0·25		0·32	0·49	0·20	0·0	0·0
34	0·31	0·47	0·22		0·30	0·47	0·23	0·0	0·0
35	0·34	0·47	0·19		0·29	0·46	0·24	0·0	0·0
36	0·37	0·47	0·16		0·29	0·46	0·26	0·0	0·0
37	0·40	0·47	0·13		0·28	0·44	0·27	0·0	0·0
38	0·43	0·46	0·11		0·29	0·43	0·28	0·0	0·0
39	0·43	0·46	0·11		0·29	0·42	0·28	0·0	0·0
40	0·43	0·46	0·11		0·30	0·42	0·28	0·0	0·0
41	0·43	0·46	0·11		0·30	0·42	0·28	0·0	0·0
42	0·45	0·45	0·10		0·31	0·41	0·28	0·0	0·0
43	0·39	0·45	0·16		0·29	0·43	0·28	0·0	0·0
44	0·47	0·43	0·10		0·32	0·40	0·28	0·0	0·0
45	0·49	0·42	0·09		0·30	0·38	0·26	0·06	0·0
46	0·49	0·42	0·09		0·30	0·38	0·26	0·06	0·0
47	0·49	0·42	0·09		0·30	0·38	0·26	0·06	0·0
48	0·45	0·37	0·08	0·10	0·30	0·38	0·26	0·06	0·0
49	0·47	0·37	0·09	0·07	0·30	0·38	0·25	0·05	0·02
50	0·49	0·37	0·09	0·05	0·29	0·37	0·25	0·04	0·05
51	0·47	0·38	0·09	0·06	0·30	0·38	0·26	0·06	0·0
52	0·52	0·37	0·09	0·02	0·28	0·36	0·24	0·03	0·08
53	0·54	0·36	0·095	0·005	0·29	0·37	0·24	0·02	0·08
54	0·55	0·35	0·098	0·48	0·29	0·38	0·25	0·02	0·07
55	0·55	0·35	0·10		0·30	0·38	0·25	0·01	0·06
56	0·56	0·34	0·10		0·30	0·39	0·25	0·01	0·05
57	0·56	0·34	0·10		0·30	0·39	0·25	0·01	0·05
58	0·57	0·33	0·10		0·31	0·40	0·25	0·01	0·05
59	0·57	0·33	0·10		0·31	0·40	0·25	0·01	0·05
60	0·57	0·33	0·10		0·31	0·40	0·25	0·01	0·05
61	0·57	0·33	0·10		0·31	0·40	0·25	0·00	0·04
62	0·57	0·33	0·10		0·31	0·40	0·25	0·00	0·04
63	0·57	0·33	0·10		0·31	0·40	0·24	0·00	0·04
64	0·57	0·33	0·10		0·31	0·40	0·25	0·00	0·04
65	0·58	0·32	0·10		0·32	0·40	0·25	0·00	0·04
66	0·58	0·32	0·10		0·32	0·40	0·25	0·00	0·04
67	0·58	0·32	0·10		0·32	0·40	0·24	0·00	0·04
68	0·58	0·32	0·10		0·32	0·40	0·24	0·00	0·04
69	0·58	0·32	0·10		0·32	0·40	0·24	0·00	0·03
70	0·58	0·32	0·10		0·32	0·40	0·24	0·00	0·03
71	0·58	0·32	0·10		0·32	0·40	0·24	0·00	0·03
72	0·58	0·32	0·10		0·32	0·40	0·24	0·00	0·03
73	0·59	0·31	0·10		0·33	0·40	0·24	0·00	0·03

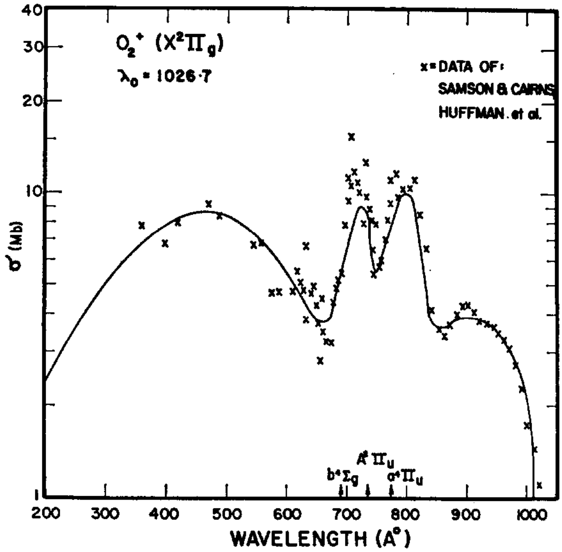

Fig. 5. $O_2^+(X^2\pi_g)$ partial cross section.

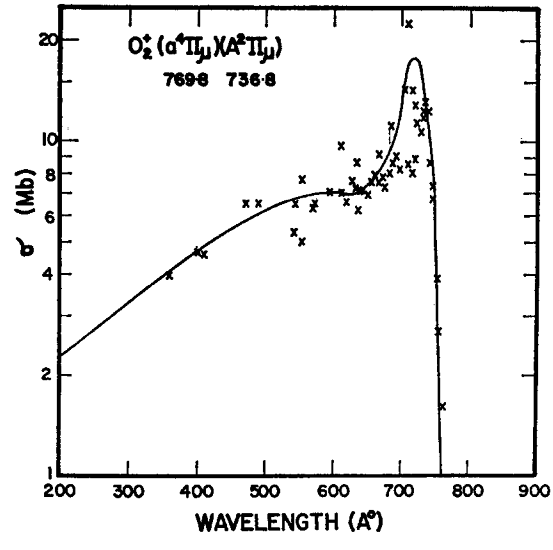

Fig. 6. $O_2^+(a^4\pi_u + A^2\pi_u)$ partial cross section.

The total photoionization cross section data is shown in Fig. 7 along with the sum of the modeled partial cross sections. Included in the total is a fit to the dissociative ionization cross section of Comes *et al.* (1968). The modeled total cross section is slightly higher than the data in just the region where the dissociative cross section is largest, raising the possibility that some of the dissociative ionization is also included in the individual state partial cross sections. Figure 8 and Table 4 give the branching ratios derived from the modeled cross sections.

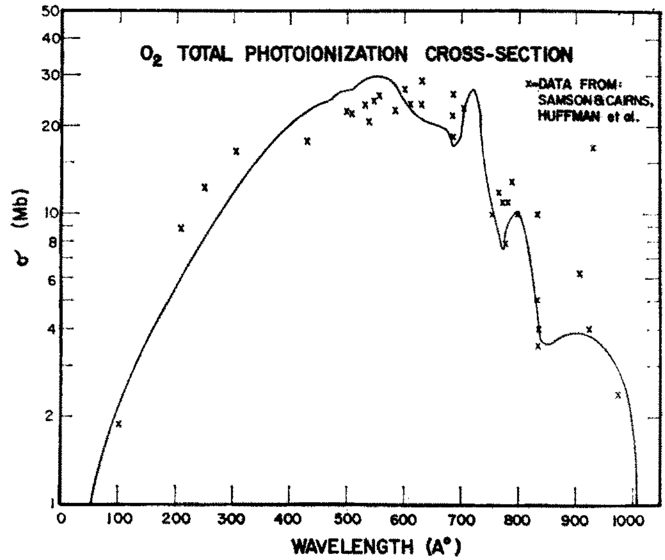

Fig. 7. O_2 total photoionization cross section.

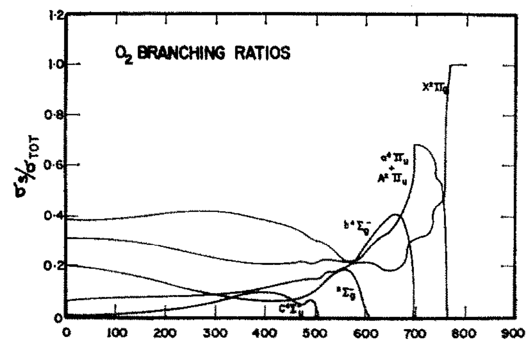

Fig. 8. O_2 branching ratios.

Samson (1971) has some data indicating the presence of higher lying states below 300 Å. These may improve the fit of the modeled sum of the cross sections to the total ionization measurements.

O

The existing information on atomic oxygen photoionization cross sections is all in the form of total cross sections. Calculations have been made by Dalgarno *et al.* (1964) and Henry (1967) and measurements by Cairns and Samson (1965) and Comes *et al.* (1968). The magnitudes of the partial cross sections were estimated from the increases at each ionization potential and the shapes assumed are given by the parameters in Table 2. At $\lambda > 500$ Å the calculations and the data of Comes

Table 4. O_2 branching ratios (first column refers to interval numbers defined in Table 1)

	Molecular oxygen					
Desig. no.	$x^2\Pi g$	$a^4\Pi u$ + $A^2\Pi u$	$b^4\Sigma^-g$	$B^2\Sigma^-g$	$c^4\Sigma^-u$	Dissoc.
25	0·65	0·35				
26	0·85	0·15				
27	0·70	0·30				
28	0·36	0·64				
29	0·29	0·64	0·07			
30	0·32	0·68	0·0			
31	0·47	0·40	0·12			0·01
32	0·20	0·33	0·40			0·07
33	0·21	0·33	0·38			0·08
34	0·22	0·31	0·35	0·01		0·11
35	0·23	0·29	0·32	0·04		0·12
36	0·22	0·26	0·26	0·14		0·12
37	0·24	0·22	0·21	0·20		0·13
38	0·29	0·23	0·18	0·15		0·15
39	0·31	0·23	0·18	0·13		0·15
40	0·31	0·22	0·17	0·11	0·05	0·14
41	0·31	0·22	0·16	0·11	0·06	0·14
42	0·35	0·22	1·15	0·08	0·06	0·14
43	0·26	0·25	0·23	0·11	0·02	0·13
44	0·38	0·22	0·12	0·07	0·09	0·12
45	0·40	0·22	0·11	0·08	0·09	0·10
46	0·40	0·22	0·11	0·08	0·09	0·10
47	0·40	0·23	0·10	0·08	0·09	0·10
48	0·41	0·23	0·10	0·09	0·08	0·09
49	0·42	0·24	0·09	0·10	0·07	0·08
50	0·42	0·25	0·09	0·10	0·06	0·08
51	0·41	0·23	0·10	0·90	0·07	0·09
52	0·42	0·25	0·09	0·12	0·05	0·07
53	0·42	0·27	0·09	0·13	0·03	0·06
54	0·41	0·28	0·08	0·14	0·03	0·06
55	0·41	0·29	0·08	0·15	0·02	0·05
56	0·39	0·30	0·08	0·17	0·01	0·05
57	0·39	0·30	0·08	0·17	0·01	0·05
58	0·39	0·31	0·08	0·17	0·01	0·04
59	0·39	0·31	0·07	0·18	0·01	0·04
60	0·39	0·31	0·07	0·18	0·01	0·04
61	0·39	0·31	0·07	0·18	0·01	0·04
62	0·39	0·31	0·07	0·18	0·01	0·04
63	0·39	0·31	0·07	0·18	0·01	0·04
64	0·39	0·31	0·07	0·18	0·01	0·04
65	0·38	0·31	0·07	0·19	0·01	0·04
66	0·38	0·31	0·07	0·19	0·01	0·04
67	0·38	0·31	0·07	0·19	0·01	0·04
68	0·38	0·31	0·07	0·19	0·01	0·04
69	0·38	0·31	0·07	0·19	0·01	0·04
70	0·38	0·31	0·07	0·19	0·01	0·04
71	0·38	0·31	0·07	0·19	0·01	0·04
72	0·38	0·31	0·07	0·19	0·01	0·04
73	0·38	0·31	0·07	0·20	0·01	0·03

et al. (1968) agree fairly well. At shorter wavelengths they begin to disagree and the assumed total cross section is shown in Fig. 9. The corresponding branching ratios are shown in Fig. 4 and Table 3.

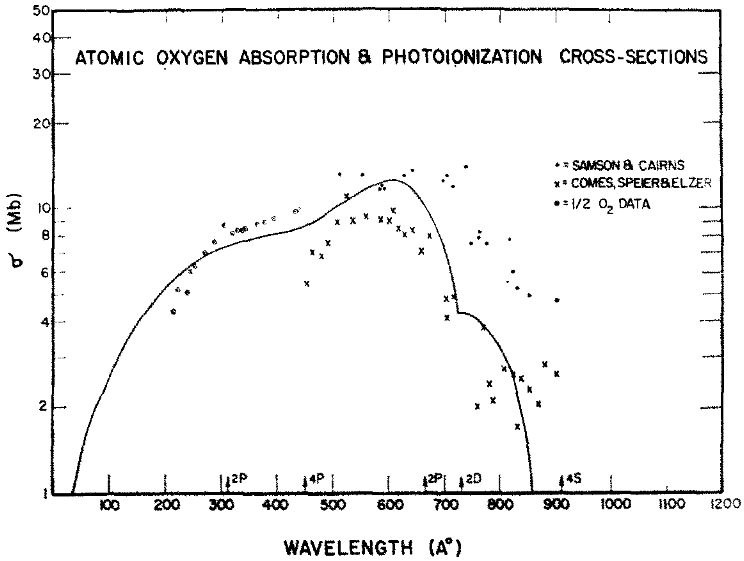

Fig. 9. Atomic oxygen total photoionization cross section.

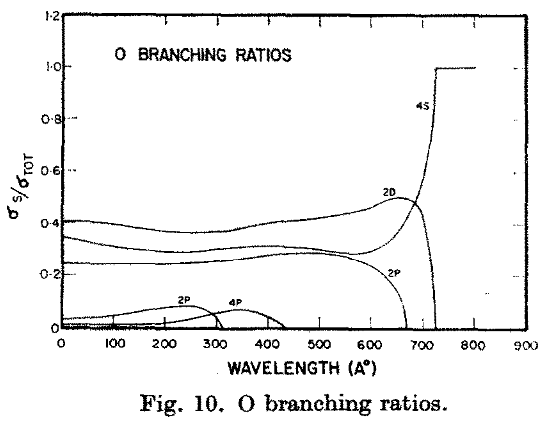

Fig. 10. O branching ratios.

3. Discussion

The cross sections presented above are not new, but they represent an attempt to organize the existing data and present it in a usuable form for those concerned with ionospheric calculations. The data available is very sparse and probably not always reliable judging by some of the disagreements between investigators. It is the needs of the users, which this paper attempts to fulfil, which will point out the areas of laboratory measurement where more and better data are needed. Hopefully, those attempting to use this data in ionospheric calculations will, through their needs for further data, stimulate further laboratory studies.

References

BERKOWITZ J. and CHUPKA W. A.	1969	*J. chem. Phys.* **51**, 2341.
BEYER K. D. and WELGE K. H.	1969	*J. chem. Phys.* **51**, 5323.
BLAKE A. J. and CARVER J. W.	1965	*Phys. Letts* **19**, 387.
BLAKE A. J. and CARVER J. W.	1967	*J. chem. Phys.* **47**, 1038.
CAIRNS R. B. and SAMSON J. A. R.	1965	*Phys. Rev.* **139**, A1403.
COMES F. J. and LESSMAN W.	1964	*Z. Naturforsch.* **19a**, 65.
COMES F. J., ELZER A. and SPEIER F.	1968	*Z. Naturforsch.* **23a**, 114.
COOK G. R. and METZGER P. H.	1964	*J. chem. Phys.* **41**, 321.
DALGARNO A., HENRY R. J. W. and STEWART A. L.	1964	*Planet. Space Sci.* **12**, 235.
GILMORE F. R.	1965	*J. Quant. Spectrosc. Rad. Trans.* **5**, 369.
HALL L. A. and HINTEREGGER H. E.	1970	*J. geophys. Res.* **75**, 6959.
HENRY R. J. W.	1967	*Planet. Space Sci.* **15**, 1747.
HINTEREGGER H. E.	1970	*Annls Géophys.* **26**, 547.
HUFFMAN R. E., TANAKA Y. and LARRABEE J. C.	1963	*J. chem. Phys.* **39**, 910 (1963).
HUFFMAN R. E.	1969	*Can. J. Chem.* **47**, 1823.
HUFFMAN R. E., LARRABEE J. C. and TANAKA Y.	1967	*J. chem. Phys.* **46**, 2213.
MARR G. V.	1967	*Photoionization Processes in Gases.* Academic Press, New York.
MCGOWAN J. W., VROOM D. A. and COMEAUX A. R.	1969	*J. chem. Phys.* **51**, 5626.
SAMSON J. A. R. and CAIRNS R. B.	1964	*J. geophys. Res.* **69**, 4583.
SAMSON J. A. R.	1970	*Phil. Trans. R. Soc. Lond.* **A268**, 141.
SCHOEN R. I.	1969	*Can. J. Chem.* **47**, 1855.
TOHMATSU T., OGAWA T. and TSURUTA H.	1965	*Rep. Ionos. Space Res. Japan* **19**, 482.
WAINFAN N., WALKER W. C. and WEISSLER G. L.	1955	*Phys. Rev.* **99**, 542.