IPPJ-AM-38

RATE COEFFICIENTS FOR THE ELECTRON-IMPACT EXCITATIONS OF C-LIKE IONS

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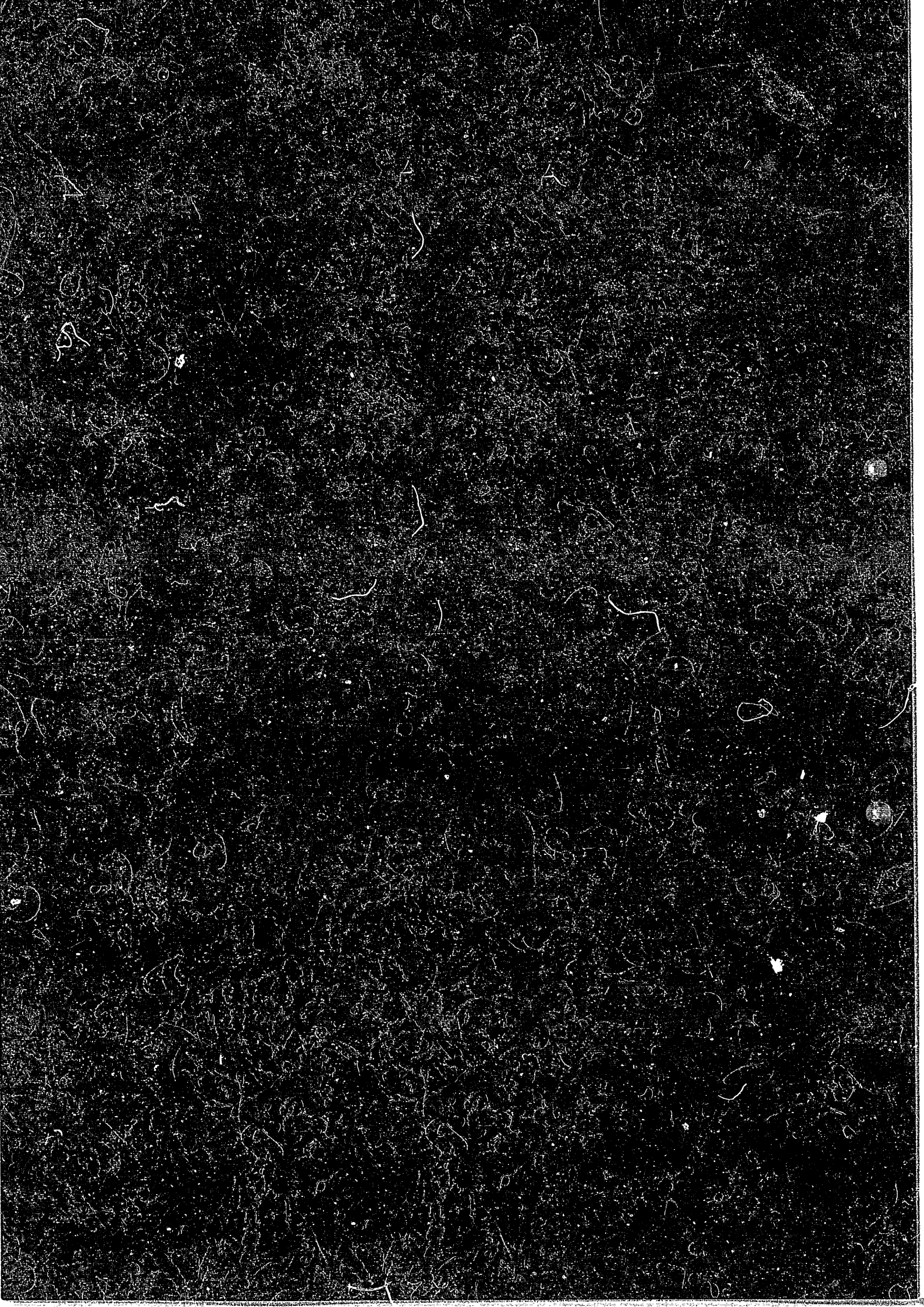

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Abstract

Cross sections have been surveyed for electron-impact excitations of C-like ions. 'Best' values of effective collision strengths are shown graphically for O III, Ne V, Mg VII, Si IX, and Ca XV over a wide range of electron temperature. They are based on the R-matrix calculation supplemented with the values obtained by distorted-wave-type methods.

1. Introduction

Electron-impact excitation of atomic ions is a fundamental process in a high-temperature plasma. Although there are very few experimental data, many theoretical values are available for the excitation cross section. Those theoretical data, however, scatter through literature and are often fragmentary. It is important to compile the data and assess their reliability. Such a task has been performed on carbon and oxygen ions and the result has been published.[1] As an extension of the previous work, a collection and evaluation of the data on C-like ions is reported in the present paper.

Because of astrophysical interest, a large number of calculations have been made on the electron-impact excitation of C-like ions. They enable us to make a rather systematic study of the excitation process along the isoelectronic sequence. Before starting the present work, we had hoped to derive a universal formula for the excitation cross section or rate coefficient applicable to ions with any nuclear charge. It turned out, however, that complicated structure due to the resonance effect makes it very difficult. In the present report, rate coefficients for several excitation processes are shown graphically only for individual species. Although a crude interpolation can be made, no universal form has been derived.

2. Data sources

An elaborate calculation based on the R-matrix theory has been carried out for O III, Ne V, Mg VII, Si IX and Ca XV.[2-11] A distorted-wave type calculation using the UCL code has been made for more than ten ion species.[12-19] Those two sets of data, listed in Table I, have been used in the present study. The R-matrix calculation is believed to be most accurate. The calculation, however, is often restricted to the region of lower electron energy. For the data to be more comprehensive and more applicable, it is desirable to extend them to higher energies. The extension is made here with the help of the values obtained by the DW method, which is more reliable at the higher electron energies. There are many other calculations for C-like ions,[20] but they are less reliable or very fragmentary.

The cross sections calculated with the UCL-DW code are mostly in fair agreement with the R-matrix result at least at the higher energies where a comparison can be made (for details, see the original literature of the R-matrix calculation[2-11]). In the case of Ca XV, however, a large discrepancy is found for the excitations of $2s2p^3\ {}^1D^o$ and ${}^1P^o$. In that case the R-matrix values are extended by using our own DW calculation,[21] which gives a very good agreement with the R-matrix result at the energies higher than the twice the excitation potential. In the DW calculation, use has been made of the same target-wave-function as in the R-matrix calculation.

3. Rate coefficients

Because of the complicated structure due to the resonance effect, it is almost impossible to show cross sections or collision strengths in a graphical form. Instead we present here an effective collision strength for a transition $i \rightarrow j$

$$\gamma_{ij} = y\, e^{y} \int_{1}^{\infty} dx\, \Omega_{ij}(x)\, e^{-yx} \qquad (1)$$

as a function of

$$y = \frac{\Delta E_{ij}}{T} \qquad (2)$$

Here Ω_{ij} is the collision strength, T is the electron temperature, and ΔE_{ij} is the transition energy. The corresponding rate coefficient is given by

$$R_{ij}(\mathrm{cm}^{3}\mathrm{sec}^{-1}) = \frac{8.010 \times 10^{-8}}{\omega_i \sqrt{T(\mathrm{ev})}}\, e^{-y}\, \gamma_{ij} \qquad (3)$$

where ω_i is the statistical weight of the initial state. It should be noted that the Maxwellian distribution has been assumed for the electron velocity.

The excitations considered are

$2s^2 2p^2\ {}^3P \longrightarrow 2s^2 2p^2\ {}^1D,\ {}^1S$

$2s2p^3\ {}^5S^o,\ {}^3D^o,\ {}^3P^o,\ {}^1D^o,\ {}^3S^o,\ {}^1P^o$.

The excitation energy, ΔE_{ij}, for the transitions is listed in Table II. Owing to the difficulty in the treatment of higher partial waves, the R-matrix method was applied first to the spin-forbidden transitions. The method is now being extended to allowed transitions, but the calculation is still in progress. The two types of the transitions, therefore, are shown separately in the following.

(1) Spin-forbidden transitions

Except for O III and the excitations of $^1P^o$ and $^1D^o$ states of Ca XV, the effective collision strength obtained by the R-matrix method is supplemented with the UCL-DW calculation. The most of the DW calculations reported give only the collision strengths at three electron energies. To calculate Υ from them, we fit the collision strengths by a formula

$$\Omega_{ij}(x) = A_{ij} + \frac{B_{ij}}{x + \xi_{ij}} + \frac{C_{ij}}{(x + \xi_{ij})^2} \qquad (4)$$

Here X is the electron energy in the threshold units, A,B,C are fit parameters depending on the nuclear charge, and ξ is a parameter appropriately chosen for each transition but independent of Z. With the use of the formula, Υ can be calculated analytically. As has been mentioned in the last section, our own DW calculation is applied to produce Ω_{ij} for the excitations

of $^1D^o$, $^1P^o$ of Ca XV. They are also fitted by the above formula. For O III, we have modified our previous recommended values [1] by taking account of the recent R-matrix result.

The resulting effective collision strengths are shown in Figs. 1 - 5. Each line in the figures has a short vertical bar on it. This indicates the boundary on the right side of which the R-matrix values are plotted. In the case of Mg VII, the R-matrix calculation has been made over a wide range of electron energy so that all the curves of Υ are based solely on that. A liitle arrow shows the position of the temperature at which the particular ion has its maximum population in the steady-state ionization balance.[22] There are a number of calculations of the ionization balance giving somewhat different results. The arrow in the figures should be taken as a rough measure of the temperature of importance in the case of ionization equilibrium. A departure from the ionization equilibrium is often seen in the case of fusion plasma, and hence rate coefficients are needed for a wide range of temperature.

(2) Allowed transitions

For allowed transitions, the R-matrix calculation has been done only for O III, Ne V and Mg VII so far. The results of the calculation are plotted in Figs. 6 - 8. Our previous recommended values[1] for O III are modified slightly on the consideration of the recent R-matrix calculation and the

resulting values are presented in the figures. For a comparison and to estimate Υ for Si IX and Ca XV, the effective collision strengths calculated from the DW result are also shown. For the allowed transitions, the collision strengths of the DW calculation are fitted by a formula

$$\Omega_{ij}(x) = A_{ij} + \frac{B_{ij}}{x + \xi_{ij}} + C_{ij}\, \ell_n\, x \qquad (5)$$

instead of Eq(4). As in the case of spin-forbidden transitions, a small arrow indicates the temperature at which each ion has its maximum population in the calculation of ionization balance.[22)]

Because no experimental data are available, it is difficult to assess the accuracy of the present effective collision strengths. From a general consideration of the theoretical methods, we conclude that the values indicated by solid lines in the figures are accurate probably within an error of 20 %.

Acknowledgements

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References

1) Y. Itikawa, S. Hara, T. Kato, S. Nakazaki, M. S. Pindzola and D. H. Crandall: Recommended data on excitation of carbon and oxygen ions by electron collisions, IPPJ-AM-27 (Institute of Plasma Physics, Nagoya University, 1983) (to be published in Atomic Data Nucl. Data Tables)

2) K. L. Baluja, P. G. Burke and A. E. Kingston: J. Phys. B 13 4675 (1980)

3) K. M. Aggarwal: J. Phys. B 16 L59 (1983)

4) K. M. Aggarwal and K. L. Baluja: J. Phys. B 16 107 (1983)

5) K. M. Aggarwal: J. Phys. B 16 2231 (1983)

6) K. M. Aggarwal: J. Phys. B 16 2405 (1983)

7) K. M. Aggarwal: Astrophys. J. Suppl. 52 387 (1983)

8) K. M. Aggarwal: Astrophys. J. Suppl. 54 1 (1984)

9) K. M. Aggarwal: Astrophys. J. Suppl. 56 303 (1984)

10) K. M. Aggarwal: Astron. Astrophys. (to be published)

11) K. M. Aggarwal: Astrophys. J. Suppl. (to be published)

12) H. E. Mason and A. K. Bhatia: Mon. Not. R. Astr. Soc. 184 423 (1978)

13) K. P. Dere, H. E. Mason, K. G. Widing and A. K. Bhatia: Astrophys. J. Suppl. 40 341 (1979)

14) H. E. Mason, G. A. Doschek, U. Feldman and A. K. Bhatia: Astron. Astrophys. 73 74 (1979)

15) A. K. Bhatia, G. A. Doschek and U. Feldman: Astron. Astrophys. 76 359 (1979)

16) A. K. Bhatia, U. Feldman and G. A. Doschek: J. Appl. Phys. 51 1464 (1980)

17) A. K. Bhatia: in A. L. Merts, J. B. Mann, W. D. Robb, and N. H. Magee, Jr., Los Alamos Scientific Laboratory Report No. LA-8267-MS (1980)

18) A. K. Bhatia: J. Appl. Phys. 53 59 (1982)

19) A. K. Bhatia and U. Feldman: J. Appl. Phys. 53 4711 (1982)

20) For bibliography on electron-ion collisions, Y. Itikawa, K. Takayanagi and T. Iwai: Atomic Data Nucl. Data Tables 31 215 (1984)

21) Y. Itikawa and K. Sakimoto: to be published

22) J. M. Shull and M. van Steenberg: Astrophys. J. Suppl. 48 95 (1982)

Table I. List of calculations using the R-matrix method and the UCL-DW code. Numbers are referred to the reference list.

	R-matrix method	DW(UCL) method
O III	7, 10	15
Ne V	2, 6, 8, 11	17
Mg VII	9, 11	12
Si IX	3, 4, 8	12
S XI		12
Ar XIII		13
Ca XV	5	13
Ti XVII		16
Mn XX		18
Fe XXI		14
Kr XXXI		19

Table II. Transition energies in eV for the processes considered. The numbers in parentheses are the corresponding values in the temperature units in 10^4 K.

	O III	Ne V	Mg VII	Si IX	Ca XV
$2s^2 2p^2\ {}^3P \rightarrow$					
$2s^2 2p^2\ {}^1D$	2.49	3.66	4.83	6.02	10.26
	(2.89)	(4.25)	(5.60)	(6.99)	(11.91)
$2s^2 2p^2\ {}^1S$	5.33	7.83	10.31	12.82	21.30
	(6.19)	(9.09)	(11.96)	(14.88)	(24.72)
$2s2p^3\ {}^5S^o$	7.48	10.93	12.98	18.05	27.41
	(8.68)	(12.68)	(15.06)	(20.95)	(31.81)
$2s2p^3\ {}^3D^o$	14.86	21.71	28.63	35.69	58.61
	(17.24)	(25.19)	(33.22)	(41.42)	(68.01)
$2s2p^3\ {}^3P^o$	17.63	25.72	33.84	42.11	69.24
	(20.46)	(29.85)	(38.92)	(48.87)	(80.35)
$2s2p^3\ {}^1D^o$	23.17	33.45	43.69	54.06	87.27
	(26.89)	(38.81)	(50.70)	(62.73)	(101.27)
$2s2p^3\ {}^3S^o$	24.42	34.54	44.65	54.87	87.17
	(28.34)	(40.08)	(51.81)	(63.67)	(101.16)
$2s2p^3\ {}^1P^o$	26.07	37.57	48.99	60.55	97.77
	(30.25)	(43.60)	(56.85)	(70.27)	(113.46)

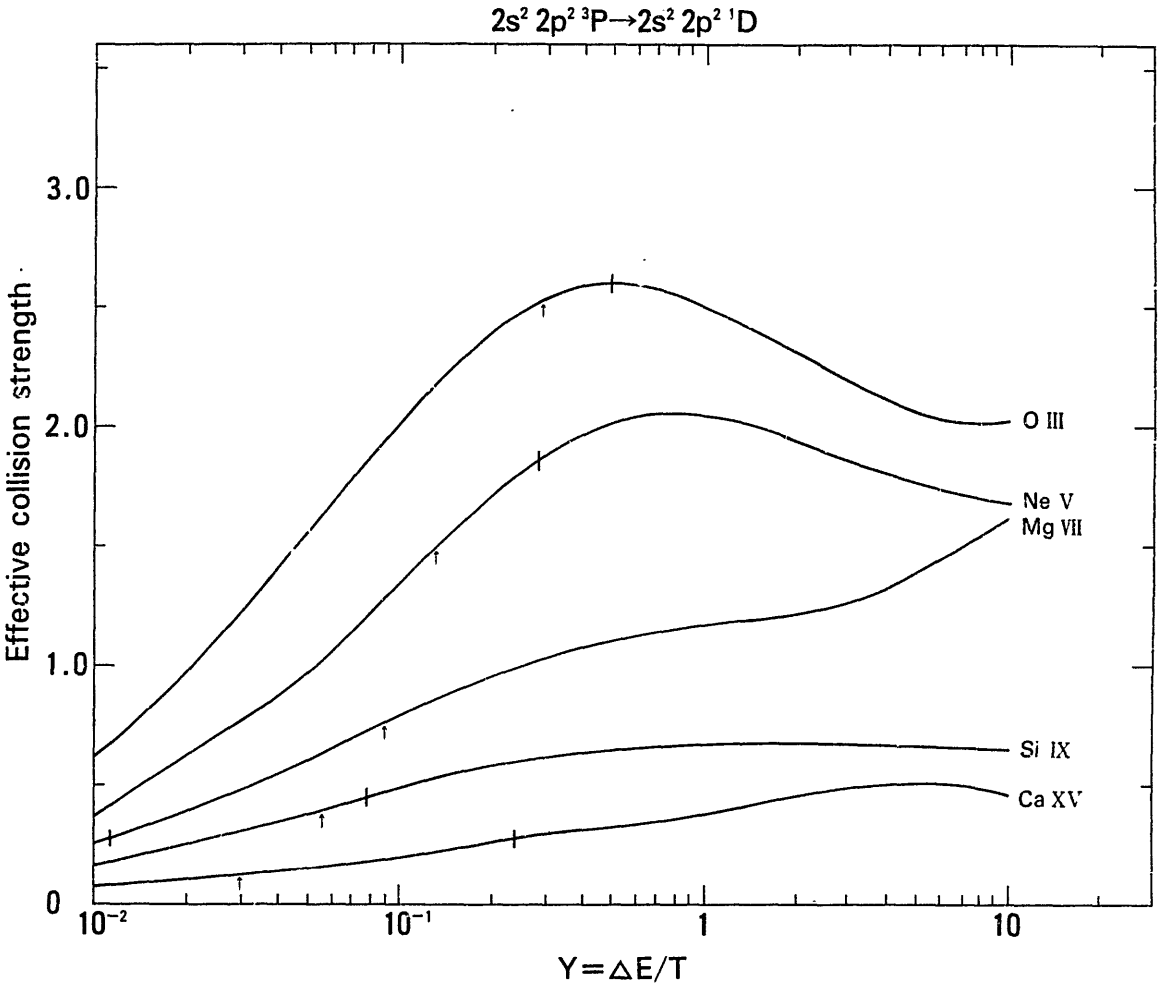

Fig. 1. Effective collision strengths for the transition $2s^2 2p^2\ ^3P \longrightarrow 2s^2 2p^2\ ^1D$ in O III, Ne V, Mg VII, Si IX and Ca XV by electron collisions. The horizontal scale denotes the inverse temperature in the units of transition energy. A small vertical bar on each curve shows the boundary on the right side of which the R-matrix values are plotted. An arrow indicates the temperature at which the respective ion has its maximum population in the calculation of steady-state ionization balance.

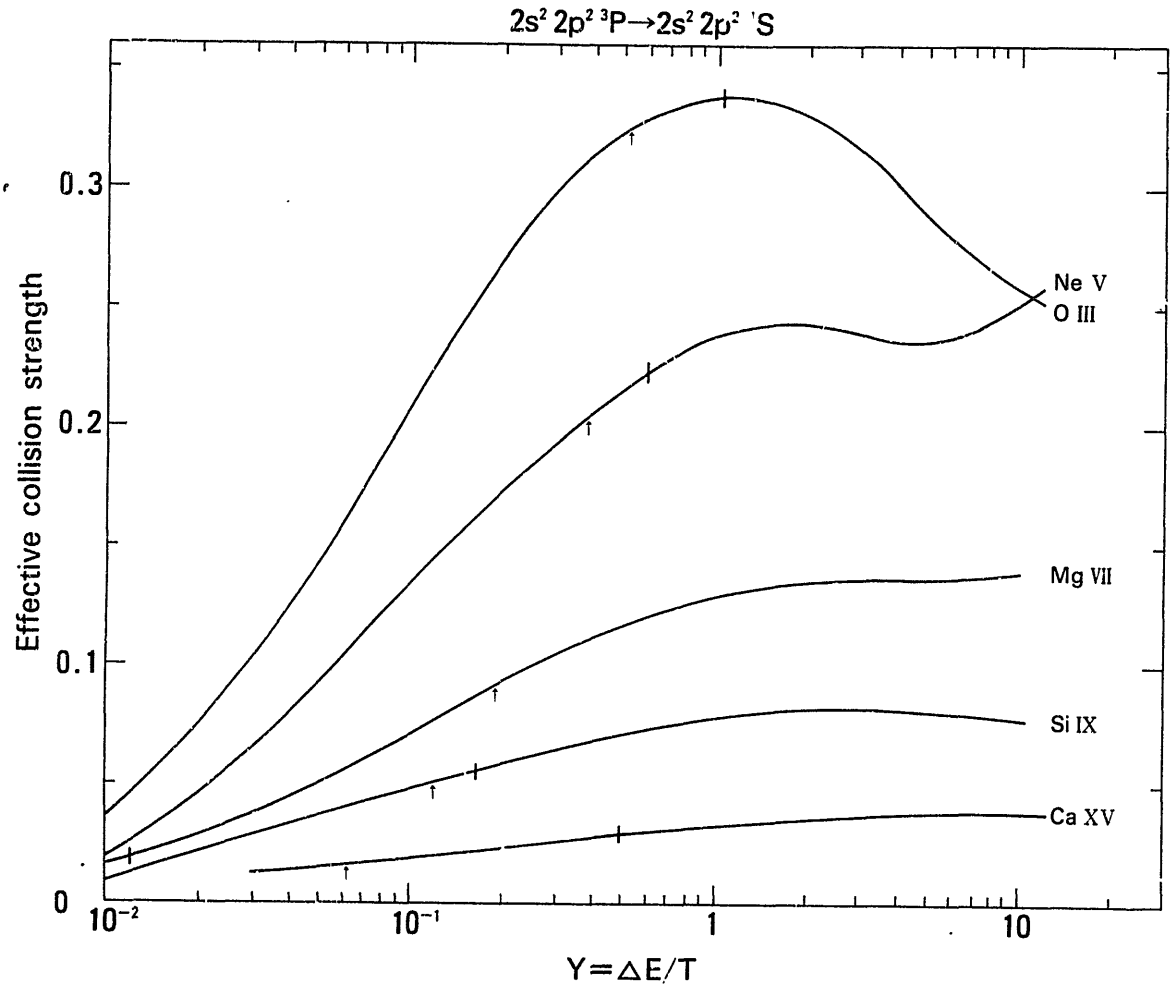

Fig. 2. Same as Fig. 1, but for the transition $2s^2 2p^2\ ^3P \longrightarrow 2s^2 2p^2\ ^1S$.

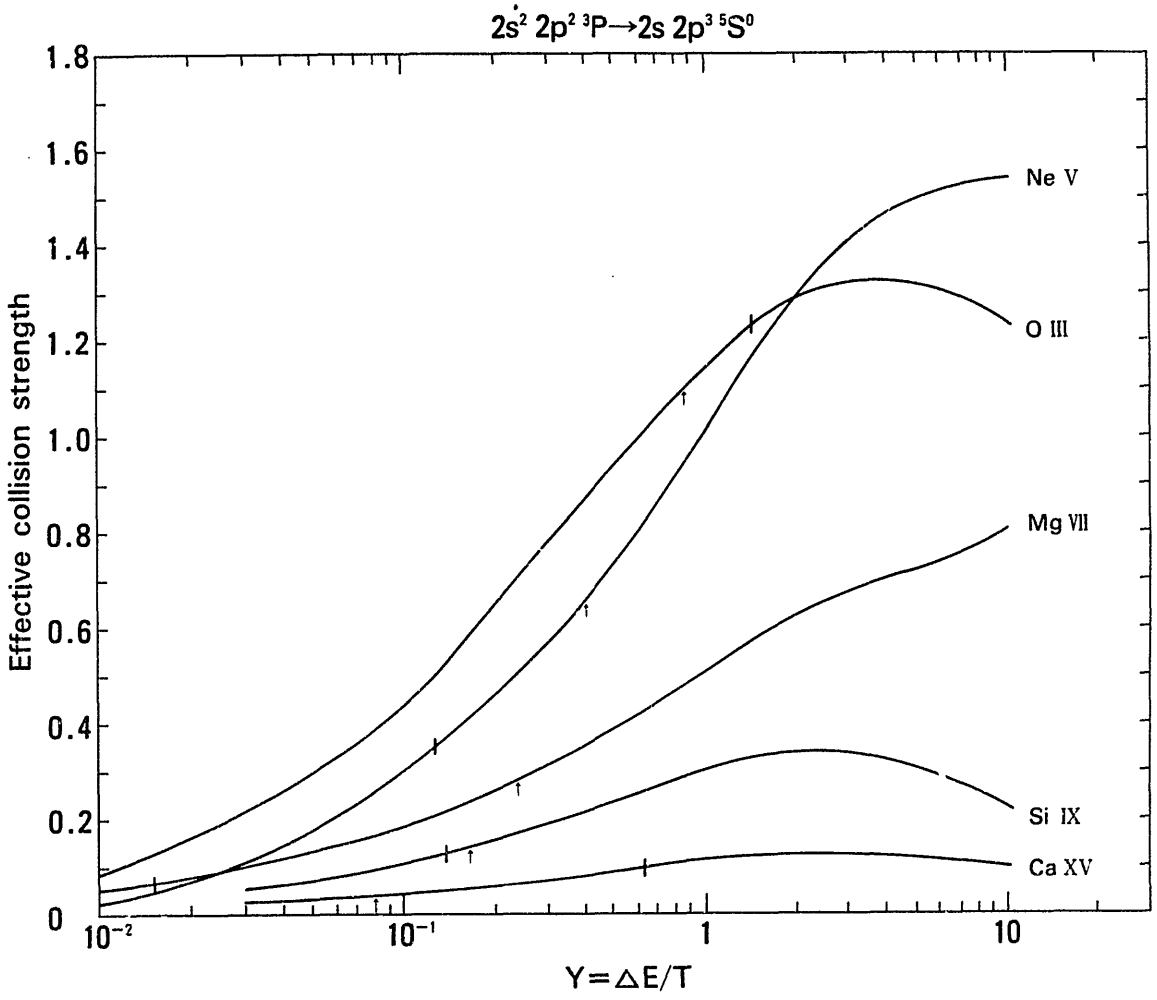

Fig. 3. Same as Fig. 1, but for the transition $2s^2 2p^2\ ^3P \longrightarrow 2s2p^3\ ^5S^o$.

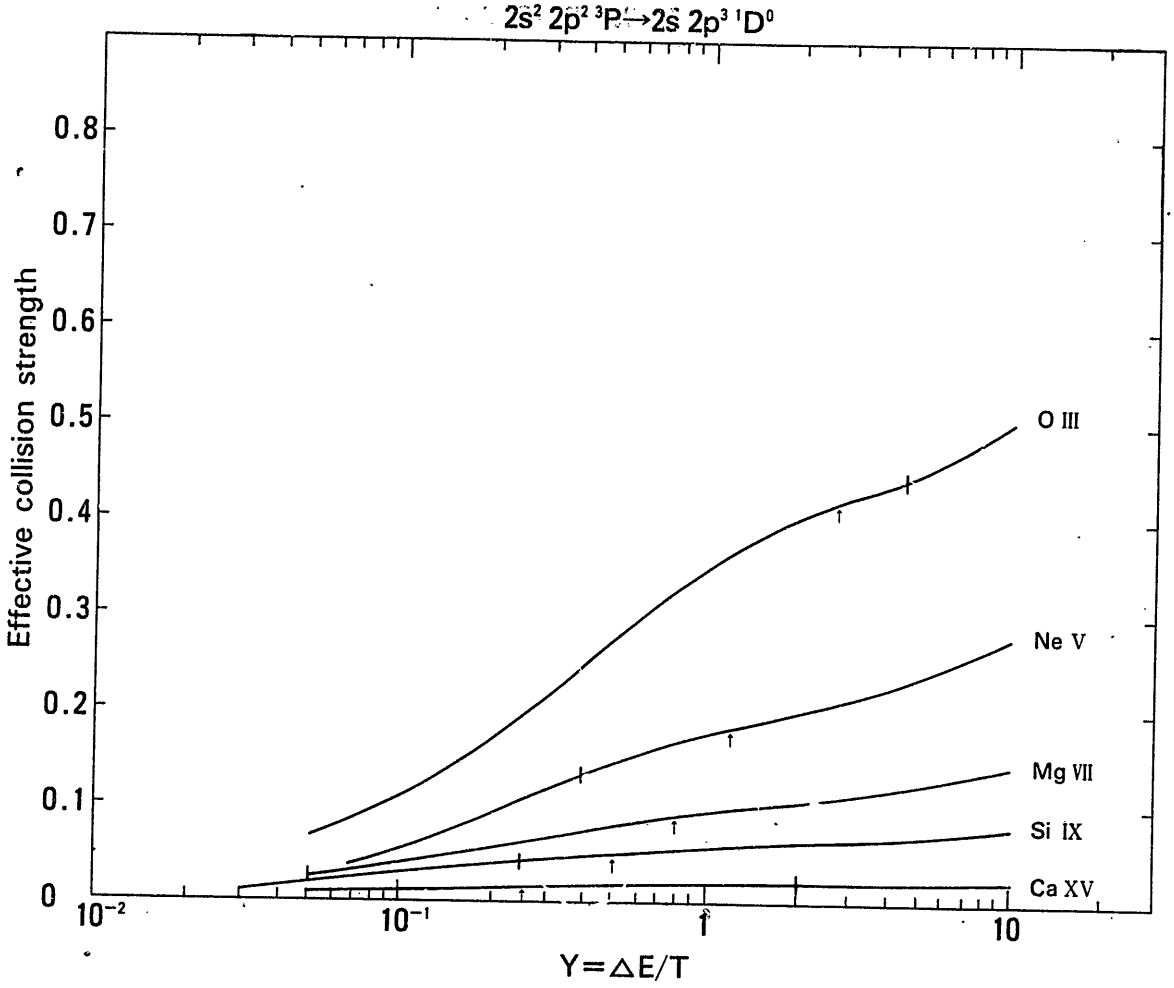

Fig. 4. Same as Fig. 1, but for the transition $2s^2 2p^2\ ^3P \longrightarrow 2s2p^3\ ^1D^o$.

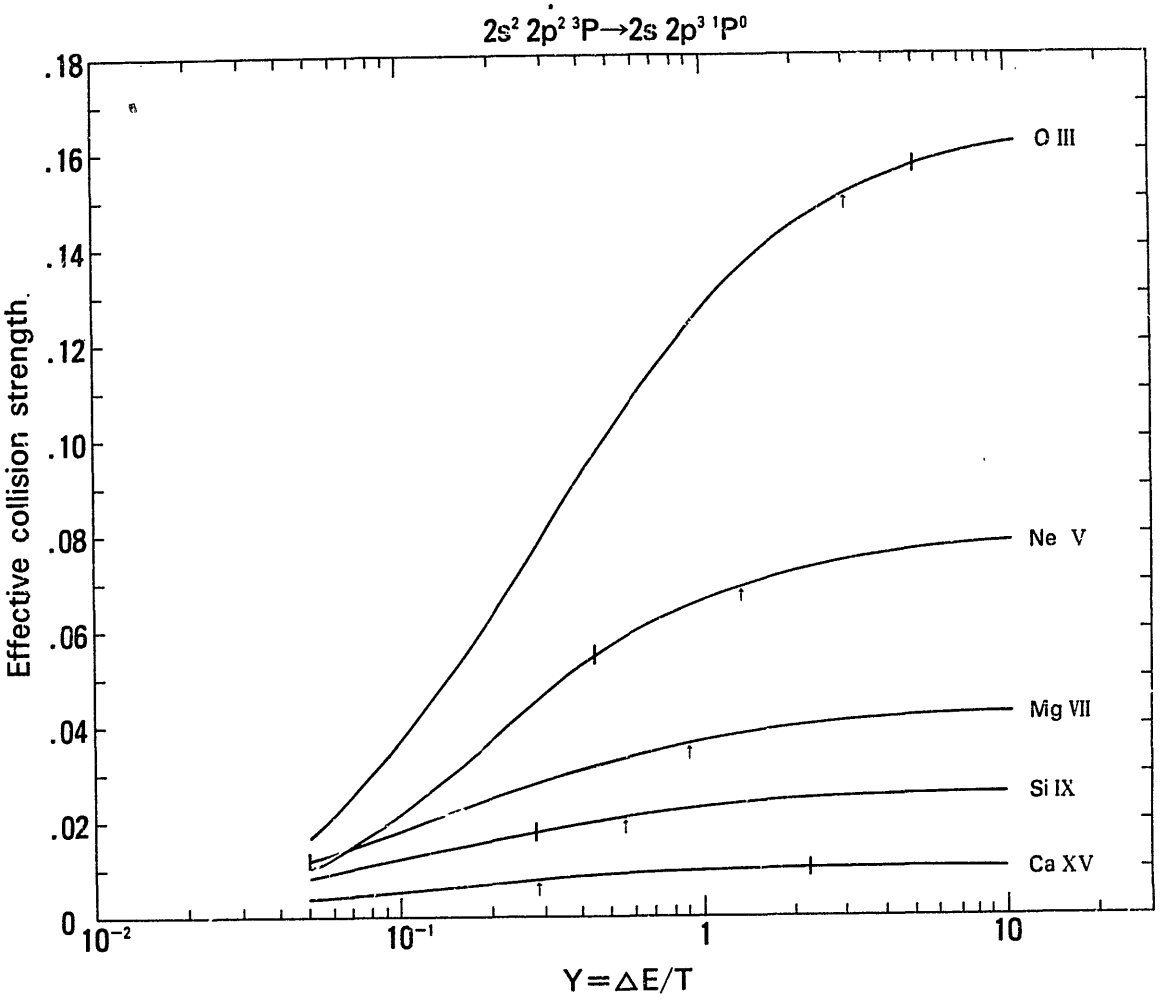

Fig. 5. Same as Fig. 1, but for the transition $2s^2 2p^2\ ^3P \longrightarrow 2s2p^3\ ^1P^o$.

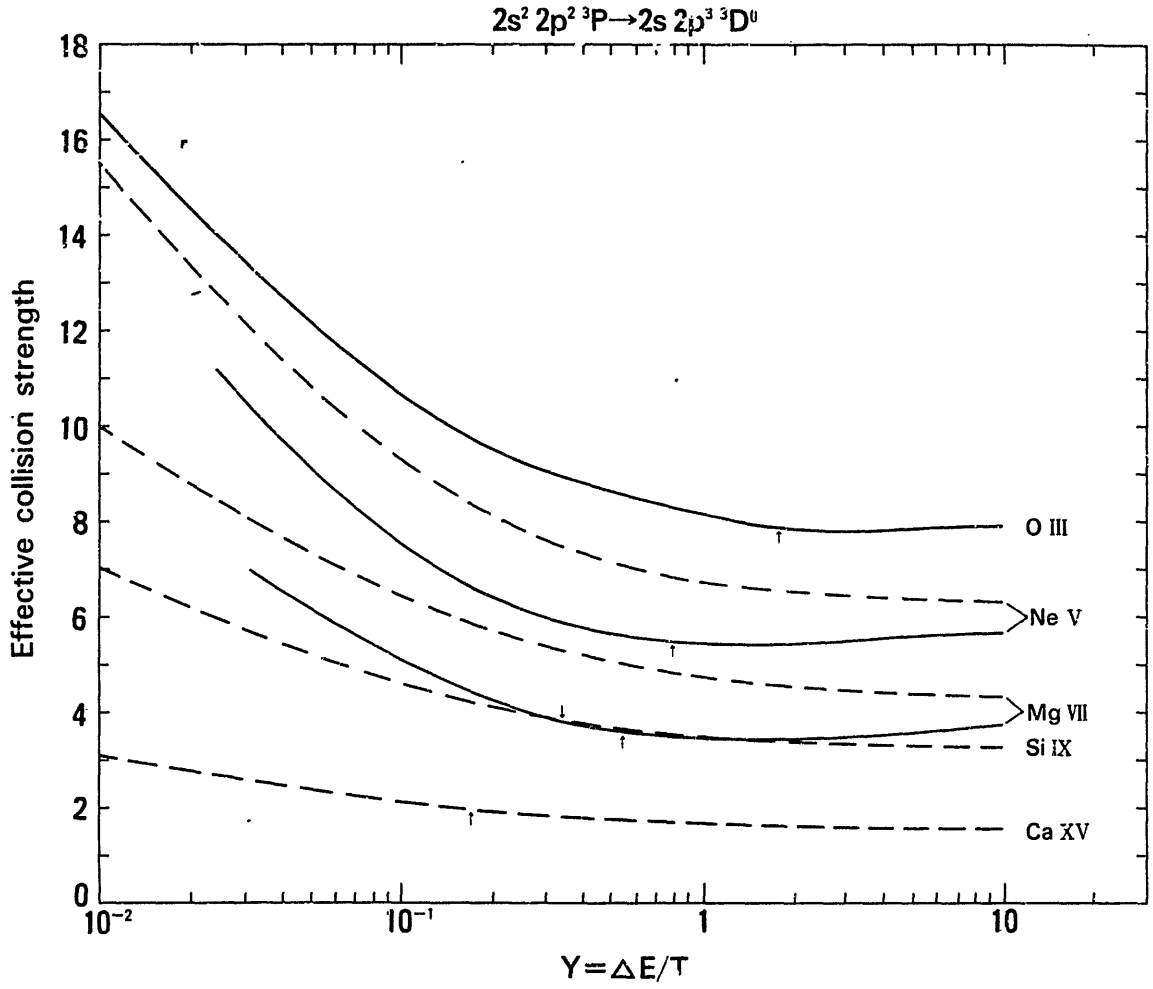

Fig. 6. Effective collision strengths for the transition $2s^2 2p^2\ ^3P \rightarrow 2s2p^3\ ^3D^o$ in O III, Ne V, Mg VII, Si IX and Ca XV by electron collisions. The horizontal scale indicates the inverse temperature in the units of transition energy. The solid lines are the results of the R-matrix method (Ne V and Mg VII) or the revised recommended values (O III, see text). The dashed lines show the results based on the distorted-wave calculation. Arrows denote the temperature at which the respective ion has its maximum population in the calculation of steady-state ionization balance.

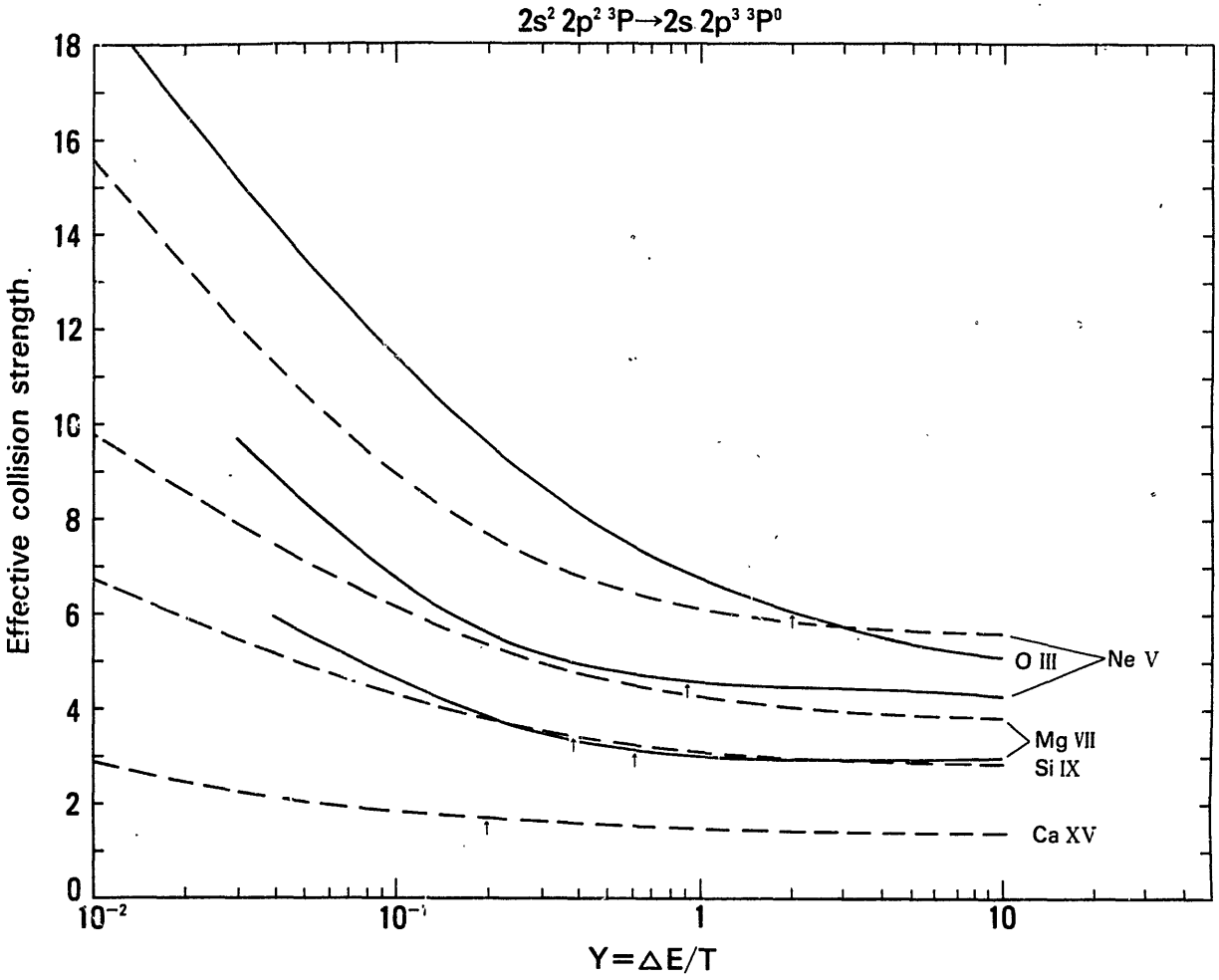

Fig. 7. Same as Fig. 6, but for the transition $2s^2 2p^2\ ^3P \longrightarrow 2s2p^3\ ^3P^o$.

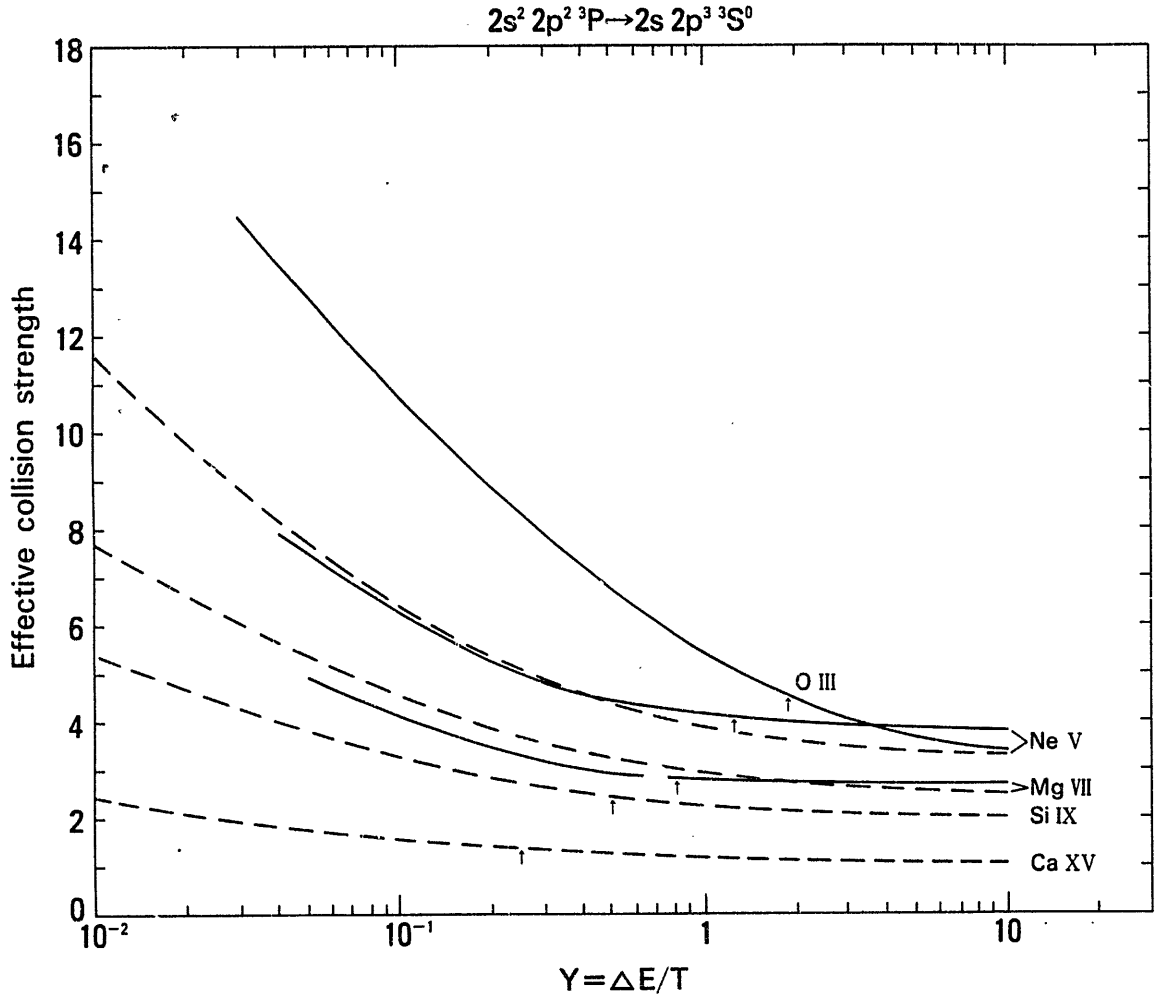

Fig. 8. Same as Fig. 6, but for the transition $2s^2 2p^2\ ^3P \longrightarrow 2s2p^3\ ^3S^o$.

LIST OF IPPJ-AM REPORTS

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