

# 電子と酸素分子の衝突 断面積データ

市川行和

J. Phys. Chem. Ref. Data 38, 1 (2009)

## Cross Sections for Electron Collisions with Oxygen Molecules

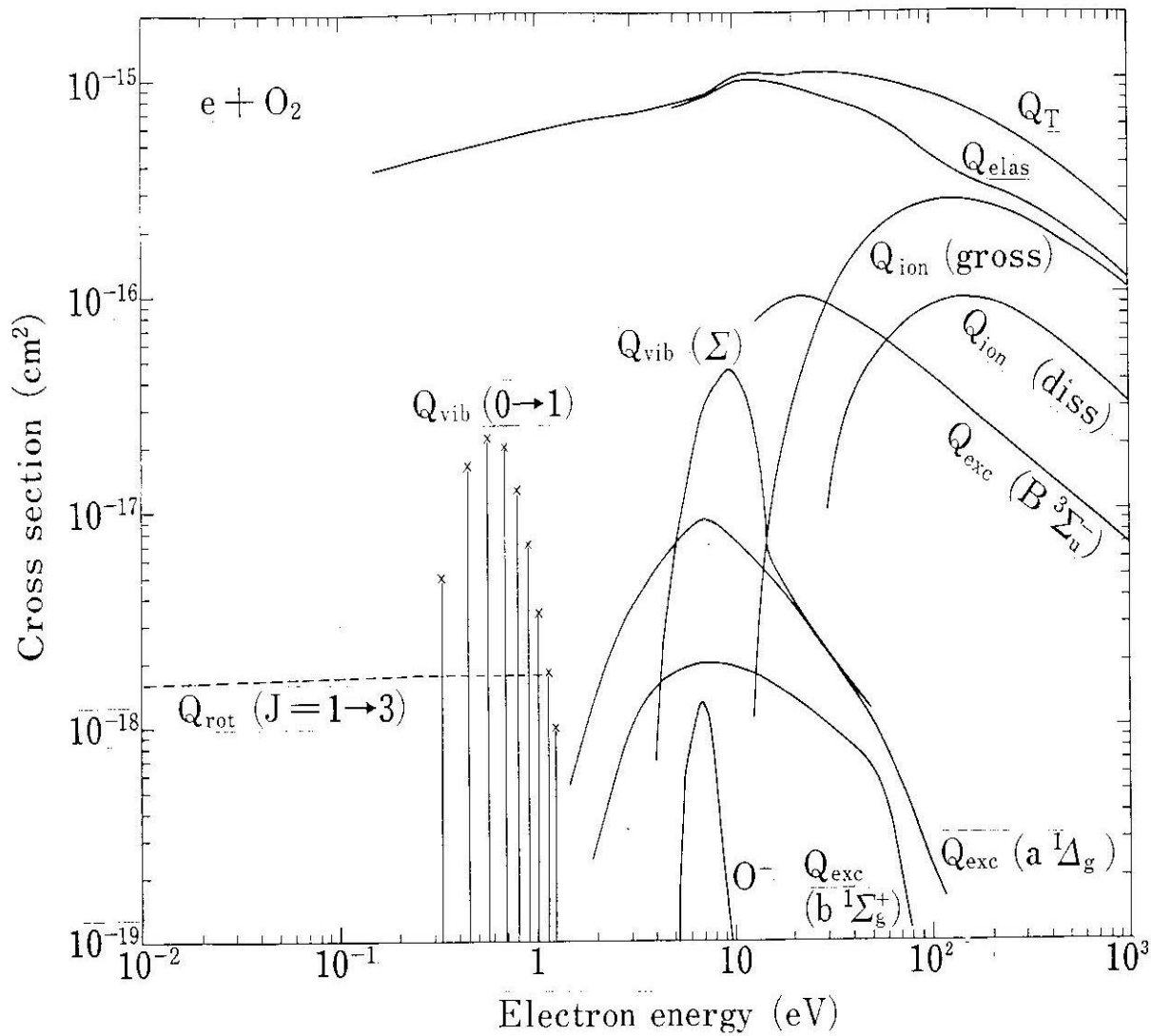
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(Received 8 July 2008; accepted 23 October 2008)

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. [DOI: 10.1063/1.3025886]

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



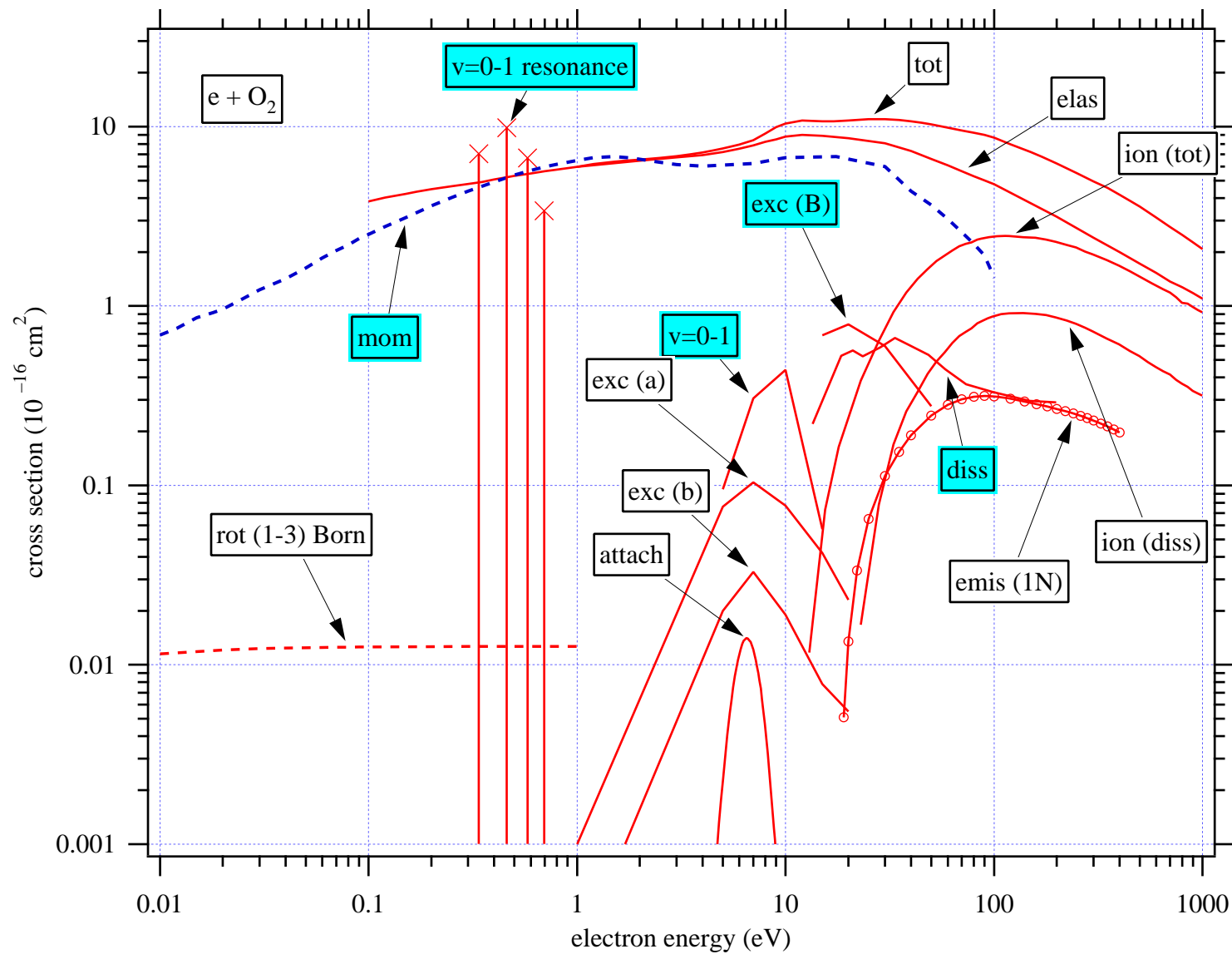
## 抜けていたもの

- $Q_{\text{vib}}$  (non-resonance,  $v=0 \rightarrow 1$ )
- $Q_{\text{ion}}$  ( $\text{O}_2^+$  生成)
- $Q_{\text{diss}}$
- $(Q_{\text{m}})$

## 大幅に修正が必要なもの

- $Q_{\text{vib}}$  (resonance)
- $Q_{\text{exc}}$

# Itikawa JPCRD 2009



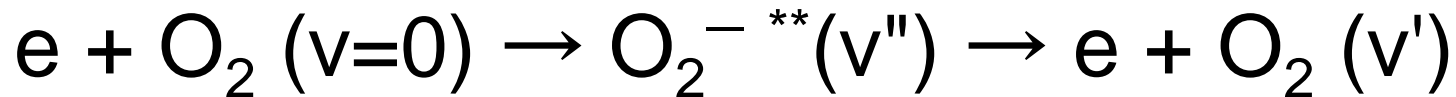
# トピックス

- (I) **共鳴** ( $< 1 \text{ eV}$ )
- (II) **解離**
- (III) **電子状態励起**

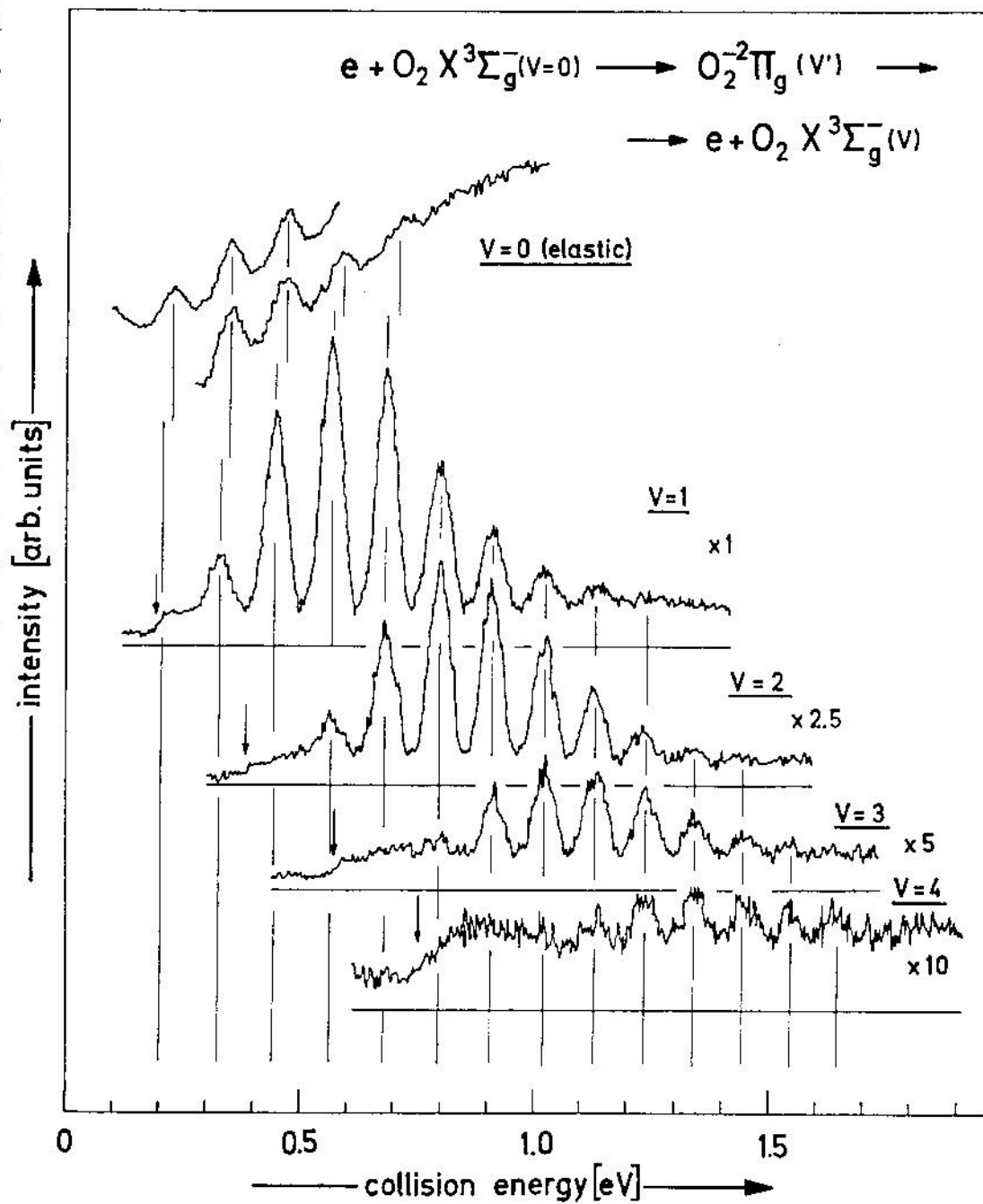
# (I) 共鳴 (< 1 eV)

**共鳴寿命 ≫ 振動周期**

**共鳴状態(負イオン)の振動構造を考慮する  
必要あり**







Linder  
 Z.Naturf. 26a, 1617  
 (1971)

Fig. 2. Measured excitation functions for vibrational excitation

# (I) 共鳴 ( $< 1 \text{ eV}$ )

共鳴幅はきわめて小さい

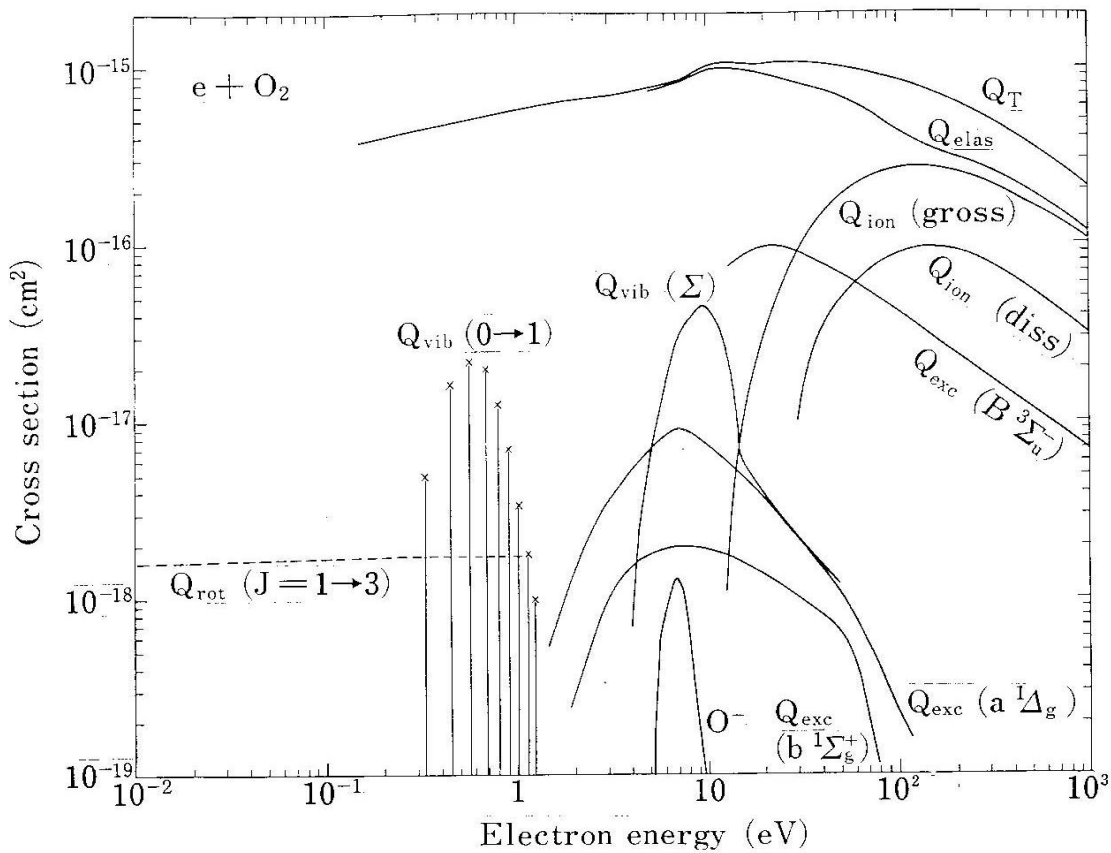
→ 実験で決めることは不可能

実験値は断面積を共鳴ピークについて積分したものの ( $Q_{\text{res}} \cdot \Delta E$ ) を与える

JPCRD89では

$\Delta E$  (理論値) を採用して  $Q_{\text{res}}$  を決めた

# JPCRD89



# (I) 共鳴 ( $< 1$ eV)

新しいデータ

実験 Allan J.Phys.B 28, 5163 (1995)

理論 Higgins J.Phys.B 28, 3391 (1995)

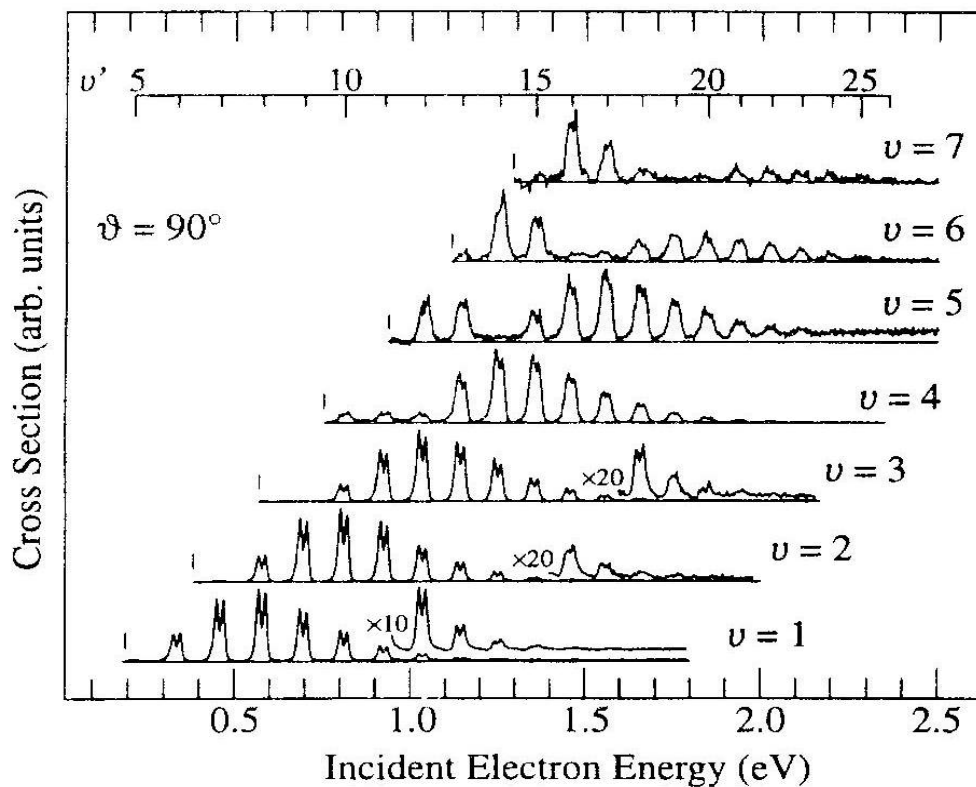
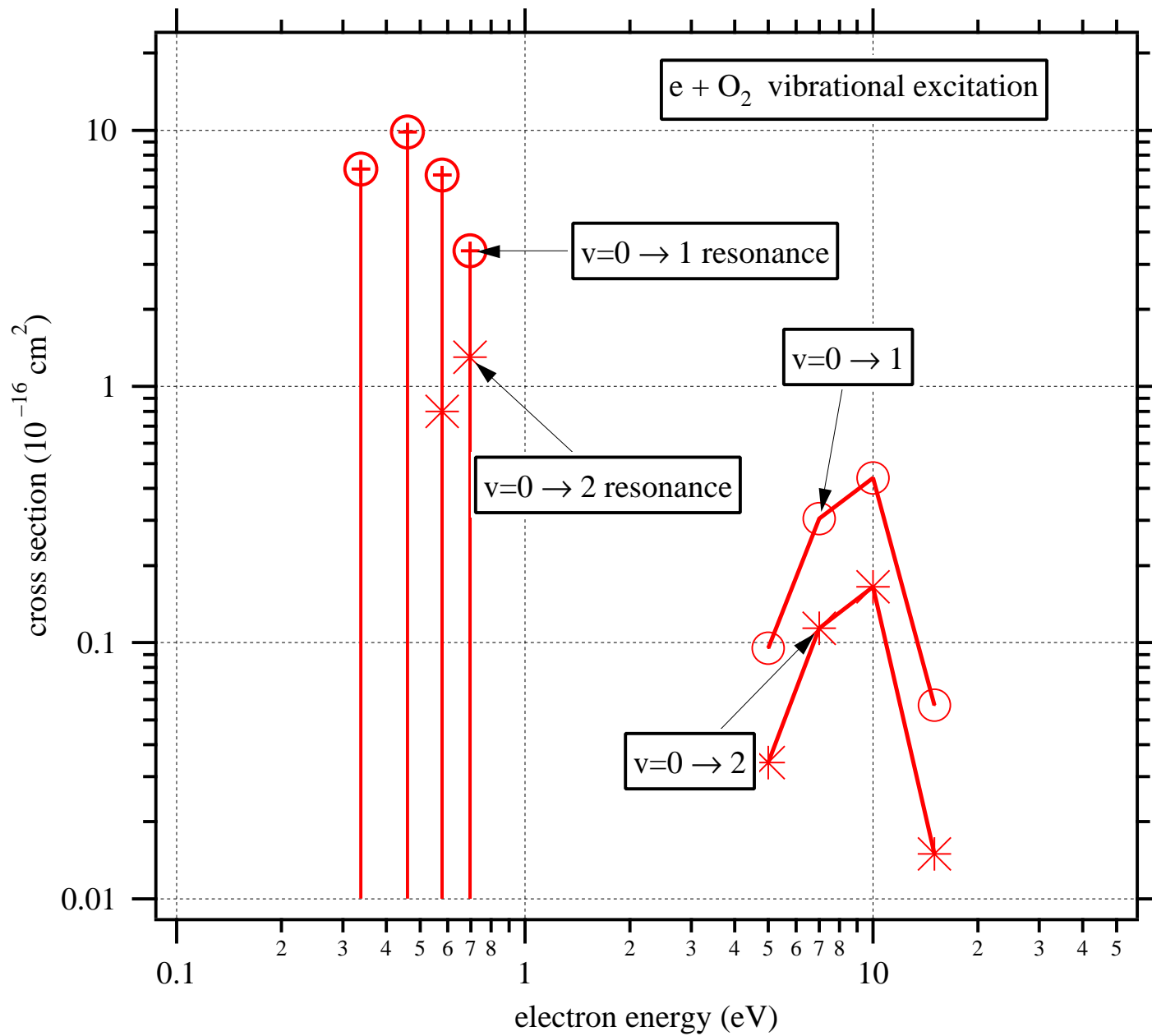


Figure 2. Vibrational excitation in the low-energy range. Levels of the  $^2\Pi_g$  resonance are identified with  $v'$  those of the  $6s^2\text{O}$  levels by  $v$ . The  $v'$  and above energies obtained

Table 5. Resonance cross section for the vibrational excitation  $\nu=0 \rightarrow \nu'$  of  $O_2$ .

The quantum number  $\nu''$  indicates the vibrational state of the resonance state and  $\Delta E$  is the width of the resonance state.

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



Allan J.Phys.B 28, 5163 (1995)

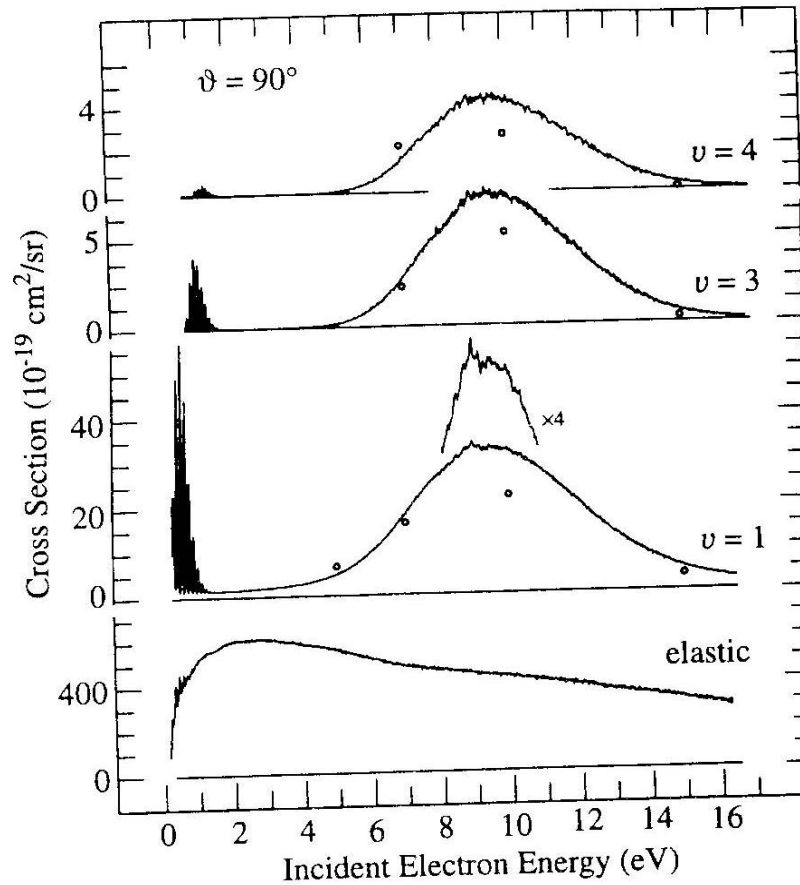
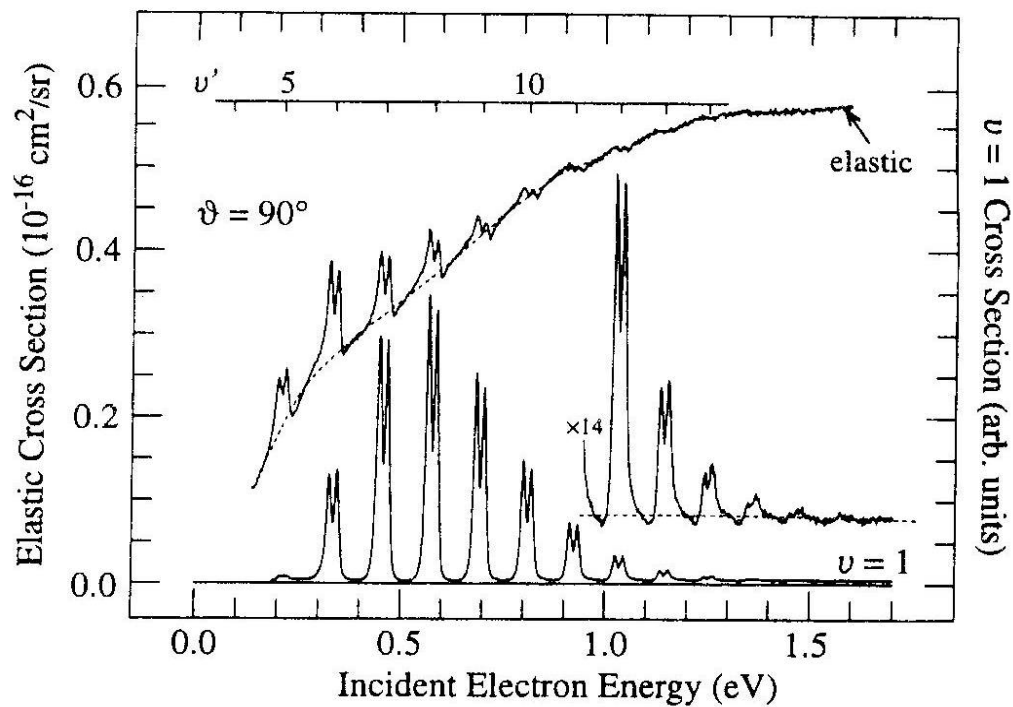


Figure 3. Elastic and vibrational DCSS over a wider energy range. Open circles indicate the results of Shyn and Sweeney (1993).





**Figure 1.** Elastic DCS (in absolute units) and  $\nu = 1$  DCS (in arbitrary units), at  $90^\circ$  and in the low-energy range dominated by the sharp  $^2\Pi_g$  resonances. The broken curves indicate approximate mean levels of the continuous part of the cross sections visualizing the 'Fano profile' shapes of the sharp resonance peaks.

# (I) 共鳴 (< 1 eV)

弾性散乱 効果あり(DCSのみデータあり)

回転励起 不明

振動励起 効果あり

全散乱断面積 あり(定性的)

応用上は影響なし? (幅が狭すぎる)

## (II) 解離



実験

P.C.Cosby,

J.Chem.Phys. 98, 9560 (1993)

# 高速標的ビームを用いた 解離断面積の測定

高速中性粒子は半導体検出器で検出可

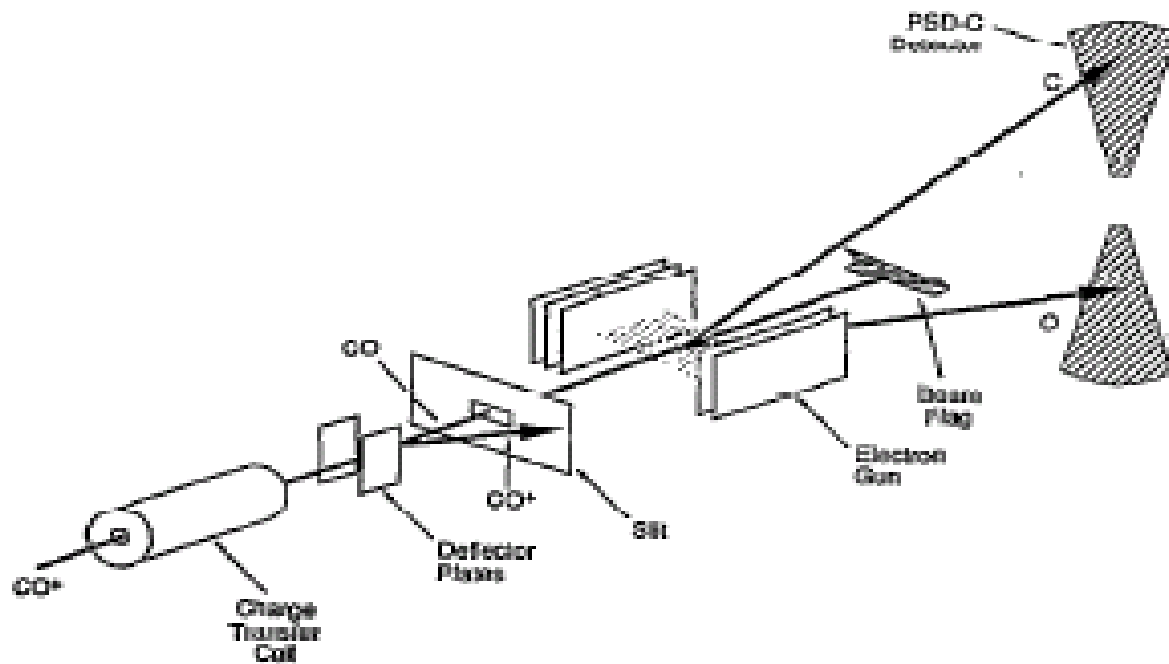


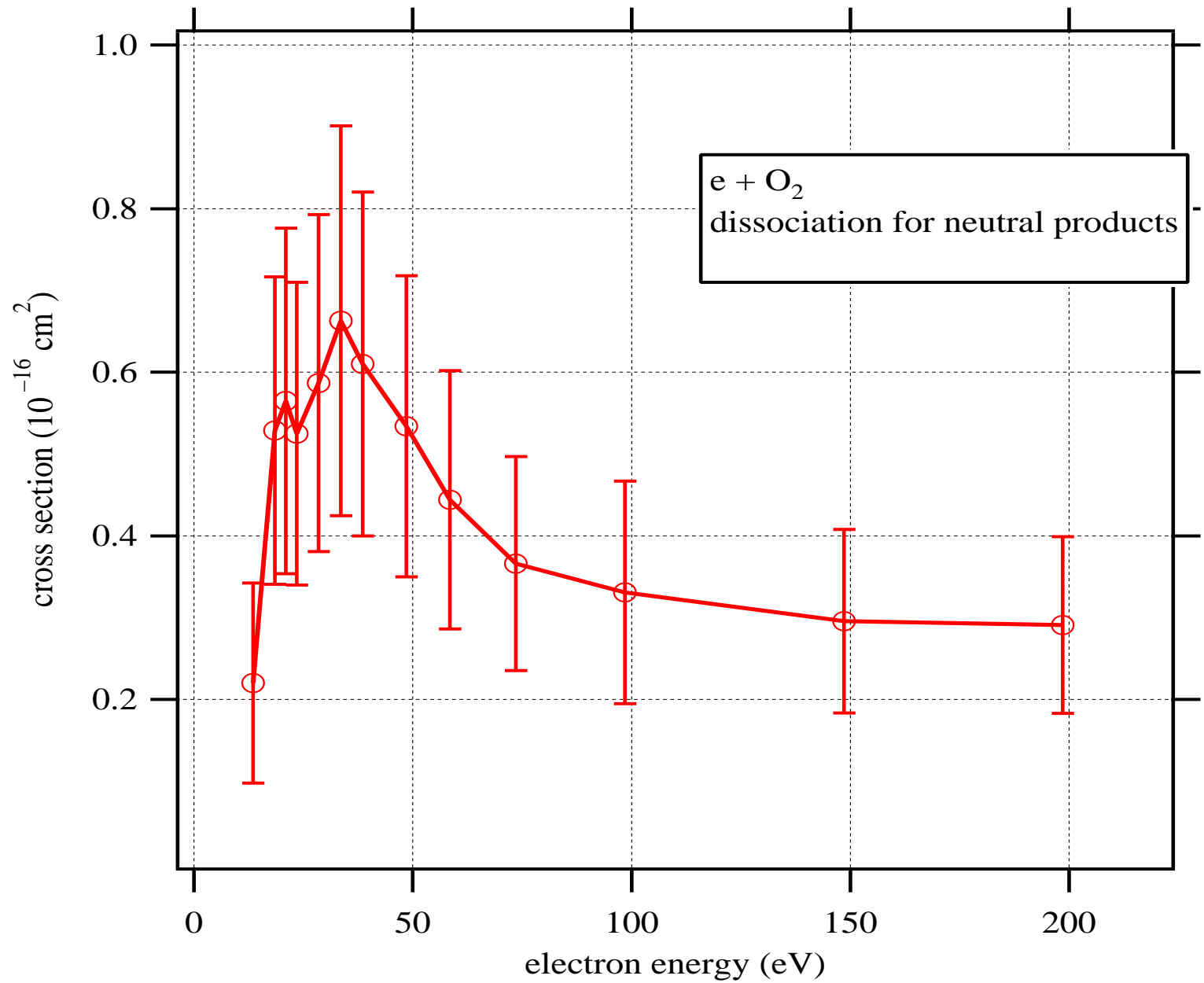
A, Bを同時に検出すれば解離断面積が求まる  
[高速の中性分子ビームは分子イオンを気体中で電荷交換して作る]

Cosby: N<sub>2</sub>, O<sub>2</sub>, CO に応用

# 高速ビーム法 (Cosby)

CO → C + O の例

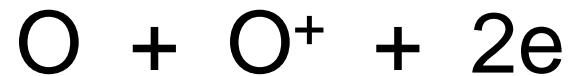




# 3種類の解離機構



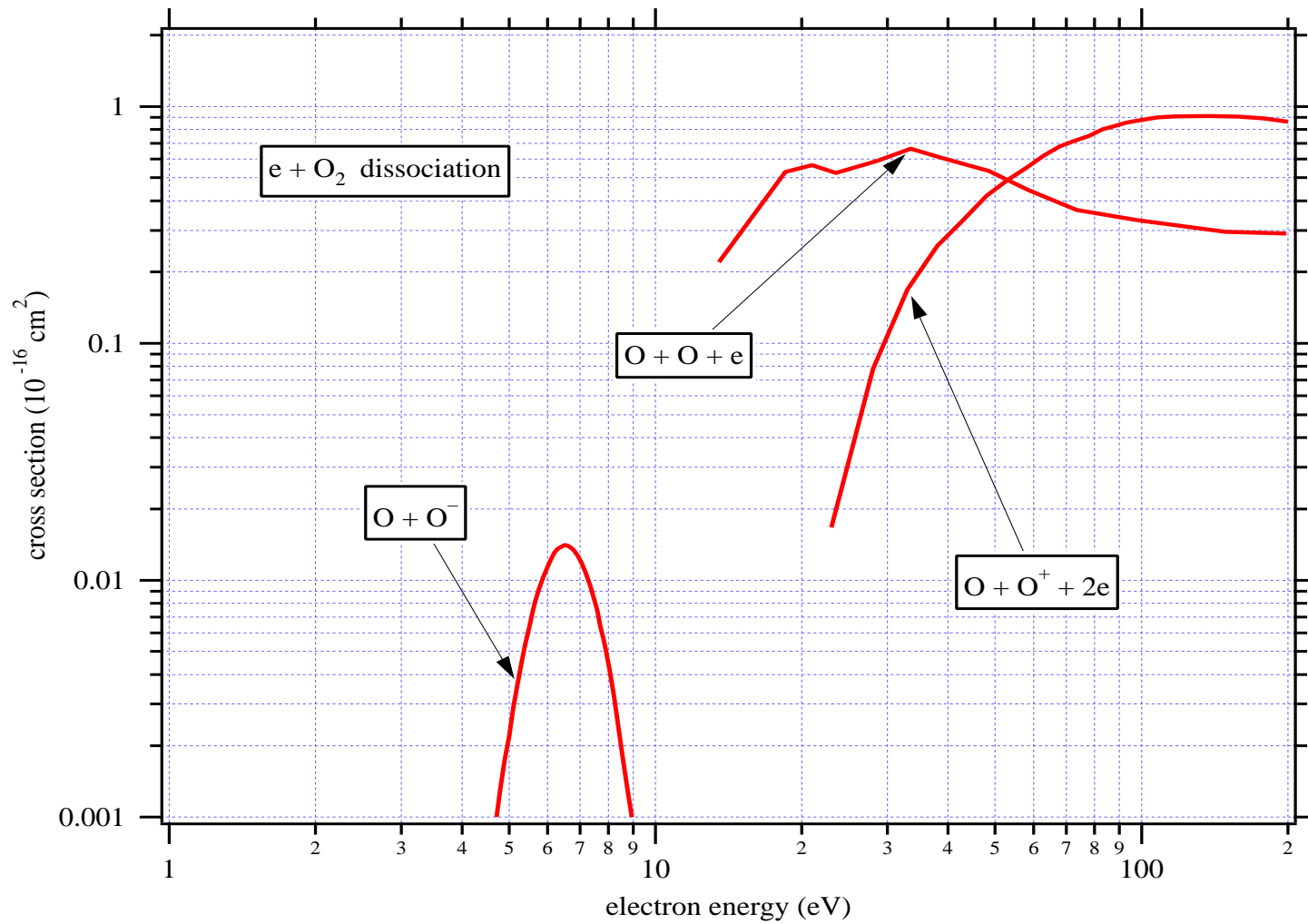
中性解離



解離イオン化



解離付着





# 解離に関する最近の review

J.W. McConkey et al.  
Phys. Rep. 466, 1 (2008)

Electron impact dissociation of oxygen-containing molecules – A critical review

dissociative excitation (emission) も含む



# (III) 電子狀態励起

520

PAUL H. KRUPENIE

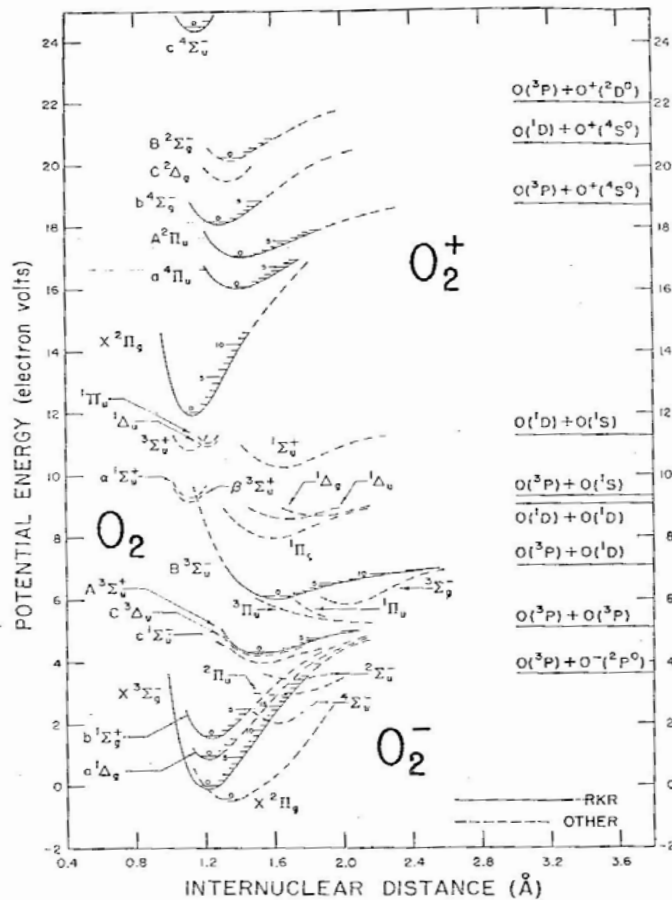


FIGURE 2. Potential energy curves for  $O_2$ ,  $O_2^+$ , and  $O_2^-$ .

\*Enlarged copies of Figure 2 may be obtained from the author upon request.  
 J. Phys. Chem. Ref. Data, Vol. 1, No. 2, 1972

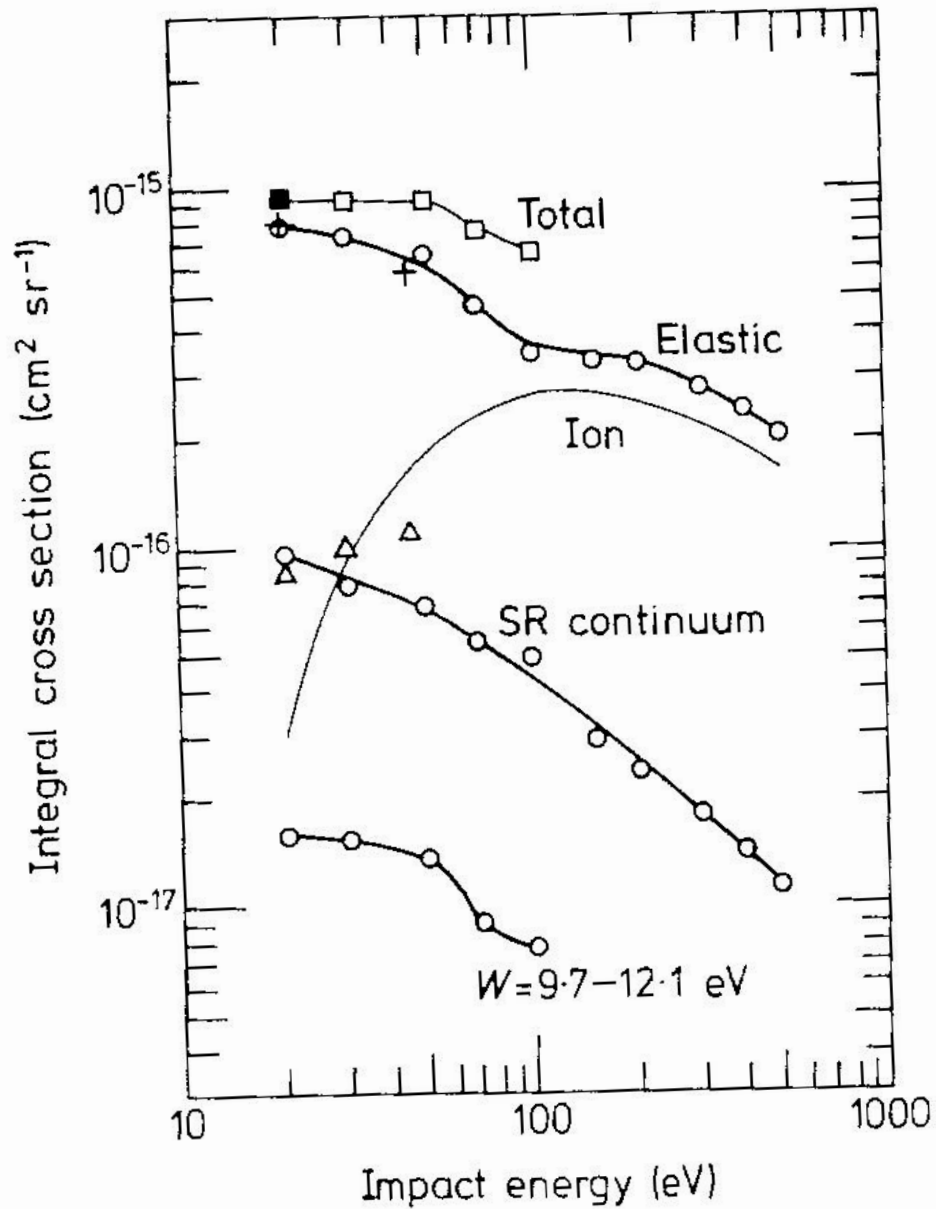
# 励起断面積データのある電子状態

状態	励起エネルギー (eV)
$B^3\Sigma_u^-$	6.120
$A^3\Sigma_u^+$	4.340
$C^3\Delta_u$	4.262
$c^1\Sigma_u^-$	4.050
$b^1\Sigma_g^+$	1.627
$a^1\Delta_g$	0.977
$X^3\Sigma_g^-$	0

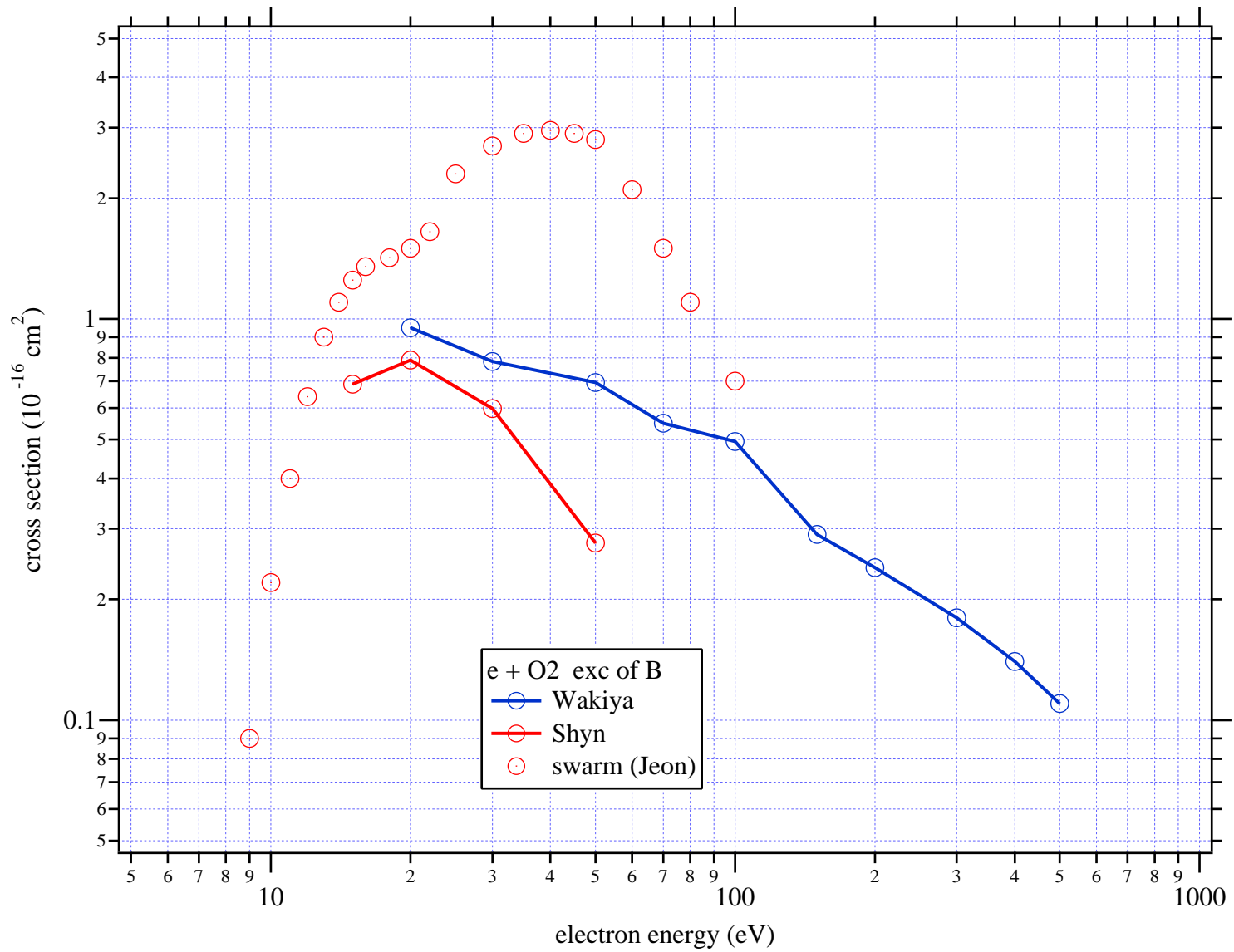


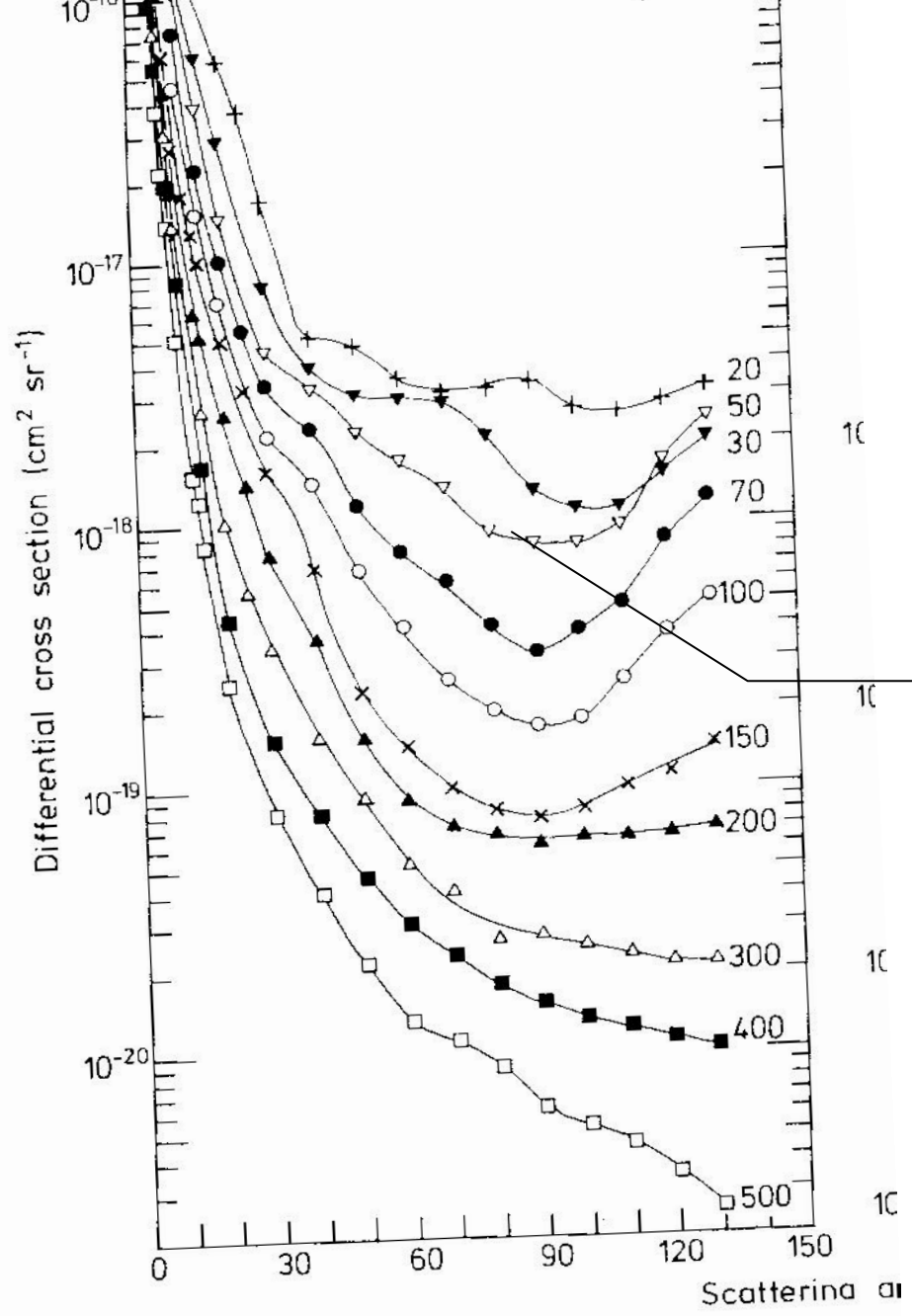
## 実験

- Wakiya J.Phys.B 11, 3913 (1978)
- Shyn et al. Phys.Rev A 50, 4794 (1994)



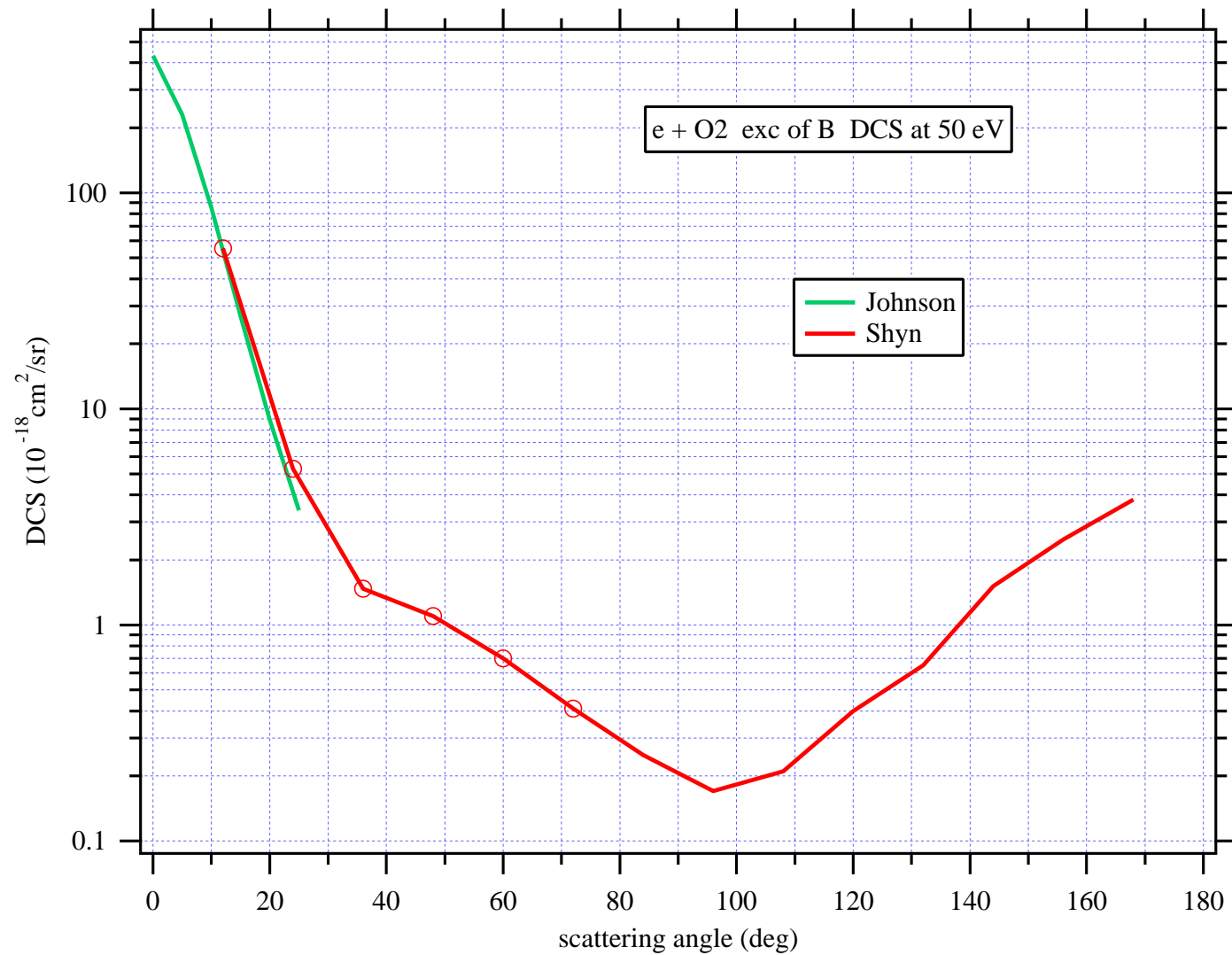
Wakiya  
J.Phys.B 11, 913 (1978)





**$e + O_2$**   
**exc of  $B^3 \Sigma_u^-$**   
**DCS measured by**  
**Wakiya (1978)**

50 eV







Wakiya78

散乱角の大きいところのDCSが大きすぎる

→ Shyn94 を採用する

**要検討！！！！**

# 分子の電子状態励起断面積

- 2原子分子( $\text{H}_2$ ,  $\text{N}_2$ , ...)  
データは多数あり  
一致は必ずしも良くない
- 多原子分子( $\text{CO}_2$ ,  $\text{H}_2\text{O}$ , ...)  
ほとんど実験値がない

# 分子の電子状態励起

**実験が困難な理由**

**多数の状態が重なっている**

**振動構造が複雑(特に、多原子分子)**

**断面積データを使う際は注意が必要**

# $e + O_2$ : 今後の問題

- **電子状態励起**  
特に、 $E > 100 \text{ eV}$
- **回転励起**  
実験なし
- **解離の詳細**  
電子状態励起との関係  
生成物

# Data compilations by Y. Itikawa

$N_2$  JPCRD 35, 31 (2006)  
 $O_2$  JPCRD 38, 1 (2009)  
 $H_2$  JPCRD 37, 913 (2008)  
 $CO_2$  JPCRD 31, 749 (2002)  
 $H_2O$  JPCRD 34, 1 (2005)

JPCRD=J. Phys. Chem. Ref. Data

**Y. Itikawa**

# **Molecular Processes in Plasmas**

**- Collisions of charged particles  
with molecules -**

**Springer, 2007**

