

Cross Sections for Electron Collisions with Oxygen Molecules

Yukikazu Itikawa

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Cross Sections for Electron Collisions with Oxygen Molecules

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Cross section data are collected and reviewed for electron collisions with oxygen molecules. Included are the cross sections for total and elastic scatterings, momentum transfer, excitations of rotational, vibrational, and electronic states, dissociation, ionization, electron attachment, and emission of radiations. For each process, the recommended values of the cross sections are presented, when possible. The literature has been surveyed through the end of 2007. © 2009 American Institute of Physics.

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Key words: attachment; cross section; dissociation; elastic scattering; electron collision; emission; excitation; ionization; molecular oxygen; momentum transfer; recommended data; total scattering.

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1. Introduction

The oxygen molecule (O₂) is one of the major components of Earth's atmosphere. It also plays an important role in various processing plasmas.^{1,2} Oxygen discharges are of practical significance particularly because O₂ is one of the simplest electronegative gases and it has low-lying metastable states. In 1989, Itikawa *et al.* published a compilation of cross section data on electron collisions with O₂.³ (We hereafter refer to the paper as JPCRD89.) Since then a number of theoretical and experimental studies have been reported on the electron collisions with O₂. The present paper is the complete update of the previous data compilation.

Since the publication of JPCRD89, a review of the cross section data for the e+O₂ system has been published several times. After a critical review of the cross section data available, Kanik *et al.*⁴ determined their recommended data for e+O₂ collisions. They reported the cross sections for total scattering, elastic scattering, ionization, and sum of all the excitation processes. Majeed and Strickland⁵ published a set of inelastic cross sections for O₂ to evaluate an energy loss of electrons in the atmosphere. Zecca *et al.*⁶ and, more recently, Brunger and Buckman⁷ published a comprehensive data compilation for electron collisions with a number of molecular species, which includes O₂. Brunger and Buckman, however, dealt with only the excitation of discrete states, besides total and elastic scatterings. In 2003, a more extensive compilation of cross section data has been published for electron-molecule collisions.⁸ It includes cross sections on total scattering, elastic scattering, momentum transfer, ionization, electron attachment, and excitations of rotational, vibrational, and electronic states. To prepare the present paper, the author consulted those previous reviews, when necessary, but independently surveyed literature (mainly those published after the publication of JPCRD89). It should be noted that the present paper has a wider scope than those previous ones. For instance, a detailed discussion is given on the emission cross section and dissociation process.

In the present paper, a set of recommended values of the cross section is determined as far as possible. In so doing, the following points are taken into account:

- In principle, experimental data are preferred to theoretical ones.
- The reliability of the experimental methods employed is critically assessed. Agreement between independent measurements of the same cross section is generally taken as an endorsement of the accuracy of the measured data.
- In cases where only a single set of data is available for a given cross section, those data are simply shown here (i.e., not designated as recommended), unless there is a strong reason to reject them. Even when

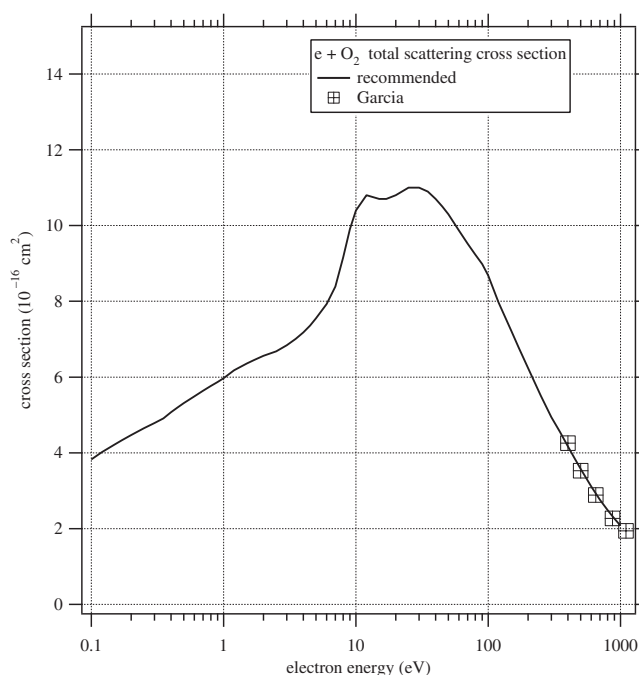


FIG. 1. Total scattering cross section for O₂. The recommended values by Karwasz *et al.*⁹ are compared with the cross section measured by Garcia *et al.*¹⁰

multiple sets of data are available, no recommendation is made if there is a significant disagreement among them or they are fragmentary (e.g., being available only at one point of collision energy).

In this way, the present paper aims to provide a more complete data set for electron collisions with O₂ than any previous publication. The literature has been surveyed through the end of 2007. Molecular properties (e.g., spectroscopic constants) of O₂ are presented in JPCRD89.

2. Total Scattering Cross Section

For oxygen molecules, a fairly large number of measurements have been performed on the total scattering cross section (Q_T). After a careful evaluation of those measurements, Karwasz *et al.*⁹ determined the recommended values of Q_T for the energy region of 0.1–1000 eV. The result is consistent with the data recommended by Kanik *et al.* in their review paper⁴ for the energy range of 1–1000 eV. The only measurement not considered by Karwasz *et al.* is that of Garcia *et al.*¹⁰ in a high-energy region (i.e., 400–5500 eV). In Fig. 1, the Q_T obtained by Garcia *et al.* are compared with the recommended values of Karwasz *et al.* The two sets of cross section well agree with each other. Here we recommend the Q_T of Karwasz *et al.* for use. Those values are presented in Table 1.

As is mentioned in Sec. 6, a shape resonance has an effect in the energy region of 0.1–1 eV. It produces very sharp peaks in the energy dependence of Q_T . The width of the peaks is too narrow for the resonance to have practical im-

TABLE 1. Recommended values of total scattering cross section

Energy (eV)	Cross section (10^{-16} cm^2)
0.1	3.83
0.12	4.02
0.15	4.22
0.17	4.33
0.2	4.47
0.25	4.65
0.3	4.79
0.35	4.91
0.4	5.07
0.45	5.20
0.5	5.31
0.6	5.49
0.7	5.64
0.8	5.77
0.9	5.87
1	5.97
1.2	6.18
1.5	6.36
1.7	6.45
2	6.56
2.5	6.68
3	6.84
3.5	7.01
4	7.18
4.5	7.36
5	7.55
6	7.93
7	8.39
8	9.16
9	9.91
10	10.4
12	10.8
15	10.7
17	10.7
20	10.8
25	11.0
30	11.0
35	10.9
40	10.7
45	10.5
50	10.3
60	9.87
70	9.52
80	9.23
90	8.98
100	8.68
120	7.97
150	7.21
170	6.78
200	6.24
250	5.51
300	4.94
350	4.55
400	4.17
450	3.85
500	3.58
600	3.11
700	2.76
800	2.49
900	2.26
1000	2.08

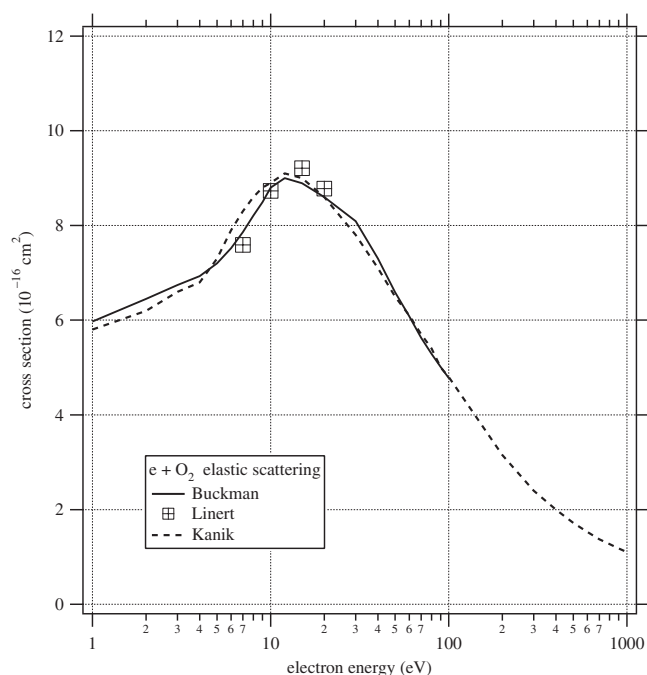


FIG. 2. Elastic scattering cross section for O_2 . Two sets of recommended values (i.e., those by Buckman *et al.*¹¹ and by Kanik *et al.*⁴) are compared with the cross sections measured by Linert *et al.*¹⁵

portance. The recommended data of Karwasz *et al.*, and hence the present ones, simply ignore those resonant peaks.

3. Elastic Scattering

Normally electron beam experiments have insufficient energy resolution to resolve each rotational state of oxygen molecules. Hence the elastic cross section experimentally obtained includes the cross sections for rotational transitions and is called the “vibrationally elastic” cross section. In the present section, Q_{elas} means such a vibrationally elastic cross section.

In 1993, Kanik *et al.*⁴ determined their recommended cross section for the electron elastic scattering from O_2 . They reported Q_{elas} for the energy region of 1–1000 eV. In 2003, Buckman *et al.*¹¹ reported their own recommended values of Q_{elas} for the energy range of 1–100 eV. They based their recommendation on the experiments done by Trajmar *et al.*,¹² Shyn and Sharp,¹³ and Sullivan *et al.*¹⁴ Buckman *et al.* also considered the data recommended by Kanik *et al.* In Fig. 2, the two sets of recommended cross sections (i.e., the results of Kanik *et al.* and Buckman *et al.*) are compared with each other.

Recently Linert *et al.*¹⁵ measured the differential cross section (DCS) for the elastic scattering in the backward direction (100° – 180°). They determined the integral elastic cross section Q_{elas} from their DCS and those measured previously by Sullivan *et al.*¹⁴ at 15° – 100° . The resulting Q_{elas} , reported at the energies of 7–20 eV, is also shown in Fig. 2. The values of Linert *et al.* well agree with the recommended data of Buckman *et al.*¹¹ The agreement is clearly better than the agreement with Kanik *et al.*⁴ Here we recommend the Q_{elas}

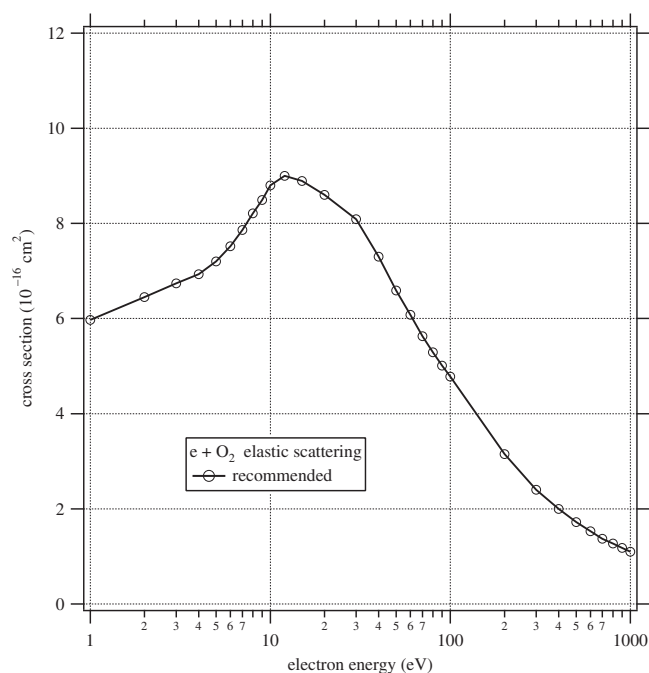


FIG. 3. Recommended values of the elastic scattering cross section for O₂.

of Buckman *et al.* for the energy range of 1–100 eV and extend them to the higher energy (100–1000 eV) with taking the data of Kanik *et al.* The recommended cross section is shown in Fig. 3 and Table 2. Buckman *et al.* claimed the uncertainty of the Q_{elas} to be within $\pm 20\%$.

As is described in Sec. 6, the elastic scattering also shows an effect of shape resonance in the region of 0.1–1 eV. The resonance appears as a series of very sharp peaks in the energy dependence of the cross section. However, no reliable experimental data, including the resonance effect, are available for the integral cross section Q_{elas} in the energy region below 1 eV (see Sec. 6 for more details).

4. Momentum-Transfer Cross Section

The (elastic) momentum-transfer cross section is defined by

$$Q_m = 2\pi \int (1 - \cos \theta) q_{\text{elas}}(\theta) \sin \theta d\theta, \quad (1)$$

where $q_{\text{elas}}(\theta)$ is the DCS for the (vibrationally) elastic scattering. The momentum-transfer cross section gives a measure of momentum transfer during the (elastic) collision.

Elford *et al.*¹⁶ presented their recommended values of Q_m for O₂. In the low-energy region (<0.3 eV), their recommendation is based on a swarm experiment. At the higher energies, they followed the result of JPCRD89.³ In the energy range of 2–20 eV, however, they modified the Q_m of JPCRD89 by using the values derived by Sullivan *et al.*¹⁴ from their beam measurement of elastic DCS. Sullivan *et al.* measured the DCSs at the scattering angles of 15°–100°. To

TABLE 2. Recommended values of elastic scattering cross section

Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
1	5.97
2	6.45
3	6.74
4	6.93
5	7.20
6	7.52
7	7.86
8	8.21
9	8.49
10	8.80
12	9.00
15	8.89
20	8.60
30	8.09
40	7.30
50	6.59
60	6.08
70	5.63
80	5.29
90	5.01
100	4.78
200	3.15
300	2.40
400	2.00
500	1.72
600	1.53
700	1.37
800	1.27
900	1.18
1000	1.10

derive the Q_m , they needed to extrapolate their DCSs in the forward and backward directions. The cross section of Elford *et al.* is shown in Fig. 4.

As is stated in Sec. 3, Linert *et al.*¹⁵ recently measured q_{elas} in the backward direction (i.e., 100°–180°). Combining their DCSs with those of Sullivan *et al.*, Linert *et al.* determined their own Q_m at the energies of 7–20 eV. In Fig. 4, the Q_m of Linert *et al.* are compared with those of Elford *et al.*¹⁶ There is a remarkable difference between the two sets of Q_m . From the definition of Q_m [see Eq. (1)], the DCS in the backward direction is very effective to Q_m . Because there is no need to extrapolate in the backward direction, the data obtained by Linert *et al.* should be more accurate than the corresponding values of Sullivan *et al.*, on which the data of Elford *et al.* are based. In conclusion, we recommend the Q_m of Elford *et al.* but modify them with taking the values of Linert *et al.* as shown in Fig. 5. The resulting values are presented in Table 3. Elford *et al.* estimated the uncertainty of their recommended data to be within 20%. The present modification has been done in this range of allowance.

In the energy region below 1 eV, a shape resonance affects q_{elas} , as is shown in Sec. 6. No experimental evidence, however, has been reported on the resonance effect on the momentum-transfer cross section so far.

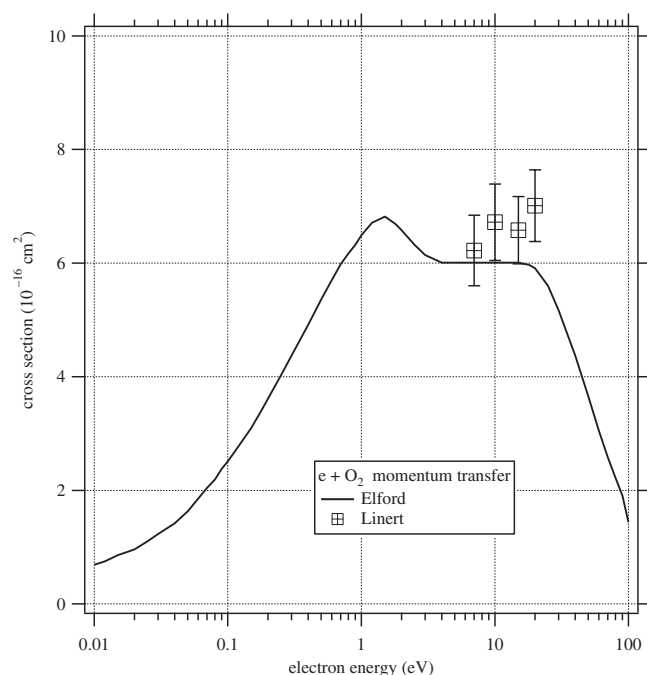


FIG. 4. Momentum-transfer cross section for O_2 . The recommended values by Elford *et al.*¹⁶ are compared with the cross section measured by Linert *et al.*¹⁵

5. Rotational Excitation

No reliable experimental information is available for the rotational excitation of O_2 . More specifically, no new (either theoretical or experimental) studies of rotational transition in O_2 have been reported since the publication of JPCRD89.³

One of the simple methods to estimate the rotational cross section Q_{rot} is the Born approximation with taking the elec-

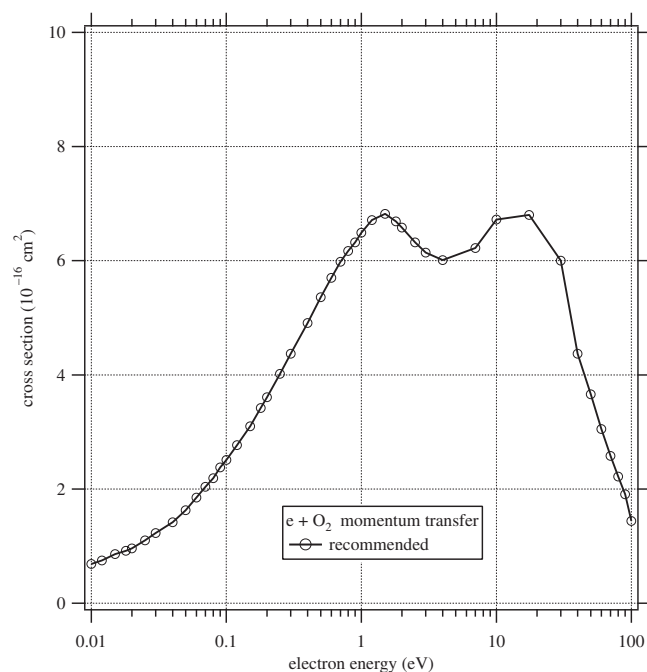


FIG. 5. Recommended values of the momentum-transfer cross section for O_2 .

TABLE 3. Recommended values of momentum-transfer cross section

Energy (eV)	Cross section (10^{-16} cm^2)
0.01	0.69
0.012	0.75
0.015	0.86
0.018	0.92
0.02	0.96
0.025	1.10
0.03	1.23
0.04	1.42
0.05	1.63
0.06	1.85
0.07	2.04
0.08	2.19
0.09	2.38
0.1	2.51
0.12	2.77
0.15	3.10
0.18	3.42
0.2	3.61
0.25	4.02
0.3	4.37
0.4	4.91
0.5	5.36
0.6	5.70
0.7	5.98
0.8	6.17
0.9	6.32
1	6.49
1.2	6.71
1.5	6.82
1.8	6.69
2	6.58
2.5	6.32
3	6.14
4	6.01
7	6.22
10	6.72
17.5	6.80
30	6.00
40	4.37
50	3.66
60	3.05
70	2.58
80	2.22
90	1.91
100	1.44

tron interaction with the molecular quadrupole moment. Due to the presence of unpaired spins, the lowest rotational level of O_2 is $J=1$. Furthermore, because of molecular symmetry, rotational transitions are allowed when $\Delta J=\text{even}$. The lowest rotational transition in O_2 , therefore, is the process $J=1 \rightarrow 3$. The Born theory, together with the electron-quadrupole interaction, gives the cross section in the form¹⁷

$$Q^{\text{Born,quad}}(1 \rightarrow 3)(\text{in a.u.}) = \frac{16\pi}{75} \sqrt{1 - \frac{10B}{E}} \langle M_2 \rangle^2. \quad (2)$$

Here B is the rotational constant in eV, $\langle M_2 \rangle$ is the quadrupole moment in a.u., and E is the electron energy in eV. For

O₂, we have $B=1.783 \times 10^{-4}$ and $\langle M_2 \rangle = -0.26$. Then we obtain the rotational cross sections $Q_{\text{rot}}(1 \rightarrow 3) = 1.15 \times 10^{-18}$ and $1.26 \times 10^{-18} \text{ cm}^2$ at $E=0.01$ and 0.1 eV , respectively. These values may give a typical example of Q_{rot} for O₂ but should be tested against any experiment (or any elaborate calculation).

6. Vibrational Excitation

According to Allan's experiment,¹⁸ the vibrational cross section Q_{vib} of O₂ shows a completely different behavior in the energy regions above about 1 eV and below that. At the energies above 1 eV , the cross section shows a broad peak at about 10 eV . In the region below 1 eV , the cross section consists of a set of very sharp peaks. In between, Q_{vib} is very small. Accordingly this section is divided into two subsections.

6.1. $E > 1 \text{ eV}$

At the publication of JPCRD89,³ no definite information was available on the cross section of individual vibrational transitions, $\nu=0 \rightarrow \nu'$. Instead, only the sum $\sum_{\nu'} Q_{\text{vib}}(0 \rightarrow \nu')$ was shown in the paper. In 1993, Shyn and Sweeney¹⁹ reported their measurement of the individual vibrational cross sections for $\nu=0 \rightarrow 1, 2, 3, 4$. They obtained the corresponding DCS at the scattering angles of 12° – 168° for the electron energies of 5 – 15 eV . A similar measurement was done by Brunger *et al.*²⁰ (The corresponding integral cross sections were given in the paper by Noble *et al.*²¹ to compare with theoretical results.) Brunger *et al.* reported the vibrational cross sections for $\nu=0 \rightarrow 1, 2, 3, 4$ at the energies of 7 – 15 eV . They obtained the DCS only in the forward directions (10° – 90°). The resulting DCSs are somewhat different from those of Shyn and Sweeney (see, e.g., Figs. 6 and 7).

Recently Linert and Zubek²² made a rather comprehensive measurement of DCS for the vibrational excitation. With the use of a magnetic angle changer, they determined DCS for a wide range of scattering angles (i.e., 15° – 180°). They obtained the cross sections for $\nu=0 \rightarrow 1, 2, 3, 4$ but only at the energy of 10 eV . Their DCS is in better agreement with those of Shyn and Sweeney¹⁹ than those with Brunger *et al.*²⁰ For the process $\nu=0 \rightarrow 1$ (see Fig. 6), the DCS of Shyn and Sweeney has a similar θ dependence but a somewhat small absolute magnitude compared with the result of Linert and Zubek. The discrepancy may be due to a rather ambiguous separation of the energy loss peak of $\nu'=1$ from the elastic peak, which is very large. For other transitions, the DCSs of the two experiments (i.e., by Shyn and Sweeney and Linert and Zubek) well agree with each other (as an example, DCS for $\nu=0 \rightarrow 2$ being shown in Fig. 7). Here we adopt as the recommended values the integral cross sections of Shyn and Sweeney except that for $\nu'=1$ at 10 eV . For $Q_{\text{vib}}(0 \rightarrow 1)$ at 10 eV , we prefer the value of Linert and Zubek to that of Shyn and Sweeney. The present recommended values of the vibrational cross sections are shown in Fig. 8 and Table 4. Considering the uncertainty claimed by the original authors, the present recommended values are correct within 20%.

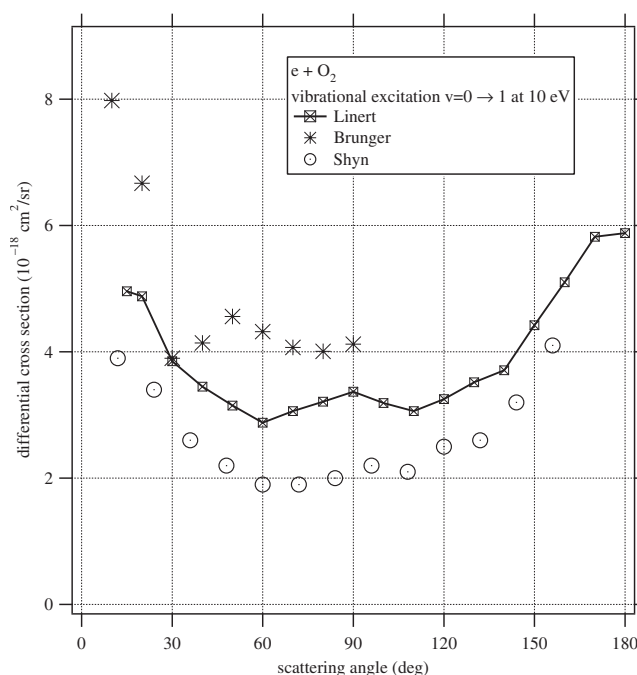


FIG. 6. DCSs for the vibrational transition $\nu=0 \rightarrow 1$ at the electron energy of 10 eV . Three sets of measurements (Linert and Zubek,²² Brunger *et al.*,²⁰ and Shyn and Sweeney¹⁹) are compared with each other.

Allan¹⁸ measured the DCS at 90° . He obtained a very detailed energy dependence of the DCS up to 16 eV . He showed that the corresponding DCS of Shyn and Sweeney¹⁹ is consistent with the result of his measurement. Furthermore, in the region of 6 – 16 eV , Allan observed excitations of very high vibrational states (up to $\nu'=8$). He concluded that the broad peak in the energy region is caused by the $^4\Sigma_u^-$ resonance.

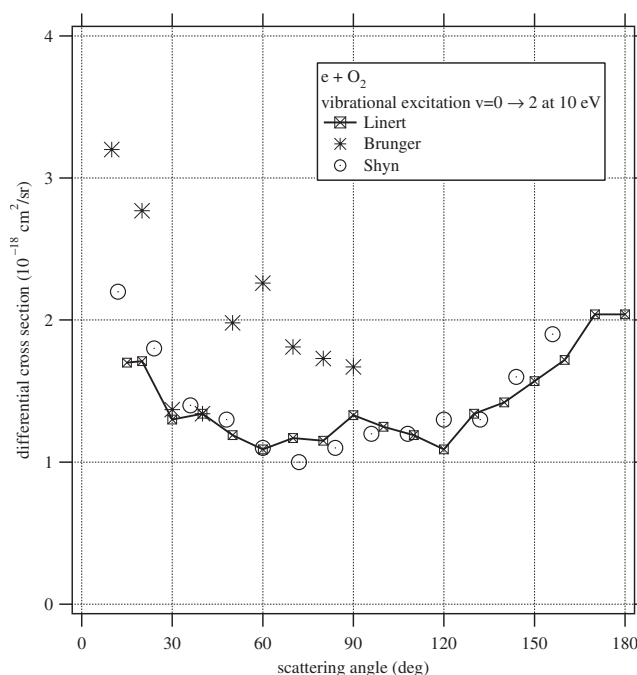


FIG. 7. DCSs for the vibrational transition $\nu=0 \rightarrow 2$ at the electron energy of 10 eV . Three sets of measurements (Linert and Zubek,²² Brunger *et al.*,²⁰ and Shyn and Sweeney¹⁹) are compared with each other.

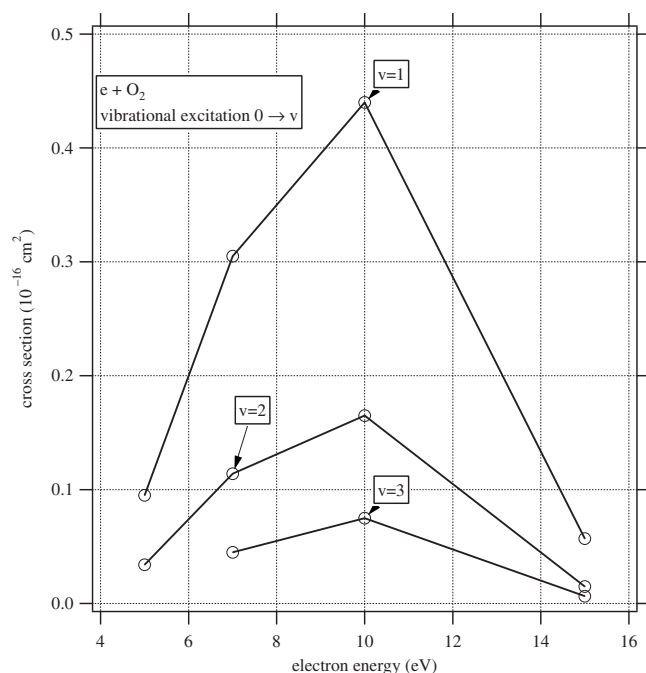


FIG. 8. Recommended values of the vibrational cross sections for the transitions $v=0 \rightarrow v'$, 1, 2, 3.

6.2. $E < 1$ eV

It is known that the vibrational cross section of O_2 has very sharp resonant peaks in the energy region of 0.2–1 eV.²³ Those peaks are due to a temporary electron capture of O_2 to form a negative ion state O_2^- ($^2\Pi_g$). Allan¹⁸ made a very detailed study of the resonance. He measured the DCS for the vibrational transitions $v=0 \rightarrow v'$ with $v' = 1-7$. All the vibrational cross sections have a sharp peak at the same position of the electron energy, which corresponds to the vibrational levels (v'') of O_2^- ($^2\Pi_g$). Allan found peaks at 0.214 eV ($v''=5$) to 2.197 eV ($v''=24$). From theoretical studies (e.g., Higgins *et al.*²⁴), the width of each peak should be very small. According to Allan, the width is narrower than the apparatus profile of his experiment. In other words, the

TABLE 4. Recommended cross sections for the vibrational transitions, $v=0 \rightarrow v'$

Energy (eV)	Cross section for $v=0 \rightarrow v'$ (10^{-16} cm ²)		
	$v'=1$	$v'=2$	$v'=3$
5	0.095	0.034	
7	0.305	0.114	0.045
10	0.44	0.165	0.075
15	0.057	0.015	0.0065

widths of the measured cross sections do not represent the real profiles of resonance. For this reason, Allan could not derive any absolute magnitude of the cross section from his measurement. Instead he derived the energy-integrated cross section, $\Delta E \cdot Q_{\text{vib}}$, where ΔE is the width of each peak. Table 5 shows an example of the energy-integrated cross section derived by Allan. JPCRD89 shows a similar table, but it is based on the measurement of $\Delta E \cdot Q_{\text{vib}}$ by Linder and Schmidt.²³ The values of Linder and Schmidt are by about three times smaller than the present ones. Allan stated that this difference is probably caused by the inadequate way of normalization used by Linder and Schmidt. There are several calculations of the resonance width. The most recent one, obtained by Higgins *et al.*,²⁴ is given in Table 5. If we adopt these theoretical values of the resonance width ΔE , the absolute value of the cross section Q_{vib} can be derived from the energy-integrated cross section $\Delta E \cdot Q_{\text{vib}}$ measured by Allan. The resulting Q_{vib} are also shown in Table 5. The resonance cross sections thus obtained for $v=0 \rightarrow 1$ and 2 are plotted in Fig. 9 with the corresponding cross sections in the higher energy region (i.e., those shown in Fig. 8).

This $^2\Pi_g$ resonance has an effect also in the cross section for other processes. Allan¹⁸ measured also the DCS (at 90°) for elastic scattering in the energy range of 0.2–16 eV. The elastic cross section has a sharp peak at the resonance corresponding to the O_2^- ($^2\Pi_g$, v'') with $v''=5-14$. Those peaks appear on a large background cross section. That is, for the

TABLE 5. Resonance cross section for the vibrational excitation $v=0 \rightarrow v'$ of O_2 . The quantum number v'' indicates the vibrational state of the resonance state and ΔE is the width of the resonance state

v''	Resonance energy ^a (eV)	$\Delta E \cdot Q_{\text{vib}}$ ^a (10^{-20} eV cm ²)			ΔE ^b (10^{-3} eV)	Q_{vib} ^c (10^{-16} cm ²)		
		$v'=1$	$v'=2$	$v'=3$		$v'=1$	$v'=2$	$v'=3$
5	0.214	(3) ^d			0.896	0.3		
6	0.338	153			2.17	7.05		
7	0.460	327	(1.6) ^d		3.32	9.85	0.05	
8	0.579	334	40		4.99	6.69	0.80	
9	0.696	238	88	(0.06) ^d	7.02	3.39	1.3	0.001
10	0.812	138	95	5.6				
11	0.925	67	76	16				

^aFrom the measurement by Allan.¹⁸

^bFrom a theoretical calculation by Higgins *et al.*²⁴

^cDerived from the $\Delta E \cdot Q_{\text{vib}}$ of Allan and ΔE of Higgins *et al.*

^dValues in the parentheses have a large uncertainty (up to a factor of 2).

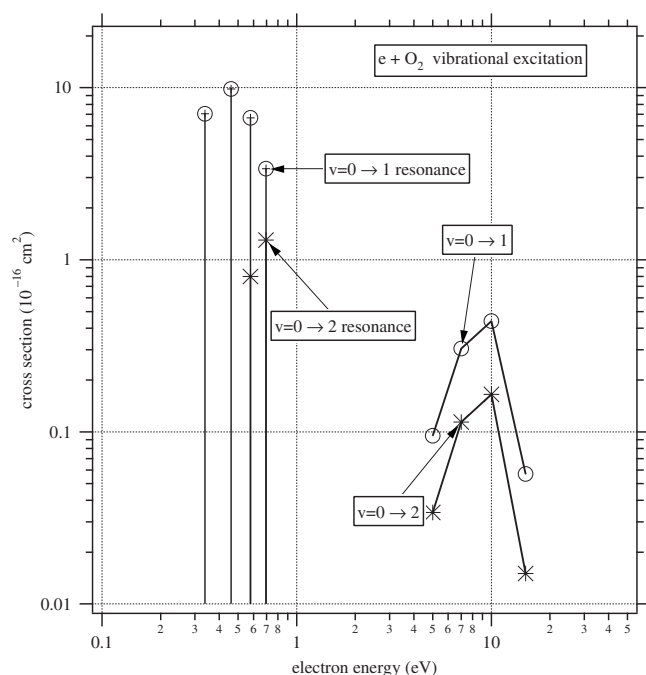


FIG. 9. Cross sections for the vibrational excitations $\nu=0 \rightarrow 1, 2$ of O_2 . In the energy region below 1 eV, typical values of the cross section due to the $^2\Pi_g$ resonance (with assuming the theoretical resonance width) are shown. Details of the resonant cross section are presented in Table 5. Cross sections in the region above 1 eV are the same as shown in Fig. 8.

elastic scattering, the contribution of the resonance is small compared with the nonresonant one. This is in remarkable contrast to the case of vibrational excitation. No quantitative estimate is available, however, for the resonance contribution to the integral cross section for the elastic scattering.

In this energy region, the total scattering cross section Q_T is given by the sum of the cross sections for elastic scattering and rotational and vibrational excitations. Thus Q_T should have an effect of the $^2\Pi_g$ resonance. Subramanian and Kumar²⁵ measured Q_T at the energies as low as 0.15 eV. However, the energy positions of their experiment were too sparse to observe such a sharp resonance as seen in the vibrational excitation. With the use of photoelectrons as an electron source, Ziesel *et al.*²⁶ performed a beam transmission experiment with a very low-energy electron beam (down to 0.012 eV). To collimate the low-energy electrons, they applied a magnetic field. With the use of this apparatus, they obtained a total scattering cross section but only for backward scattering. The result shows a resonance structure very similar to that in the elastic DCS found by Allan.¹⁸

7. Excitation of Electronic States

An experimental study of excitation of electronic state of O_2 has been limited to several lowest states. Table 6 shows those states for which experimental data on the excitation cross section are available. Each of the states is separately discussed below. In the last subsection (Sec. 7.4), related information about higher states is also given. In JPCRD89,³ the excitation cross sections of the electronic states, Q_{exc} ,

TABLE 6. Electronic states of O_2 for which the cross section data are available (a more detailed list of the energy levels is given in JPCRD89³)

State	T_0 (eV) ^{a,b}	Figure	Table
a $^1\Delta_g$	0.977	11	7
b $^1\Sigma_g^+$	1.627	13	7
c $^1\Sigma_u^-$	4.050	14	8
A' (C) $^3\Delta_u^c$	4.262	14	8
A $^3\Sigma_u^+$	4.340	14	8
B $^3\Sigma_u^-$	6.120	16	9

^aEnergy of the lowest vibrational state relative to the ground level $X \ ^3\Sigma_g^-$ ($\nu=0$).

^bCited from JPCRD89.

^cIn JPCRD89, this state is designated as C.

were reviewed on the basis of rather old experimental data (mostly published in the 1970s). In the present paper, more recent data are collected and evaluated to produce the recommended cross sections.

7.1. a $^1\Delta_g$

After the publication of JPCRD89, five groups reported the measurement of their cross section for the excitation of a $^1\Delta_g$ state. The following shows the authors and the energy regions of those experiments:

- Middleton *et al.*,^{27,28} 5–20 eV;
- Doering,²⁹ 2.6–28.6 eV;
- Shyn and Sweeney,³⁰ 5–20 eV;
- Allan,³¹ 1–18 eV (only DCS at 30° and 90°);
- Linert and Zubek,³² 10 eV.

Figure 10 compares the DCSs measured at 10 eV by four of the groups (Doering reporting no data at 10 eV). For comparison, the figure also shows the result of the most recent calculation by Tashiro *et al.*^{33,34} Linert and Zubek obtained the most comprehensive set of DCSs (i.e., cross sections for the scattering angles up to 180°). The result of Allan is in good agreement with the DCS of Linert and Zubek. The data of Shyn and Sweeney agree fairly well with the value of Linert and Zubek except at the angles smaller than 30°. The cross section of Middleton *et al.*, which is measured only at the angles less than 90°, significantly deflects from the values of Linert and Zubek. Finally the theoretical values of Tashiro *et al.* are consistent with the experimental data obtained by Linert and Zubek. [It should be noted here that the DCSs of Allan and Linert and Zubek are the cross sections corresponding to the excitation of the vibrationally ground level ($\nu=0$) of the a $^1\Delta_g$ state. Those groups also obtained the cross section for other vibrational levels of the state. According to the authors, however, the $\nu=0$ cross section is more than 90% of the vibrationally summed cross section of the state, which is the value obtained by other experimental groups.]

In Fig. 11, we show the integral cross section for the excitation of the a $^1\Delta_g$ state. There are three sets of experimental data and one calculation. Note that Linert and Zubek³² give their cross section only at 10 eV. Here we do not show

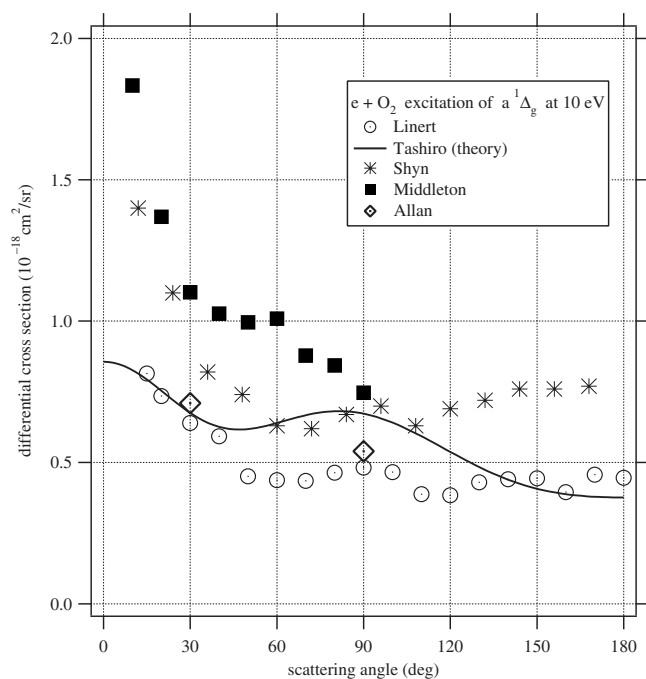


FIG. 10. DCSs for the excitation of the $a^1\Delta_g$ state of O_2 at the collision energy of 10 eV. Four sets of measurements (Linert and Zubek,³² Shyn and Sweeney,³⁰ Middleton *et al.*,²⁸ and Allan³¹) and a calculation (Tashiro *et al.*,³⁴) are compared with each other.

the cross section measured by Middleton *et al.*²⁷ because they may have a large uncertainty due to their extrapolation of DCS in a wide range of scattering angles. Those three sets of experimental data shown in Fig. 11 are consistent with

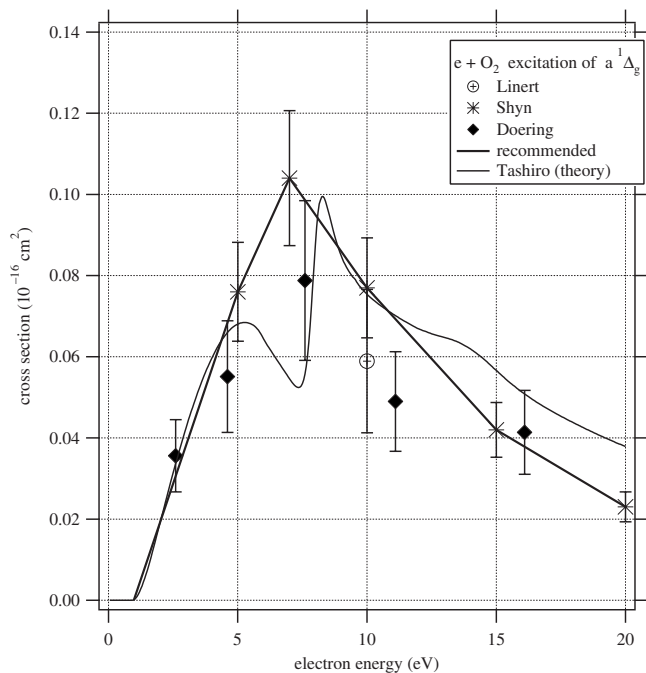


FIG. 11. Cross sections for the excitation of the $a^1\Delta_g$ state of O_2 . Three sets of experimental data (Linert and Zubek,³² Shyn and Sweeney,³⁰ and Doering²⁹) are compared with the theoretical result of Tashiro *et al.*³³ The present recommended values are indicated with a thick solid line.

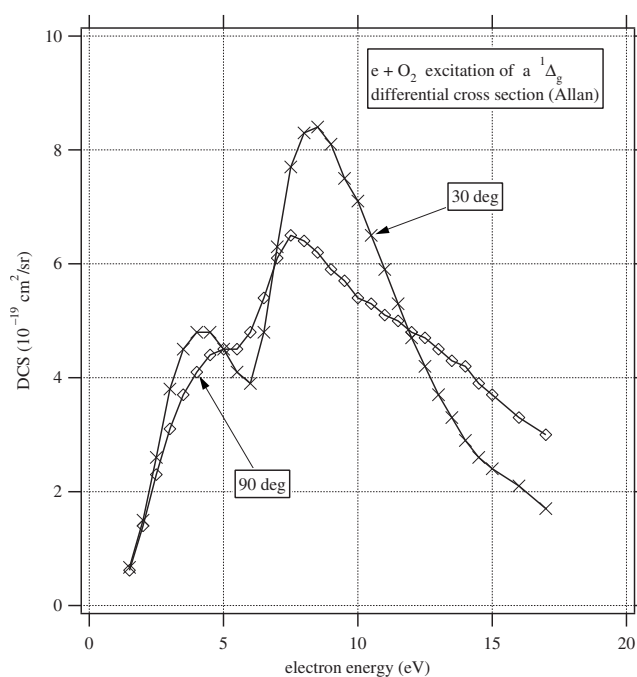


FIG. 12. Energy dependence of the DCSs for the excitation of the $a^1\Delta_g$ state of O_2 measured by Allan³¹ at the scattering angles of 30° and 90°.

each other. Furthermore they are in overall agreement with the result of the calculation of Tashiro *et al.*³³ The theoretical cross section shows a rapidly changing structure due to resonance. The calculation was based on the fixed nuclei approximation. The resonance structure may depend on the internuclear distance. Hence the structure may be smoothed out when the nuclear dependence is taken into account in the calculation. Allan³¹ measured a detailed energy dependence of the DCS at 30° and 90°. Each set of his DCSs shows the resonance structure similar to the theoretical result. Allan shows, however, that the structure is changed with the scattering angle (see Fig. 12). Therefore, the integral cross section should have a slight effect of the resonance, if any. In conclusion,³⁰ we here adopt the cross sections of Shyn and Sweeney³⁰ as the recommended ones. They are presented in Table 7. Shyn and Sweeney evaluated the uncertainty of their cross sections to be $\pm 16\%$.

7.2. $b^1\Sigma_g^+$

The two states, $a^1\Delta_g$ and $b^1\Sigma_g^+$, have the same configuration of molecular orbitals. The corresponding excitation

TABLE 7. Recommended cross sections for the excitations of the electronic states, $a^1\Delta_g$ and $b^1\Sigma_g^+$

Energy (eV)	Cross section (10^{-16} cm^2)	
	$a^1\Delta_g$	$b^1\Sigma_g^+$
5	0.076	0.020
7	0.104	0.033
10	0.077	0.019
15	0.042	0.0078
20	0.023	0.0055

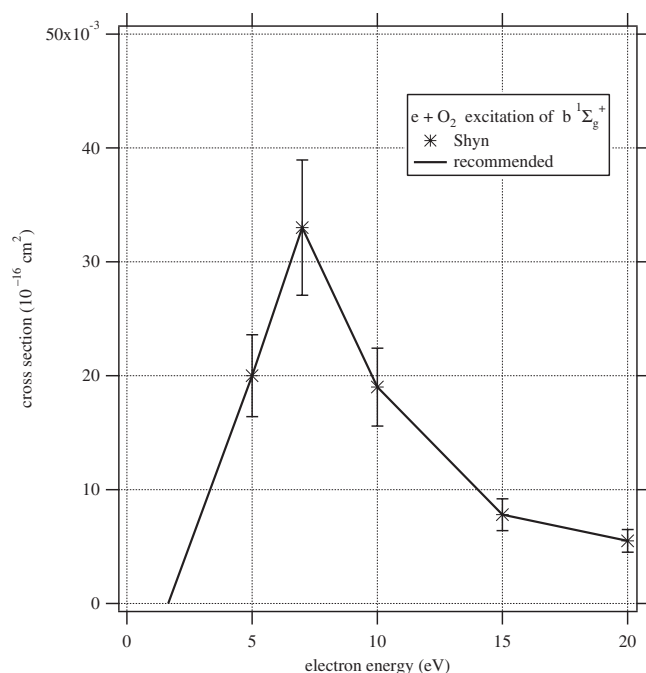


FIG. 13. Recommended values of the cross section for the excitation of the $b\ ^1\Sigma_g^+$ state of O_2 based on the experimental data obtained by Shyn and Sweeney³⁰.

energies are not much different from each other. Thus we expect that the excitation cross sections are not much different for the two states. We have three sets of measurements of the cross section for this state.^{27,30,31} Assuming the same situation as in the case of the $a\ ^1\Delta_g$ state, we select the data of Shyn and Sweeney³⁰ as the recommended values for the excitation of the $b\ ^1\Sigma_g^+$ state. Those data are shown in Fig. 13 and Table 7. The uncertainty of the cross section was estimated by Shyn and Sweeney to be $\pm 18\%$.

7.3. $A\ ^3\Sigma_u^+$, $A'\ ^3\Delta_u$, $c\ ^1\Sigma_u^-$

The threshold energies of the excitations of these three states are very close. Normally in the electron energy loss measurement, the energy loss peaks corresponding to these excitations are overlapped with each other. Shyn and Sweeney³⁵ attempted to decompose the loss peak into individual components. Their conclusion, however, may have a large uncertainty (see Green *et al.*³⁶). Tashiro *et al.*^{33,34} made a detailed calculation of the excitation of the electronic states of O_2 and obtained cross sections each for the excitation of the A , A' , and c states. The calculation shows that the excitation cross section for the A' state, $Q_{\text{exc}}(A')$, is very large compared with the other two cross sections, $Q_{\text{exc}}(A)$ and $Q_{\text{exc}}(c)$, which have almost the same magnitude. On the other hand, Shyn and Sweeney obtained two large cross sections [$Q_{\text{exc}}(A)$ and $Q_{\text{exc}}(A')$] and one small one [$Q_{\text{exc}}(c)$]. Thus we have no definite information on the relative magnitudes of the three cross sections. In the following, only the sum of the three cross sections [denoted by $Q_{\text{exc}}(A+A'+c)$] is presented.

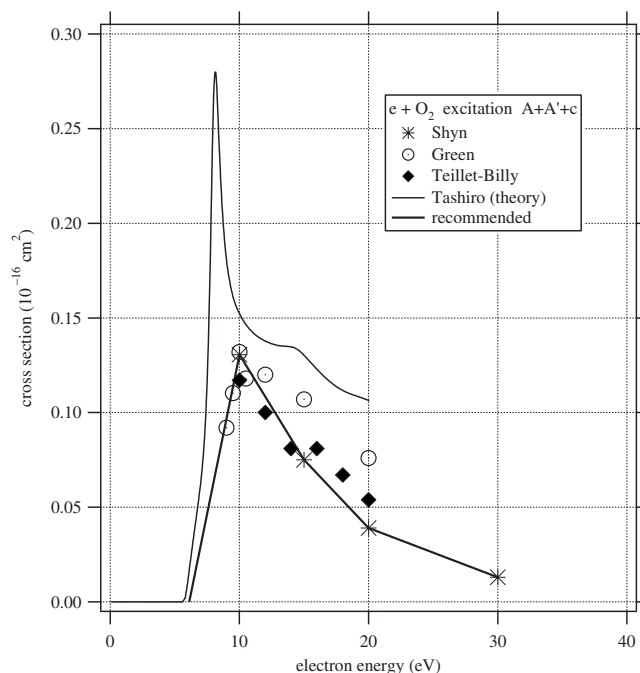


FIG. 14. Combined cross sections for the excitations of the states $A\ ^3\Sigma_u^+$, $A'\ ^3\Delta_u$, and $c\ ^1\Sigma_u^-$ of O_2 . Three sets of experimental data (Shyn and Sweeney,³⁵ Green *et al.*,³⁶ and Teillet-Billy *et al.*³⁷) are compared with the theoretical result of Tashiro *et al.*³³ The present recommended values are indicated with a thick solid line.

In Fig. 14, we show the results of three measurements reported after the publication of JPCRD89 (i.e., those of Teillet-Billy *et al.*,³⁷ Shyn and Sweeney,³⁵ and Green *et al.*^{36,38}). The values of Shyn and Sweeney are the sum of their cross sections separately reported for the A , A' , and c states. The cross sections of Green *et al.*³⁶ were derived from the DCS reported by them.³⁸ They measured the DCS only up to 90° . Because of the wide-range extrapolation, their integral cross section may have a large uncertainty. Here we adopt the cross section of Shyn and Sweeney as the recommended data. Those cross sections are tabulated in Table 8. They are in good agreement with the experimental data of Teillet-Billy *et al.* In Fig. 14, we also plot the theoretical cross section obtained by Tashiro *et al.*³³ The theoretical values have a sharp resonant peak at around 9 eV. The calculation was based on the fixed nuclei approximation. The potential curves for the upper three states (i.e., A , A' , and c) have a minimum at the internuclear distance much larger than the minimum position of the ground state, so that the fixed nuclei approximation might be unreliable in this sys-

TABLE 8. Recommended cross sections for the excitations of the electronic states, $A\ ^3\Sigma_u^+ + A'\ ^3\Delta_u + c\ ^1\Sigma_u^-$

Energy (eV)	Cross section (10^{-16} cm^2)
10	0.1305
15	0.075
20	0.039
30	0.013

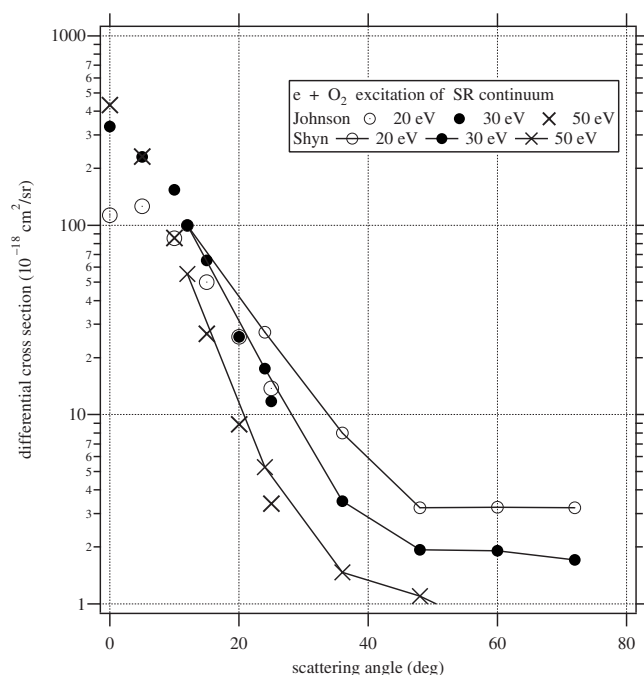


FIG. 15. DCSs for the excitation of the SR continuum of O_2 measured at 20, 30, and 50 eV by Johnson and Kanik⁴⁰ and Shyn *et al.*³⁹

tem. Allan³¹ measured the DCS at 90° for this process over the collision energies of 6–20 eV. His experimental result shows no evidence of resonance. Probably the effect of resonance, if any, is small in the case of excitations of the A, A', and c states.

7.4. $B^3\Sigma_u^-$ (Schumann-Runge Continuum) and Higher States

The electron energy loss spectrum for O_2 shows a broad peak ranging from 7 to 9.5 eV. This is called the Schumann-Runge (SR) continuum and caused by the excitation of the $B^3\Sigma_u^-$ state. Assuming that two other states also have contributions to this broad peak, Shyn *et al.*³⁹ derived cross sections for the three individual states. However, the decomposition of the loss peak is rather arbitrary. Here the sum of the three cross sections is designated as the cross section of the SR continuum obtained by Shyn *et al.*

Johnson and Kanik⁴⁰ made a measurement of DCSs for the SR continuum. They obtained the DCSs for the scattering angles of 0° – 25° and at the electron energies of 20, 30, 50, and 100 eV. Figure 15 compares the DCSs obtained by Shyn *et al.*³⁹ and Johnson and Kanik at $E=20, 30, 50$ eV. The two sets of cross section are consistent with each other. Since Johnson and Kanik gave no integral cross section, the Q_{exc} of Shyn *et al.* are chosen as the recommended data here. The result is shown in Fig. 16 and Table 9. Shyn *et al.* gave no information of the uncertainty of their summed cross section. If considering similar experiments of their group, however, the uncertainty of the present recommended data is around $\pm 20\%$.

Shyn *et al.*⁴¹ extended their measurement to the excitation of higher states. They obtained the cross sections for the

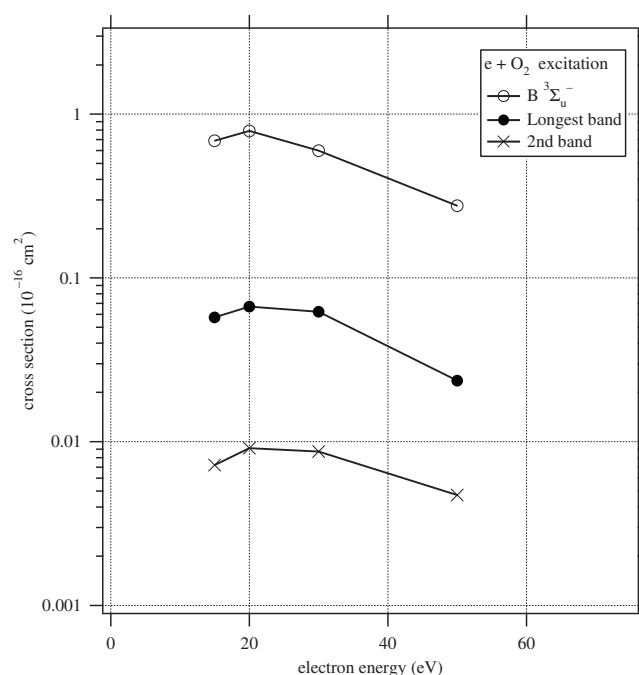
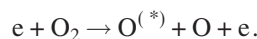


FIG. 16. Cross sections for the excitations of the SR continuum, the LB, and the 2B measured by Shyn *et al.*^{39,41}

excitations of the longest band (LB) and the second band (2B) in the energy loss spectrum. Those cross sections are also shown in Fig. 16 and Table 9. Johnson and Kanik⁴⁰ also measured the DCSs for these two bands. Their result is in quite good agreement with the corresponding ones of Shyn *et al.* Shyn *et al.* estimated the uncertainty of their data to be $\pm 20\%$ for LB and $\pm 23\%$ for 2B band.

8. Dissociation for Neutral Products

Here we are concerned with the process



One or both of the product atoms can be in its excited state. In the following, we present

- the total dissociation cross section for neutral products and
- the cross section for the production of $O(^1S)$

When the product atom emits radiation, we can measure the

TABLE 9. Recommended cross sections for the excitations of the electronic state $B^3\Sigma_u^-$ the LB, and the 2B

Energy (eV)	Cross section (10^{-16} cm^2)		
	$B^3\Sigma_u^-$	LB	2B
15	0.687	0.0575	0.007 20
20	0.790	0.0669	0.009 15
30	0.598	0.0622	0.008 71
50	0.2764	0.0236	0.004 72

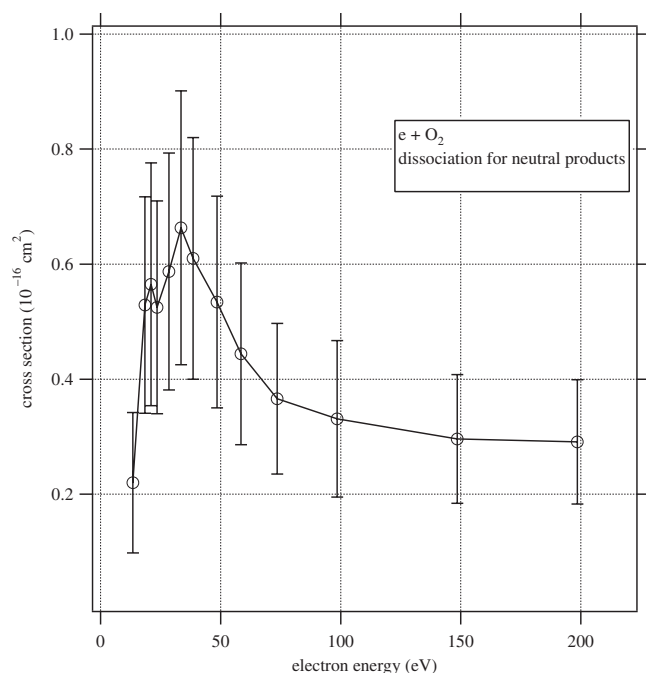


FIG. 17. Dissociation cross section for the neutral products (i.e., $e + \text{O}_2 \rightarrow e + \text{O} + \text{O}$) measured by Cosby⁴².

emission cross section for the radiation of specific wavelength. Those emission cross sections are dealt with in Sec. 11.

8.1. Total Dissociation Cross Section for Neutral Products

With the use of a fast O_2 beam, Cosby⁴² directly detected the dissociation fragment, O. He determined the total dissociation cross section by detecting the two fragment atoms in coincidence. His result is shown in Fig. 17 and Table 10. Cosby claimed the uncertainty of his data to be $\pm 34\%$.

The excitation of the SR continuum is known to contribute to a neutral dissociation [i.e., $\text{O} (^3\text{P}) + \text{O} (^1\text{D})$]. In fact, the

TABLE 10. Dissociation cross section for the neutral products measured by Cosby⁴²

Energy (eV)	Cross section (10^{-16} cm^2)
13.5	0.220
18.5	0.529
21.0	0.565
23.5	0.525
28.5	0.587
33.5	0.663
38.5	0.610
48.5	0.534
58.5	0.444
73.5	0.366
98.5	0.331
148.5	0.296
198.5	0.291

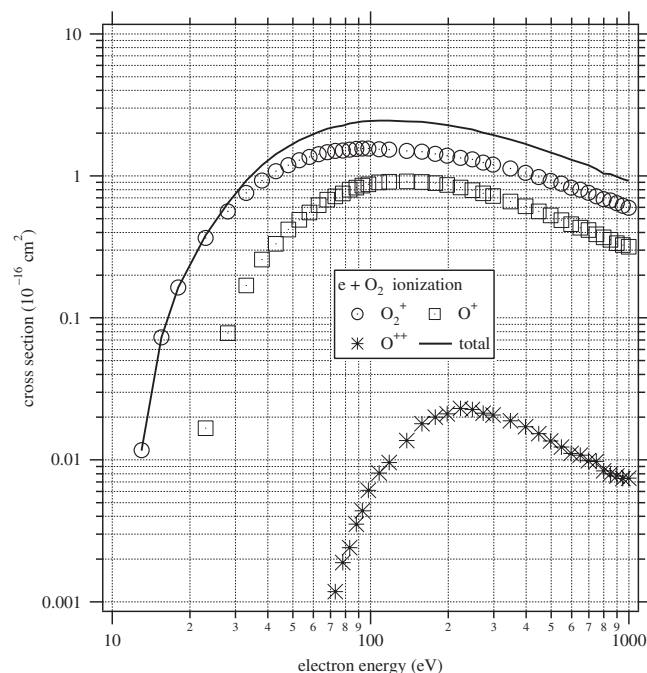


FIG. 18. Recommended values of ionization cross section of O_2 . Total ionization cross section and partial cross sections for the production of O_2^+ , O^+ , and O^{++} are shown.

present total dissociation cross section has a magnitude of the same order of the excitation cross section for the SR continuum shown in Fig. 16. As the electron energy increases, many higher excited states can lead to dissociation, so that the total dissociation cross section does not decrease rapidly.

8.2. Production of $\text{O} (^1\text{S})$

With the use of a Xe surface detector, LeClair and McConkey⁴³ could selectively detect $\text{O} (^1\text{S})$ upon electron-impact dissociation of O_2 . Comparing to a similar measurement of $\text{O} (^1\text{S})$ from N_2O and applying the Born-Bethe calibration technique to the latter experiment, LeClair and McConkey obtained an absolute value of the cross section for the process $\text{O}_2 \rightarrow \text{O} (^1\text{S})$. The result is shown in Fig. 22, together with the emission cross section for $\text{O}_2 \rightarrow \text{O}^*$. It is noted that the production of $\text{O} (^1\text{S})$ is a very minor process in the dissociation of O_2 .

9. Ionization

After evaluating all the available experimental data, Lindsay and Mangan⁴⁴ determined their recommended data set for the partial and total ionization cross sections of O_2 . Their values were based on the time of flight (TOF) measurement of each product ion by Straub *et al.*,⁴⁵ with a slight modification due to a recent recalibration of the experimental apparatus. Since no more recent experimental data are available, we here adopt the values recommended by Lindsay and Mangan. Those cross sections are shown in Fig. 18 and Table 11. In the figure, the cross sections are plotted for the pro-

TABLE 11. Recommended values of ionization cross sections

Energy (eV)	Cross section (10^{-16} cm^2)			Total
	O_2^+	O^+	O^{++}	
13	0.0117			0.0117
15.5	0.0730			0.0730
18	0.164			0.164
23	0.366	0.0167		0.383
28	0.563	0.0781		0.641
33	0.758	0.169		0.927
38	0.929	0.258		1.19
43	1.08	0.333		1.42
48	1.19	0.419		1.61
53	1.29	0.490		1.78
58	1.36	0.553		1.91
63	1.42	0.621		2.04
68	1.47	0.679		2.15
73	1.50	0.717	0.001 18	2.22
78	1.51	0.751	0.001 89	2.26
83	1.53	0.801	0.002 41	2.34
88	1.55	0.827	0.003 52	2.38
93	1.56	0.855	0.004 38	2.42
98	1.56	0.871	0.006 10	2.43
108	1.54	0.900	0.008 08	2.45
118	1.53	0.910	0.009 56	2.45
138	1.50	0.913	0.013 7	2.42
158	1.48	0.905	0.018 0	2.40
178	1.43	0.891	0.020 0	2.34
198	1.39	0.864	0.021 1	2.28
223	1.34	0.830	0.023 0	2.19
248	1.31	0.794	0.022 6	2.12
273	1.24	0.755	0.021 3	2.01
298	1.20	0.721	0.020 7	1.94
348	1.13	0.659	0.018 9	1.80
398	1.05	0.611	0.017 1	1.68
448	0.983	0.562	0.015 3	1.56
498	0.923	0.526	0.013 6	1.46
548	0.882	0.487	0.012 3	1.38
598	0.827	0.457	0.011 1	1.30
648	0.800	0.432	0.010 8	1.24
698	0.761	0.415	0.009 87	1.19
748	0.720	0.388	0.009 77	1.12
798	0.686	0.369	0.008 37	1.06
848	0.671	0.355	0.007 99	1.03
898	0.643	0.336	0.007 70	0.987
948	0.617	0.326	0.007 40	0.950
998	0.597	0.317	0.007 43	0.922

ductions of O_2^+ , O^+ , and O^{++} and their sum as the total ionization cross section $Q_{\text{ion}}(\text{tot})$. The uncertainty in each cross section was determined by Lindsay and Mangan to be $\pm 5\%$, $\pm 5\%$, $\pm 6\%$, and $\pm 5\%$, respectively. It should be noted that the cross section for O^+ production includes the cross section for the production of O_2^{++} because the TOF technique cannot discriminate the ions with the same mass/charge ratio.

The total ionization cross section can be directly derived from the measurement of total ion current. Figure 19 com-

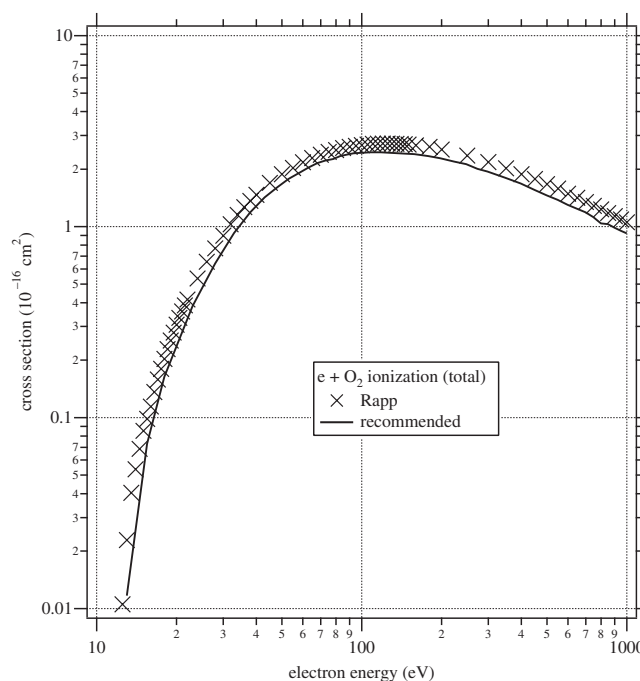


FIG. 19. Total ionization cross section of O_2 . The present recommended values are compared with the experimental data of Rapp and Englander-Golden⁴⁶.

pares the present recommended values of $Q_{\text{ion}}(\text{tot})$ with those obtained from the ion current measurement by Rapp and Englander-Golden.⁴⁶ The present values are systematically smaller (by about 10%–15%) than the ones of Rapp and Englander-Golden. Rapp and Englander-Golden reported that, due to chemical effects on metal surfaces, they had difficulty in normalizing the O_2 cross section (see the paper by Rapp and Englander-Golden for details). They estimated a large uncertainty (about $\pm 10\%$) for that. If we take into account this situation, the two sets of total ionization cross sections in Fig. 19 are consistent with each other. In JPCRD89, $Q_{\text{ion}}(\text{tot})$ was taken as the same as those of Rapp and Englander-Golden. At the publication of the paper, no reliable experimental data were available on $Q_{\text{ion}}(\text{O}_2^+)$. Then $Q_{\text{ion}}(\text{O}_2^+)$ was estimated as the difference, $Q_{\text{ion}}(\text{tot}) - [Q_{\text{ion}}(\text{O}^+) + Q_{\text{ion}}(\text{O}^{++})]$. Because of the difference between the two sets of $Q_{\text{ion}}(\text{tot})$ as shown in Fig. 19, the $Q_{\text{ion}}(\text{O}_2^+)$ in JPCRD89 is larger than the present values of $Q_{\text{ion}}(\text{O}_2^+)$.

When electrons ionize O_2 , molecular ions in several different electronic states [designated as $\text{O}_2^+(n)$] may be produced. By collecting all the secondary electrons, Doering and Yang⁴⁷ determined the cross section for the production of $\text{O}_2^+(n)$ with $n = X^2\Pi_g$, $a^4\Pi_u$, and $b^4\Sigma_g^-$ at the impact of electrons of 100 eV. The cross sections are shown in Table 12. Doering and Yang could not obtain the cross section for the $A^2\Pi_u$ state, so that the upper limit of the cross section is given for the state. As is shown in Sec. 11, Terrell *et al.*⁴⁸ measured the emission cross sections for the electron collision with O_2 . In particular, they obtained the Q_{emis} for the first negative band system $b \rightarrow a$ and the second negative band system $A \rightarrow X$ of O_2^+ . In Table 12, those emission cross

TABLE 12. Cross sections for the production of O_2^+ in specific electronic states at the 100 eV electron impact with O_2

Ionization excitation ^a		Emission ^b	
State of O_2^+	Cross section (10^{-18} cm ²)	Transition	Cross section (10^{-18} cm ²)
$X^2\Pi_g$	92.2		
$a^4\Pi_u$	50.8		
$b^4\Sigma_g^-$	22.1	$b^4\Sigma_g^- \rightarrow a^4\Pi_u$	32.8
$A^2\Pi_u$	<2	$A^2\Pi_u \rightarrow X^2\Pi_g$	10.2

^aObtained by Doering and Yang.⁴⁷

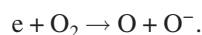
^bObtained by Terrell *et al.*⁴⁸

sections at 100 eV are compared with the ionization-excitation cross sections obtained by Doering and Yang. The emission cross sections may include cascade effects so that they should be larger than the ionization-excitation cross sections. In this sense, the two sets of cross sections in Table 12 are consistent with each other. In principle, it is very difficult to completely detect the relevant secondary electrons. Hence the ionization-excitation cross section obtained by Doering and Yang may include a large uncertainty.

A measurement of the energy distribution of the secondary electrons ejected upon electron-impact ionization is necessary when one evaluates the energy loss of the incident electron in a gas. JPCRD89 showed the data, i.e., the so-called singly differential cross sections (SDCSs) for ionization, measured by Opal *et al.*⁴⁹ at the incident-electron energies of 50, 100, 200, 300, 500, 1000, and 2000 eV. In 1991, Shyn and Sharp⁵⁰ reported their experimental data on the SDCSs of O_2 at the energies of 25, 50, 75, 100, 150, and 250 eV. When compared at 50 and 100 eV, the result of Shyn and Sharp is consistent with the previous data of Opal *et al.* Figure 20 shows the SDCSs of Shyn and Sharp, together with the values of Opal *et al.* at 100 eV. An integration of SDCSs over the energies of the secondary electron should give the total ionization cross section. Shyn and Sharp confirmed that their SDCS gives the total ionization cross section measured by other authors.

10. Dissociative Attachment

There are two, rather old, papers reporting the cross section for the process



One is the measurement of total negative ion current by Rapp and Briglia⁵¹ and the other is the swarm-beam experiment of Christophorou *et al.*⁵² The resulting cross sections of the two experiments are in good agreement with each other. (Christophorou⁵³ showed the comparison and discussed other earlier experiments.) Here we take the cross section of Rapp and Briglia as the recommended data. They are shown in Fig. 21 and Table 13.

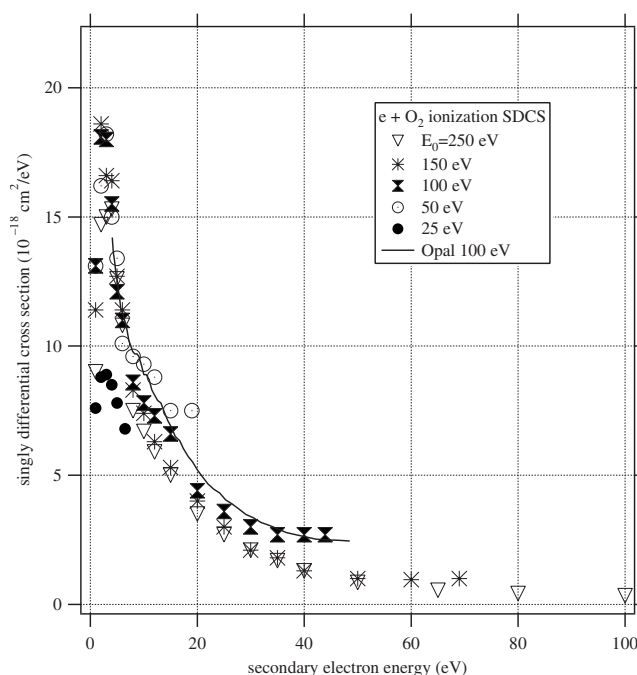


FIG. 20. Energy distribution of the secondary electrons ejected upon electron-impact ionization of O_2 . The energy of the incident electron is denoted by E_0 . The values obtained by Shyn and Sharp⁵⁰ are plotted with the data measured at $E_0=100$ eV by Opal *et al.*⁴⁹ for comparison.

11. Emission Cross Sections

When electrons collide with O_2 , radiations of various wavelengths are emitted. They are associated with dissociation (i.e., from O^* and O^{+*}) and ionization (i.e., from O_2^{+*}). No significant emission from neutral molecules (i.e., O_2^*) is

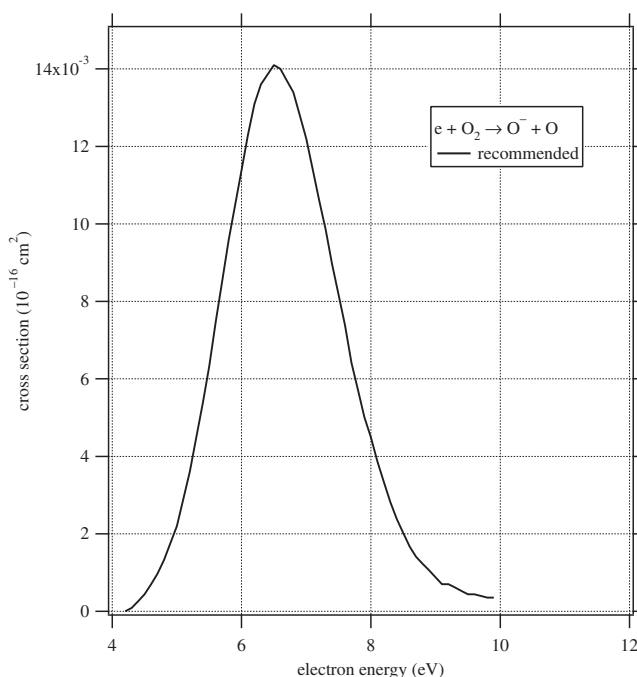


FIG. 21. Recommended cross sections for dissociative electron attachment of O_2 : $e + O_2 \rightarrow O^- + O$.

TABLE 13. Recommended cross sections for dissociative electron attachment

Energy (eV)	Cross section (10^{-16} cm ²)
4.2	0
4.3	0.000 088
4.4	0.000 264
4.5	0.000 440
4.6	0.000 704
4.7	0.000 968
4.8	0.001 32
4.9	0.001 76
5	0.002 20
5.1	0.002 90
5.2	0.003 61
5.3	0.004 49
5.4	0.005 37
5.5	0.006 33
5.6	0.007 48
5.7	0.008 53
5.8	0.009 59
5.9	0.010 5
6	0.011 4
6.1	0.012 3
6.2	0.013 1
6.3	0.013 6
6.5	0.014 1
6.6	0.014 0
6.7	0.013 7
6.8	0.013 4
6.9	0.012 8
7	0.012 2
7.1	0.011 4
7.2	0.010 6
7.3	0.009 85
7.4	0.008 97
7.5	0.008 18
7.6	0.007 39
7.7	0.006 42
7.8	0.005 72
7.9	0.005 01
8	0.004 49
8.1	0.003 87
8.2	0.003 34
8.3	0.002 82
8.4	0.002 38
8.5	0.002 02
8.6	0.001 67
8.7	0.001 41
8.8	0.001 23
8.9	0.001 06
9	0.000 880
9.1	0.000 704
9.2	0.000 704
9.3	0.000 616
9.4	0.000 528
9.5	0.000 440
9.6	0.000 440
9.8	0.000 352
9.9	0.000 352

known. Emission cross sections Q_{emis} have been measured many times for electron collisions with O₂. JPCRD89 summarizes those reported before 1989. After the publication of JPCRD89, several new measurements have been made. The results of those recent measurements are given below.

11.1. Emission from Dissociation Fragments (O*, O⁺*)

Using a new apparatus with a high resolution spectrometer, Kanik *et al.*⁵⁴ obtained absolute cross sections for the emissions of 135.6, 130.4, and 115.2 nm lines from atomic oxygen. The transitions for those emissions are shown in Table 14. Among them, the 135.6 nm line corresponds to a forbidden transition with a long lifetime (180 μ s). Special care was taken to detect all the emission from the transition. The Q_{emis} obtained by Kanik *et al.* are shown in Fig. 22 and Table 15 (and also in Table 14 for comparison with other lines). Kanik *et al.* estimated the overall error of their result to be $\pm 23\%$. Particularly for the 130.4 nm line, many experimental studies have been reported (see JPCRD89³). Kanik *et al.* claimed that their new result is in good agreement with those previous ones.

Wilhelmi and Schartner⁵⁵ measured emission spectra in the VUV (46–131 nm) and the near UV/visible (340–665 nm) ranges upon electron collisions with O₂. Their electron energy ranged from 200 to 2000 eV. From their spectra, Wilhelmi and Schartner determined absolute emission cross sections for the lines listed in Table 14. Those emission cross sections were measured previously by several other experimental groups. When a comparison is made between the Q_{emis} of Wilhelmi and Schartner and those of the previous experiments, some disagreements exist. In Figs. 23 and 24, for example, the Q_{emis} obtained by Ajello and Franklin⁵⁶ are plotted for the 98.9 nm line of O* and 83.3 nm line of O⁺*, together with the corresponding values measured by Wilhelmi and Schartner. The Q_{emis} of Ajello and Franklin are the same as those cited in JPCRD89 but renormalized according to the recommendation of van der Burgt *et al.*⁵⁷ Clearly the Q_{emis} of Wilhelmi and Schartner is larger than the values of Ajello and Franklin, even if the respective experimental uncertainties are considered. Wilhelmi and Schartner said nothing about the reason of this discrepancy. Probably this reflects the difficulty inherent in the measurement of the absolute value of the emission cross section.

Terrell *et al.*⁴⁸ measured emission spectra in the region of 222–660 nm upon electron collisions with O₂. Besides two emission bands from O₂⁺ (see Sec. 11.2), they observed many lines from O* and O⁺*. From those lines, they determined the absolute emission cross sections at the electron energy of 100 eV. All of Q_{emis} measured have a magnitude less than 10^{-18} cm². According to Terrell *et al.*, the sum of the emission cross sections they obtained (at 100 eV) are 0.46×10^{-18} and 1.45×10^{-18} cm² for O* and O⁺*, respectively.

TABLE 14. Emission from dissociation fragments (O*, O⁺)

Species	Wavelength (nm)	Transition	Q_{emis} at 200 eV (10 ⁻¹⁸ cm ²) ^a	Q_{emis} at 200 eV (10 ⁻¹⁸ cm ²) ^b
O*	135.6	$2p^3(^4S^o)3s\ ^5S^o \rightarrow 2p^4\ ^3P$		4.79
	130.4	$2p^3(^4S^o)3s\ ^3S^o \rightarrow 2p^4\ ^3P$		2.10
	115.2	$2p^3(^2D^o)3s\ ^1D^o \rightarrow 2p^4\ ^1D$		0.298
	102.7	$2p^3(^4S^o)3d\ ^3D^o \rightarrow 2p^4\ ^3P$	0.90	
	99.9	$2p^3(^2P^o)3s\ ^1P^o \rightarrow 2p^4\ ^1D$	0.49	
	98.9	$2p^3(^2D^o)3s\ ^3D^o \rightarrow 2p^4\ ^3P$	2.13	
	87.9	$2p^3(^2P^o)3s\ ^3P^o \rightarrow 2p^4\ ^3P$	0.72	
	79.2	$2s2p^5\ ^3P^o \rightarrow 2p^4\ ^3P$	0.016	
O ⁺	83.3	$2s2p^4\ ^4P \rightarrow 2s^22p^3\ ^4S^o$	3.57	
	79.7	$2s2p^4\ ^2D \rightarrow 2s^22p^3\ ^2P^o$	0.071	
	71.9	$2s2p^4\ ^2D \rightarrow 2s^22p^3\ ^2D^o$	0.49	
	67.3	$2s^22p^2(^3P)3s\ ^2P \rightarrow 2s^22p^3\ ^2P^o$	0.14	
	64.4	$2s2p^4\ ^2S \rightarrow 2s^22p^3\ ^2P^o$	0.096	
	61.7	$2s^22p^2(^3P)3s\ ^2P \rightarrow 2s^22p^3\ ^2D^o$	0.61	
	58.1	$2s2p^4\ ^2P \rightarrow 2s^22p^3\ ^2P^o$	0.013	
	53.9	$2s^22p^2(^3P)3s\ ^4P \rightarrow 2s^22p^3\ ^4S^o$	1.38	

^aObtained by Wilhelmi and Schartner.⁵⁵^bObtained by Kanik *et al.*⁵⁴

11.2. Emission from O₂⁺

When electrons collide with O₂, the following emission bands are observed:

first negative band system

$b\ ^4\Sigma_g^- \rightarrow a\ ^4\Pi_u$ of O₂⁺ at 450–850 nm,

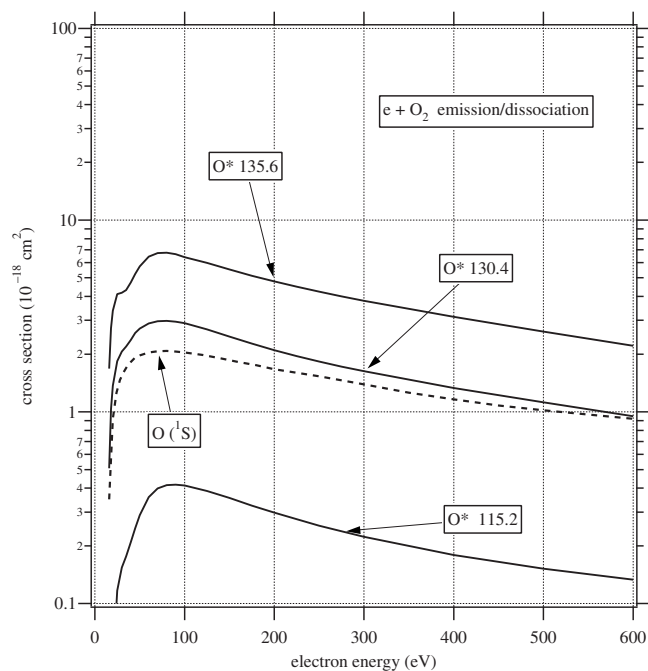


FIG. 22. Cross sections for the emission of 135.6, 130.4, and 115.2 nm lines of O, measured by Kanik *et al.*⁵⁴ upon electron collisions with O₂. For comparison, cross section for the production of O(¹S) from O₂ obtained by LeClair and McConkey⁴³ is also shown.

TABLE 15. Emission cross sections for the radiation from O* measured by Kanik *et al.*⁵⁴

Energy (eV)	Emission cross section (10 ⁻¹⁸ cm ²)		
	115.2 nm	130.4 nm	135.6 nm
16	0.002 19	0.507	1.68
18	0.027 3	1.03	2.73
20	0.049 6	1.37	3.37
25	0.117	1.84	4.11
30	0.154	2.06	4.18
35	0.176	2.19	4.32
40	0.209	2.37	4.72
45	0.247	2.58	5.24
50	0.289	2.72	5.74
60	0.359	2.89	6.45
70	0.398	2.97	6.74
80	0.414	2.98	6.76
90	0.417	2.95	6.65
100	0.413	2.90	6.40
125	0.386	2.69	5.98
150	0.355	2.47	5.52
175	0.324	2.27	5.13
200	0.298	2.10	4.79
225	0.275	1.95	4.49
250	0.255	1.83	4.23
275	0.238	1.72	4.00
300	0.223	1.63	3.79
400	0.179	1.33	3.13
500	0.152	1.12	2.62
600	0.133	0.947	2.21

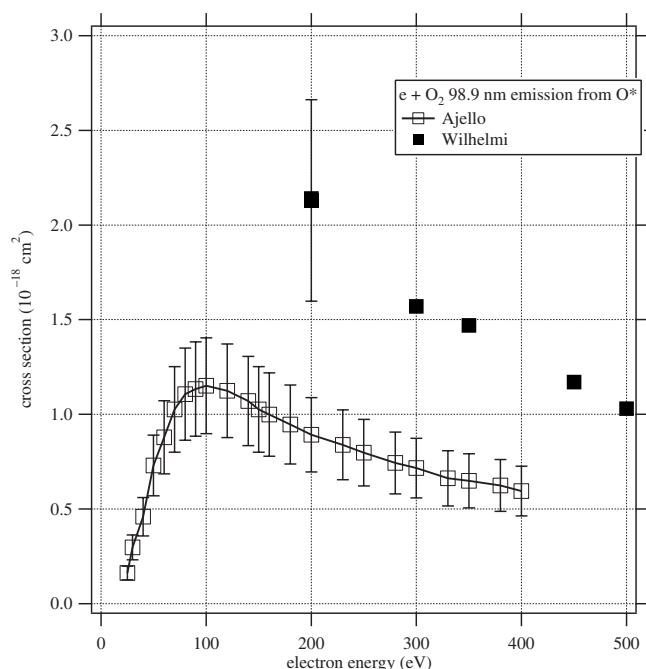
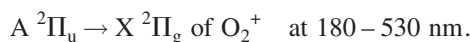


FIG. 23. Emission cross section for the 98.9 nm line of O^* measured upon electron collisions with O_2 . Two sets of experimental data (those of Ajello and Franklin⁵⁶ and of Wilhelmi and Schartner⁵⁵) are compared with each other.

second negative band system



Terrell *et al.*⁴⁸ observed the molecular emissions in the re-

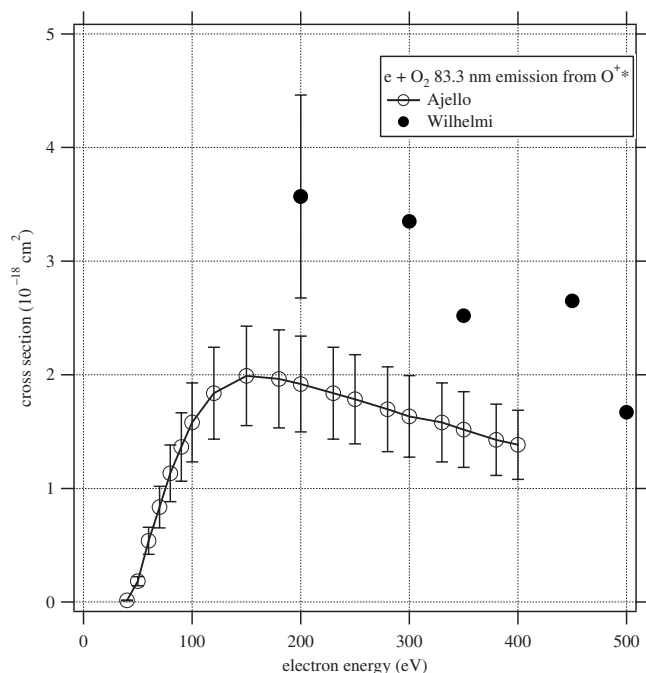


FIG. 24. Emission cross section for the 83.3 nm line of O^{+*} measured upon electron collisions with O_2 . Two sets of experimental data (those of Ajello and Franklin⁵⁶ and of Wilhelmi and Schartner⁵⁵) are compared with each other.

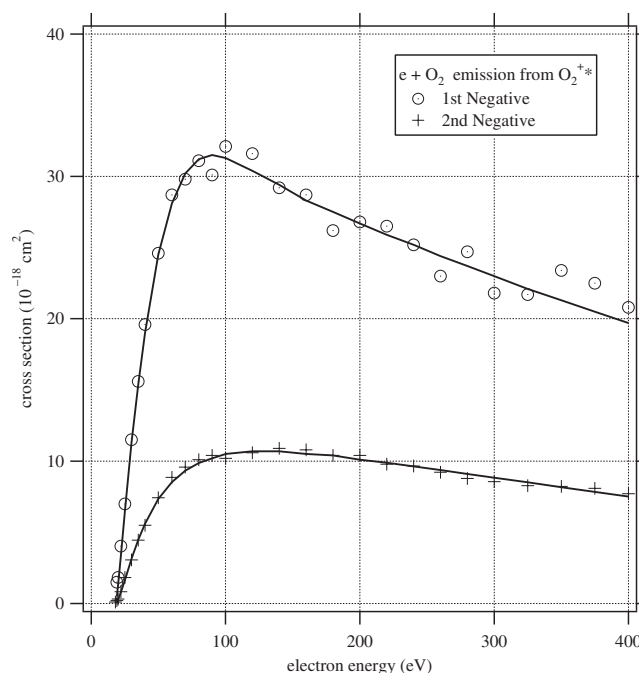


FIG. 25. Emission cross sections for the first and second negative band systems of O_2^{+*} measured by Terrell *et al.*⁴⁸ upon electron collisions with O_2 . Symbols indicate the original experimental data and solid lines are the result of analytical fitting of those data.

gion of 222–660 nm for the electron energies from the respective threshold to 400 eV. On the basis of the measured spectra and the relevant Franck-Condon factors, Terrell *et al.* made a model spectrum for the entire wavelength range of each band system. That is, they theoretically extended the spectra outside of their measurement. From this model, Terrell *et al.* determined the absolute value of the emission cross section for the whole band system. The resulting cross section is shown in Fig. 25 and Table 16. The experimental error of their values was estimated to be $\pm 24\%$. Their measured data were analytically fitted within this uncertainty. The resulting fitted curve is also shown in Fig. 25.

The previous paper, JPCRD89, cited the emission cross section for the (1,0) band of the first negative system $b \rightarrow a$ measured by Borst and Zipf.⁵⁸ Terrell *et al.*⁴⁸ showed that their cross section for the first negative band system is twice the value given by Borst and Zipf. However, they also showed that the excitation function (i.e., the energy dependence) of the emission cross section for the first negative band system of the two experiments coincides with each other.

12. Summary and Future Problems

Cross sections recommended for electron collisions with O_2 are summarized in Fig. 26. They are:

- (i) the total scattering cross section (Table 1),
- (ii) the elastic scattering cross section (Table 2),
- (iii) the momentum-transfer cross section (Table 3),
- (iv) the vibrational cross section for the transition $v=0 \rightarrow 1$ (Table 4) (For the $^2\Pi_g$ resonance in the region of

TABLE 16. Emission cross sections for the radiation from O_2^{+*} measured by Terrell *et al.*⁴⁸

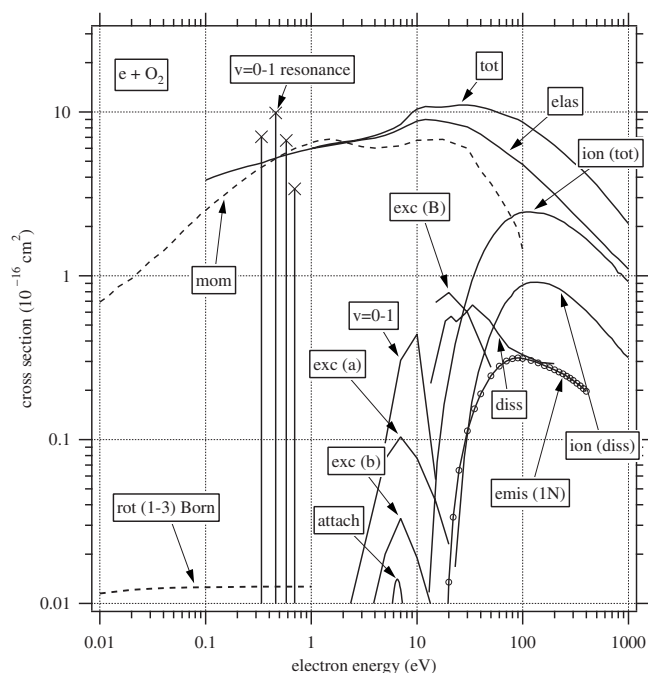
Energy (eV)	Emission cross section (10^{-18} cm^2)	
	First negative band system	Second negative band system
18		0.097
19	1.5	0.21
20	1.84	0.32
22	4.03	0.84
25	7.00	1.82
30	11.5	3.07
35	15.6	4.45
40	19.6	5.50
50	24.6	7.44
60	28.7	8.86
70	29.8	9.58
80	31.1	10.1
90	30.1	10.4
100	32.1	10.2
120	31.6	10.6
140	29.2	10.9
160	28.7	10.8
180	26.2	10.4
200	26.8	10.4
220	26.5	9.79
240	25.2	9.66
260	23.0	9.22
280	24.7	8.78
300	21.8	8.57
325	21.7	8.28
350	23.4	8.23
375	22.5	8.09
400	20.8	7.72

0.1–1 eV, only the schematic representation of the cross section is shown, see Sec. 6.2),

- (v) a few representative cross sections for the excitation of electronic states (i.e., the excitation of a $^1\Delta_g$, $b^1\Sigma_g^+$, and $B^3\Sigma_u^-$ states) (Tables 7 and 9),
- (vi) the cross section for neutral dissociation (Table 10),
- (vii) the total ionization cross section (Table 11),
- (viii) the ionization cross section for the production of O^+ (Table 11),
- (ix) the dissociative electron-attachment cross section (Table 13),
- (x) the emission cross section for the first negative band system of O_2^+ (Table 16).

As is stated in Sec. 5, no reliable data are available for rotational transitions. To show an expected magnitude of the rotational cross section, Fig. 26 includes the theoretical result of $Q_{\text{rot}}(1 \rightarrow 3)$ obtained with the Born approximation.

When compared with the previous compilation, JPCRD89,³ almost all the conclusions in that paper have been revised. Particularly experimental data are now available for the vibrational excitation of individual states (i.e.,

FIG. 26. Summary of the cross sections for electron collisions with O_2 .

$v=0 \rightarrow 1, 2, 3, 4$), dissociation for neutral products, production of molecular ion (O_2^+), and emission of the second negative band system of O_2^+ .

As is usual, further studies are needed to make the cross section data more comprehensive and more accurate. In particular, the following problems should be addressed.

- (i) There are no reliable experimental data on rotational cross sections.
- (ii) Excitations of electronic states have been studied rather extensively but still need more experiments. Particularly needed are the studies of excitations of higher states and/or excitations at higher energies (say, >100 eV).
- (iii) More detailed study is necessary to make clear the relation between excitation of electronic states and dissociation.
- (iv) The available electron-attachment cross section is too old.

13. Acknowledgments

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