

CONF-790360--1

LA-UR-79-660

TITLE: PARTIAL PHOTOIONIZATION CROSS SECTIONS AND RADIATIVE RECOMBINATION RATE COEFFICIENTS FOR Li-LIKE IONS - II

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SUBMITTED TO: The International Symposium on Atomic, Molecular, and Solid State Theory, Flagler Beach, Florida, March 11 through March 17, 1979

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Partial Photoionization Cross Sections and Radiative Recombination

Rate Coefficients for Li-Like Ions - II

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ABSTRACT

A non-hydrogenic single-electron-transition model with Dirac-Slater SCF wave functions and all necessary multipoles has been used to obtain partial photoionization cross sections for C⁺³, O⁺⁵, Al⁺¹⁰, Fe⁺²³, and Mo⁺³⁹ for principal quantum number $n = 10$ and all ℓ , $h\nu \gtrsim 200$ keV, supplementing results reported elsewhere for $n = 2, 3, 4$, and 6 . The partial cross sections for the isoelectronic sequence are represented approximately by a simple analytical form:

$$\ln [(Z - s_{n\ell})^2 \sigma^{n\ell} (h\nu)] = \sum_0^3 a_i(n\ell)x^i$$

(Z = nuclear charge; $x = \ln [h\nu/(Z - 2)^2]$.) n^{-3} scaling is used to obtain partial cross sections for other values of n ($6 < n < 10$, $10 < n < 100$). Radiative recombination rate coefficients (summed over ℓ and $n < 100$) have been calculated from the partial photoionization cross sections for $kT = .01, .03, 0.1, 0.3, 1.0, 3.0$ and 10.0 keV. The results have application to ionization balance calculations for the solar corona and for TOKAMAKS.

Partial photoionization cross sections for Li-like ions of C, O, Al, Fe and Mo for principal quantum number $n = 2, 3, 4$ and 6 and $\ell < n$ calculated on the basis of a single-electron-transition model [1] were reported previously ([2], referred to below as I). This paper extends those results to $n = 10$, and introduces a different method for scaling the single-electron-transition model results to other values of n , in order to obtain recombination rate coefficients summed over n and ℓ .

The single-electron-transition model used as the basis of the calculations reported here is described in (I), where also comparisons are made with results of other authors and with non-relativistic dipole hydrogenic model results. In the cases of Li-like Al, Fe and Mo it was found empirically that the cross section for photoionization from an excited orbital is given with small error by using the wave function for the corresponding orbital in the ground state configuration. Enough multipole terms were used to ensure a calculated cross section converged to within $\pm 1\%$.

Partial photoionization cross sections for a typical case (0^{+5} , $n = 10$) are shown in Fig. 1. Coefficients of polynomials for interpolating the partial cross sections to intermediate values of Z (= nuclear charge),

$$z^2 \sigma(Z, h\nu_i^*) = \begin{cases} N_i^{-1} \sum_{j=0}^3 b_{ij} z^{-j} & (6 \leq Z \leq 26) \\ N_i^{-1} \sum_{j=0}^2 c_{ij} z^{-j} & (26 \leq Z \leq 42) \end{cases} \quad (1)$$

are given in Table I, which also tabulates the normalization constants N_i and the coefficients in

$$z^2 h\nu_i^*(Z) = A_i + B(z^{-1} - z_1^{-1}) + C(z^{-2} - z_1^{-1}) \quad (i = 1, 2, 3, \dots) \quad (2)$$

The quadratic splines match the slopes and values of the cubics at $Z = z_1 = 26$. An example illustrating the use of the interpolating polynomials is given in (I).

Less accurately, the partial photoionization cross section data for the isoelectronic sequence can be represented by the simple form (compare [3])

$$\ln[(Z - s_{n\ell})^2 \sigma^{n\ell}(Z, h\nu)] = \sum_{i=0}^3 a_i(n\ell) x^i \quad (3)$$

where $x = \ln[h\nu/(Z - 2)^2]$. (Figure 2 is a typical plot.) The coefficients a_i and screening constants $s_{n\ell}$ (Table II) were determined by a least-squares procedure so as to keep the fractional error $|\sigma_{\text{fit}} - \sigma|/\sigma$ less than about 5% near threshold. The error increases at higher photon energies. Figure 3 is a typical error plot.

The partial cross sections scale approximately as n^{-3} for $\ell \geq 3$ (Figs. 4, 5; also, figures in [4]). (Compare Eq. 71.20 of [5].)

Radiative recombination rate coefficients [6] were calculated from the partial photoionization cross sections. n^{-3} scaling from $n = 10$ was used to generate cross sections for $6 < n < 10$ and $10 < n$ in order to sum the rate coefficients over empty and partially-filled shells with $n < 100$. The contribution of terms with $9 < \ell$ was neglected (Fig. 5). For $10 < n$ an extrapolation to energies below the $n = 10$ edge is also required: Compare Fig. 4. Quadratic extrapolation on the logarithms -- i.e., $\log \sigma$ vs. $\log h\nu$ -- was used. (For the higher temperatures ($.01 \text{ keV} < kT$ for C; $3 \text{ keV} < kT$ for Mo) the contributions of $3 < \ell < 9$ and the partial integral below the $n = 10$ edge are each less than 10%.) Figure 6 shows the convergence of the sums in a typical case.

The calculated summed rate coefficients differ only slightly* from the

*Differences are hardly detectable on the scale of Fig. 2 of (I).

curves of Fig. 2 of (I), where a different method was used to approximate the contribution of terms with $6 < n$.

The summed recombination rates can be approximated with error < 1% by

$$kT \sum_{n,\ell} \alpha^{n\ell}(T) = \sum_{i=0}^3 B_i [\log_{10}(kT/\text{keV})]^i \quad (4)$$

where the coefficients are given in Table IV. Table V gives ratios of the summed coefficients to Kramers' semiclassical model ([7] and (I)) values. Although the partial photoionization cross sections may differ substantially from dipole hydrogenic values (I, and Table III),* the Kramers model predicts the summed recombination rate coefficients fairly accurately in most cases.

The partial cross sections and recombination rate coefficients reported here have application to ionization balance calculations for the solar corona and for TOKAMAKS.

Acknowledgment

The SCF bound state wave functions were obtained with a computer program developed by Liberman, Waber and Cromer [8].

The author thanks Dr. W. F. Huebner for commenting on the manuscript.

*Differences are probably mainly due to higher multipoles: The ratio of photon wave length to orbital diameter is $0.5\lambda/\langle r \rangle_{nl}$

$$\approx 23(Z-2) \text{ keV } (\hbar\nu)^{-1} [3n^2 - \ell(\ell + 1)]^{-1}.$$

For a 10p orbital this ratio is .08(Z-2) keV/hν.

Table I - Constants (A_i , B , C , Z_1) for Eq. (2) of text, normalization constants (N_i), coefficients (b_0 , b_1 , b_2 , b_3) of cubic polynomials (in Z^{-1}) for interpolation in the range $6 < Z < 26$, and coefficients (c_0 , c_1 , c_2) of quadratic splines (in Z^{-1}) for interpolation in the range $26 < Z < 42$. (The slope and value of the spline at $Z^{-1} = 26^{-1}$ match the cubic.) Units for A_i and N_i are keV and 10^{24} cm^{-2} , respectively.

* For these cases the polynomial fits should not be used for $Z < 8$.

Table II - Screening parameters (s_{nl}) and coefficients for Eq. (3) of text.

$\langle x_0 \rangle$ = Z-average of x corresponding to edge.

Table IV - Coefficients for fits (Eq. 4 of text) giving temperature dependence of summed recombination rate coefficients, $\sum_{nl} \alpha^{nl}(T)$ (cm^3/s), for ions that are Li-like after recombination.

Table V - Ratios of summed recombination rate coefficients to Kramers model values. (The ion stage is that of the recombined ion.)

Figure Captions

Fig. 1. Partial photoionization cross sections for O^{+5} , $n = 10$, calculated on basis of single-electron-transition model.

Fig. 2. Partial photoionization cross sections for Li-like ions (6d shell) multiplied by $(Z - s)^2$. The curve is a least-squares fit. (Units: barns, keV)

Fig. 3. Fractional error $(\sigma_{\text{fit}} - \sigma)/\sigma$ of fit in Fig. 2.

Fig. 4. Partial photoionization cross sections for $Al + 10$, $n = 10$, calculated by single-electron-transition model. Also shown are points scaled (n^{-3}) from $n = 6$. The arrow indicates the 6s edge.

Fig. 5. Single-electron-transition model calculations of partial photoionization cross sections for Al^{+10} , $n = 10$, multiplied by statistical weight factor g_i/g_{i+1} (see I) and partial summed on ℓ . Also shown are points (Δ , o) scaled (n^{-3}) from single-electron-transition model results for $n = 6$, and a point (x) corresponding to extrapolation from $n = 4$ and 6 by Lee-Pratt method [9]. The asymptotic value given by the hydrogenic expression 71.20 of [5] is also indicated (B/S). The $n = 10$ edge is approximately $h\nu \approx .017$ keV.

Fig. 6. Partial sum on n , ℓ of radiative recombination rate coefficients for Al^{+10} , $kT = .03$, 1.0 keV, calculated by single-electron-transition model ($n = 2, 3, 4, 6, 10$) and n^{-3} scaling. $L = \min(n-1, 9)$.

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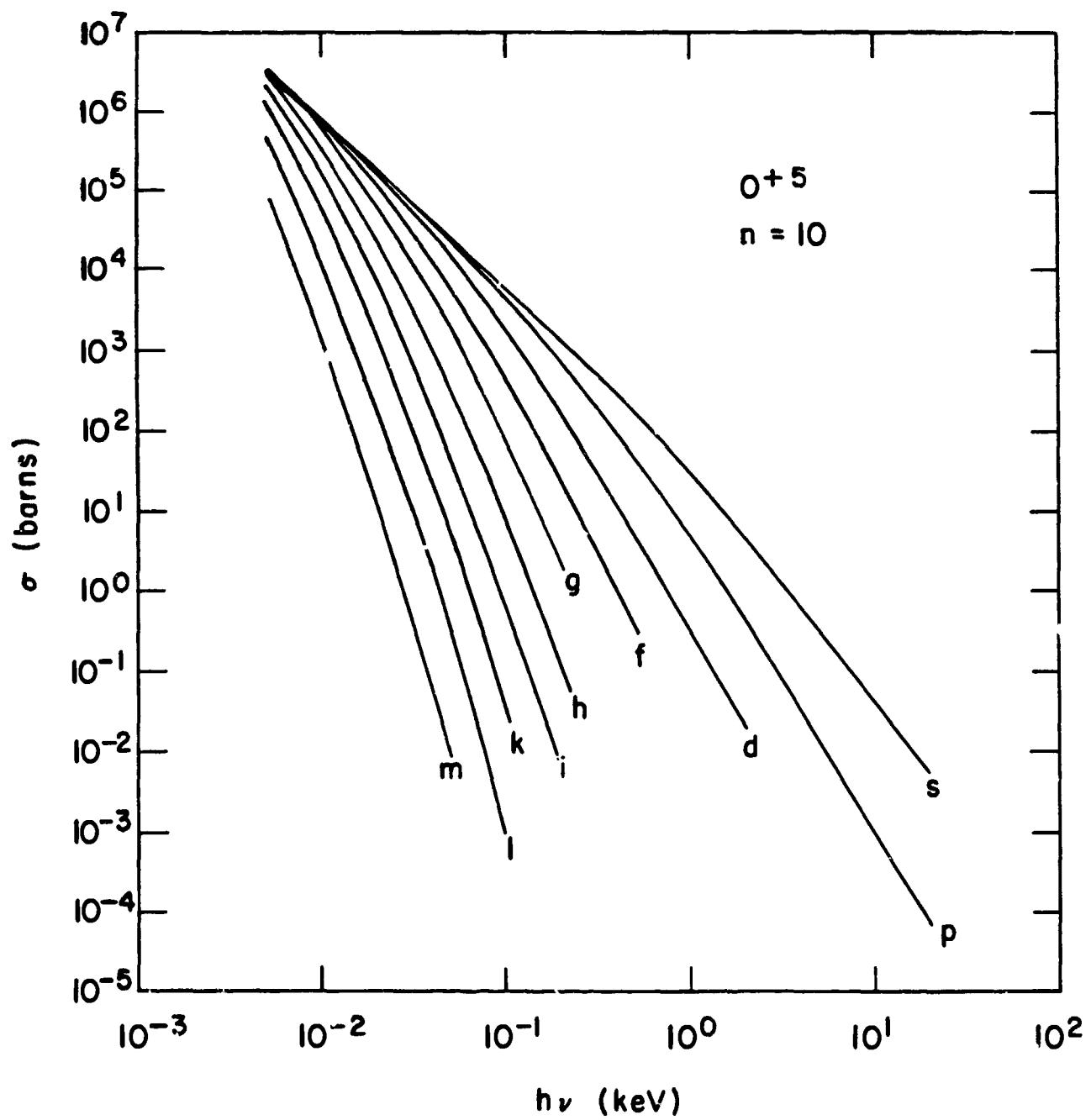


Fig. 1. Partial photoionization cross sections for O^{+5} , $n = 10$, calculated on basis of single-electron-transition model.

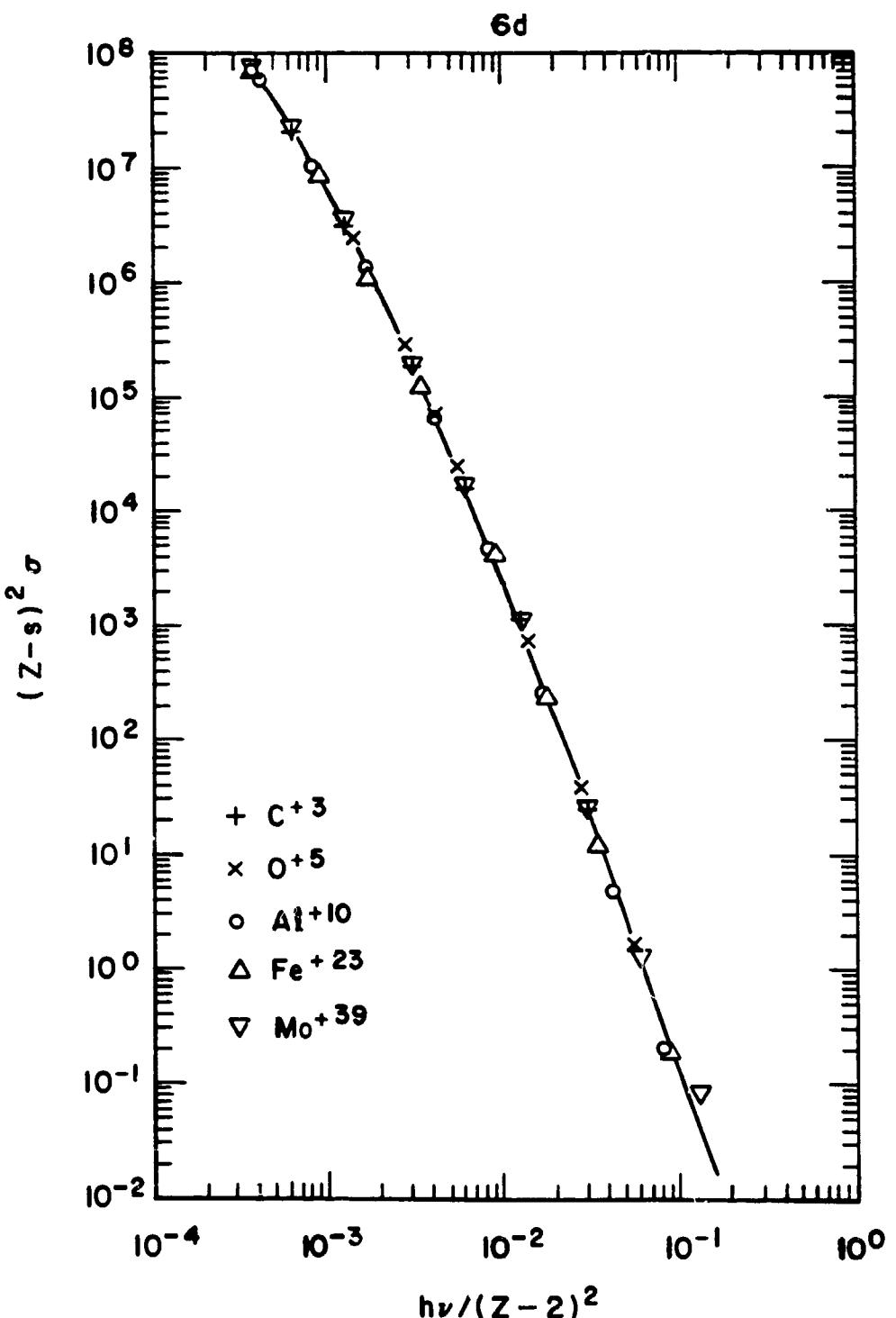


Fig. 2. Partial photoionization cross sections for Li-like ions (6d shell) multiplied by $(Z-s)^2$. The curve is a least-squares fit. (Units: barns, keV)

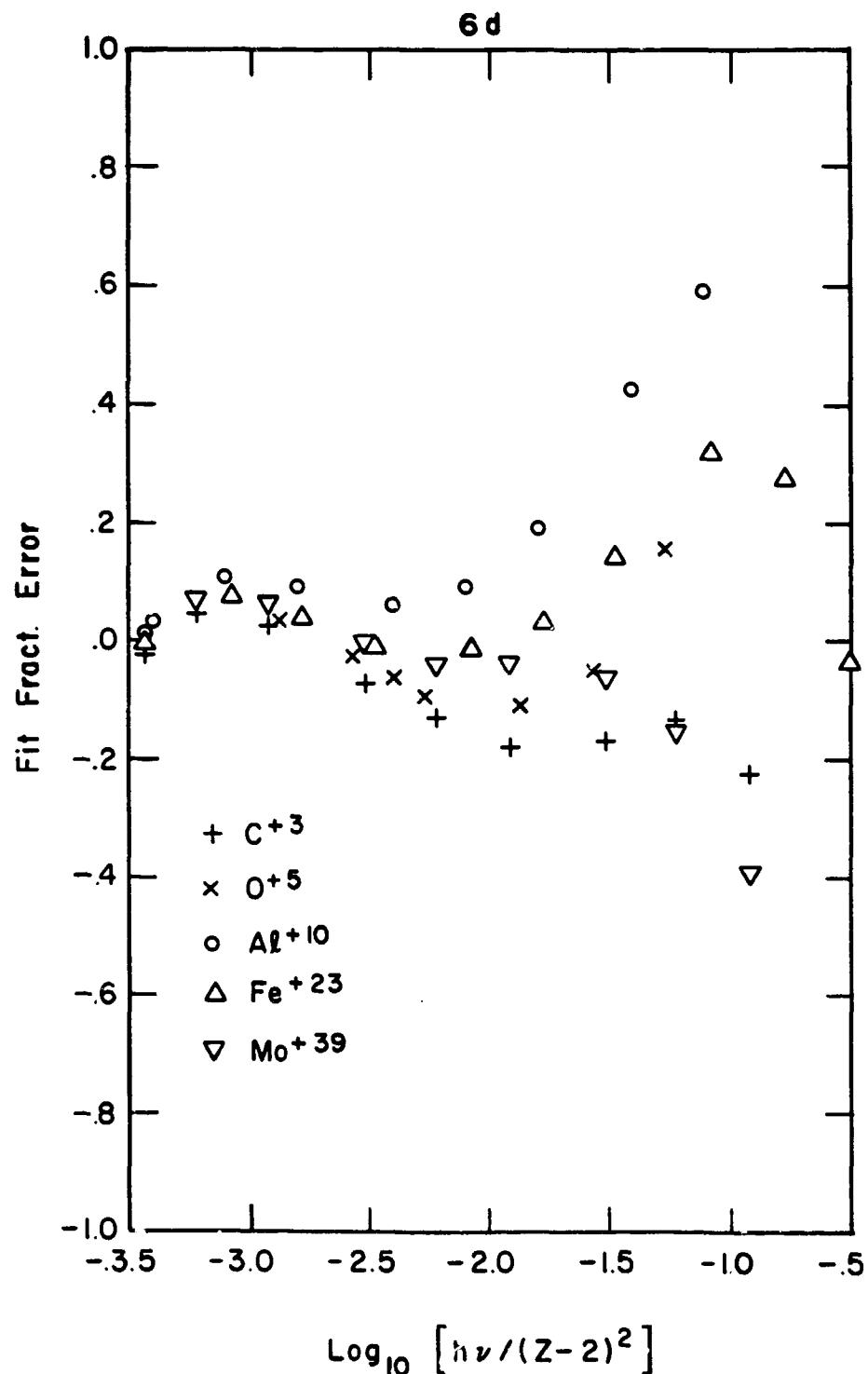
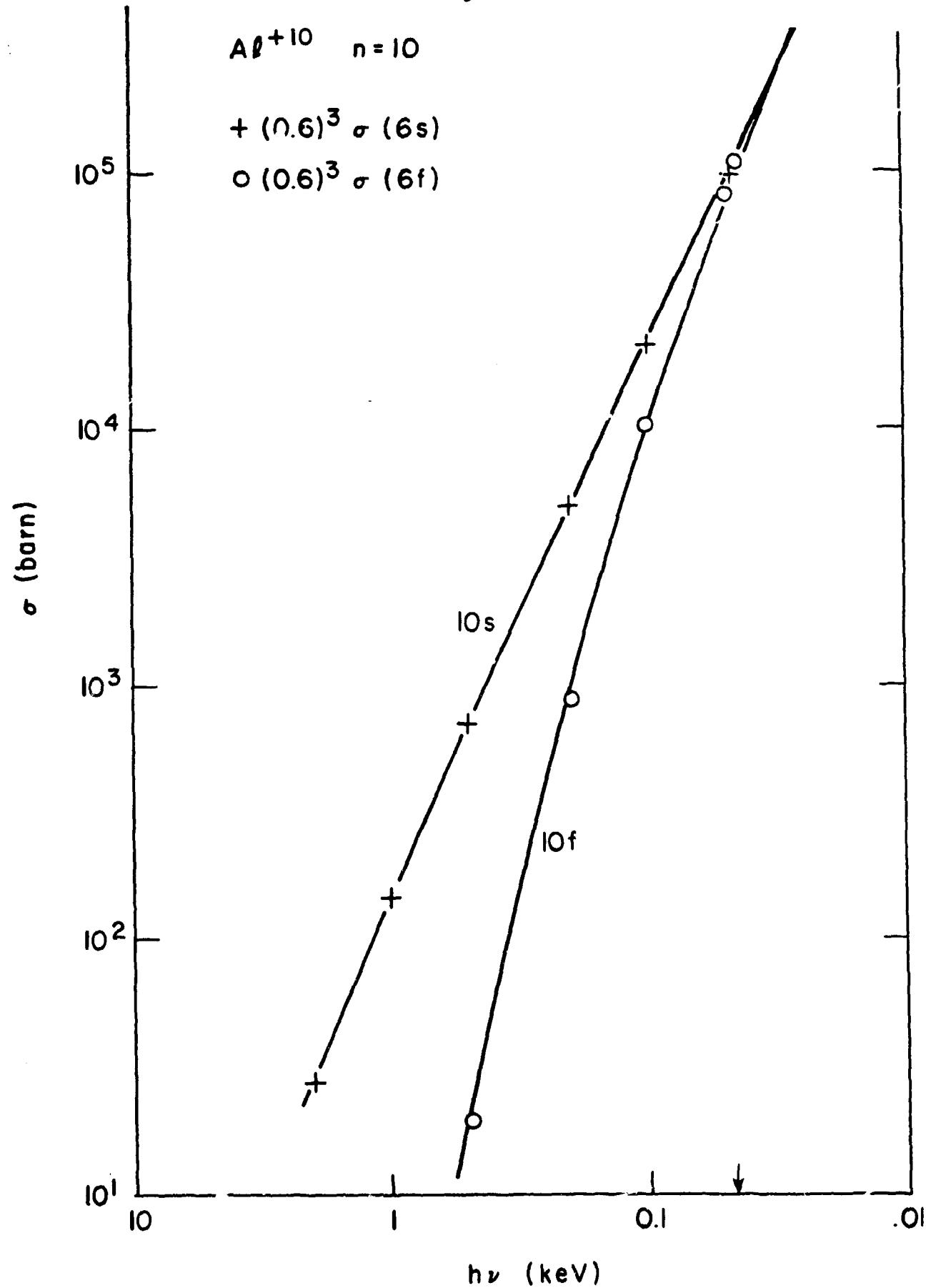


Fig. 3. Fractional error $(\sigma_{fit} - \sigma)/\sigma$ of fit in Fig. 2.

Fig. 4. Partial photoionization cross sections for Al + 10, n = 10, calculated
by single-electron-transition model. Also shown are points scaled (n^{-3}) from
n = 6. The arrow indicates the 6s edge.



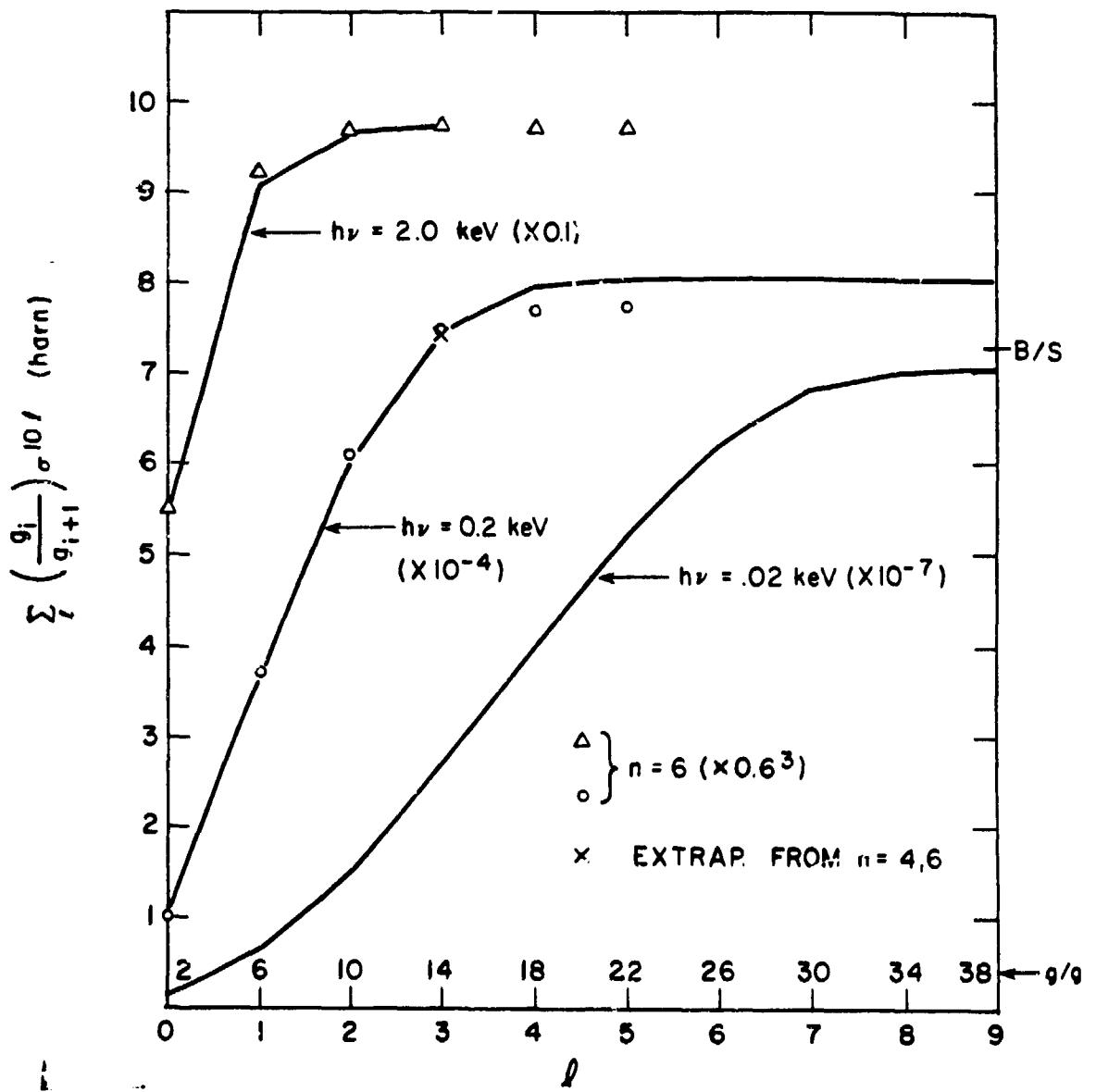


Fig. 5. Single-electron-transition model calculations of partial photoionization cross sections for Al^{+10} , $n = 10$, multiplied by statistical weight factor g_i/g_{i+1} (see I) and partial summed on i . Also shown are points (Δ , \circ) scaled (n^{-3}) from single-electron-transition model results for $n = 6$, and a point (\times) corresponding to extrapolation from $n = 4$ and 6 by Lee-Pratt method [9]. The asymptotic value given by the hydrogenic expression 71.20 of [5] is also indicated (B/S). The $n = 10$ edge is approximately $h\nu \approx .017$ keV.

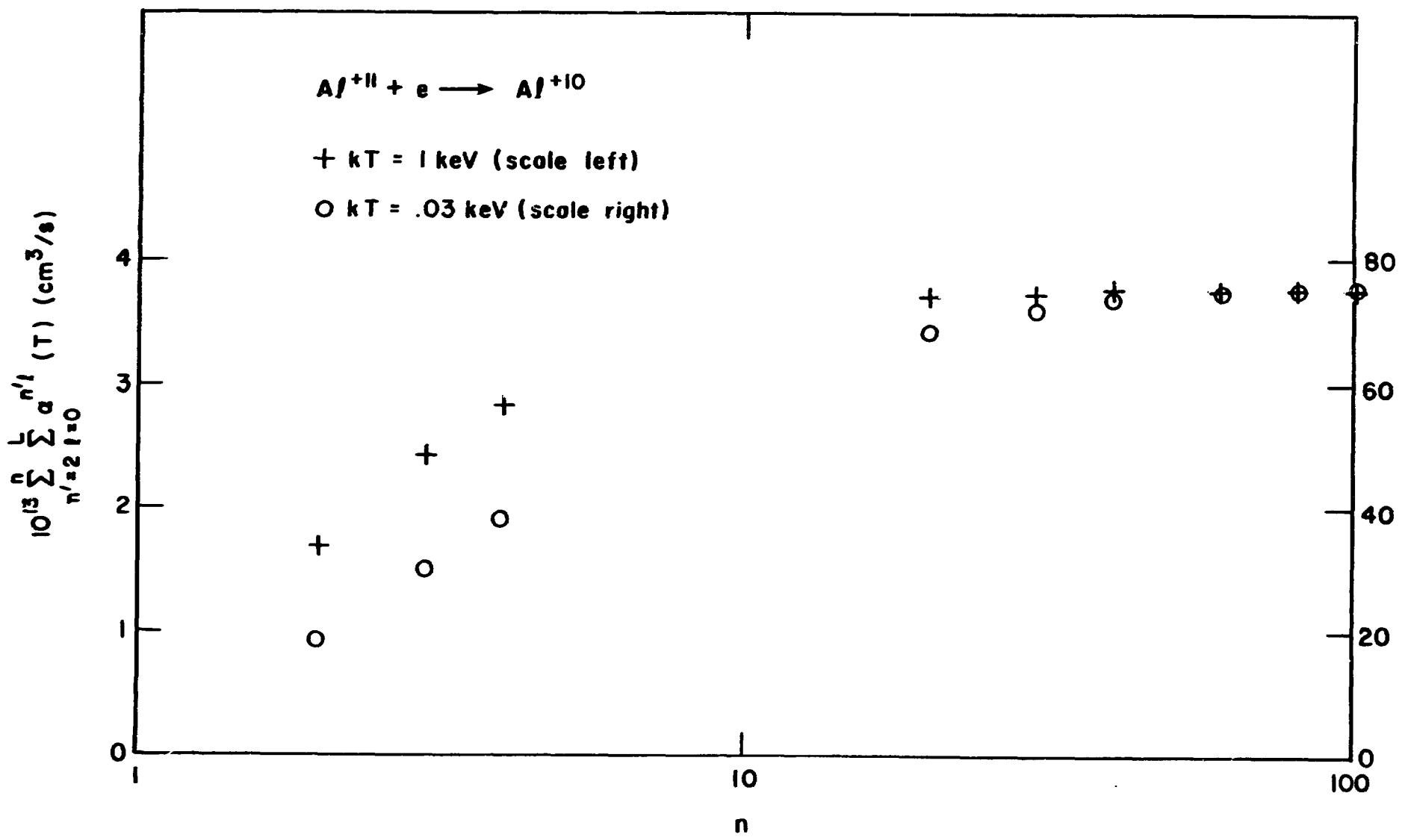


Fig. 6. Partial sum on n , l of radiative recombination rate coefficients for Al^{+10} , $kT = .03, 1.0 \text{ keV}$, calculated by single-electron-transition model ($n = 2, 3, 4, 6, 10$) and n^{-3} scaling. $L = \min(n-1, 9)$.

		b = -.000548 kev	c = .000553 kev	z1 = 26	
1	7.8455e-02	3.2672e-09	5.7578e-01 -1.6460e+00	5.5517e+01 -1.8221e+02	4.5287e-01 5.0145e+00 -4.1583e+01
2	1.0000e-01	8.9372e-09	7.7904e-01 7.0230e-01	9.5581e+00 -3.4004e+01	9.4613e-01 -7.9346e+00 1.1982e+02
3	2.0000e-01	7.3379e-08	1.2506e+00 -9.6592e+00	5.7259e+01 -1.8188e+02	8.9428e-01 9.1450e+00 -1.9764e+02
4	4.0000e-01	7.1293e-07	1.2066e+00 -1.0780e+01	4.5770e+01 -1.1956e+02	1.3796e+00 -1.9598e+01 1.5351e+02 *
5	7.0000e-01	6.1418e-06	1.1631e+00 -1.0073e+01	2.1242e+01 -4.7339e+00	1.6093e+00 -3.3271e+01 3.2254e+02 *
6	1.0000e+00	2.8478e-05	1.2511e+00 -1.3431e+01	4.5961e+01 -5.6087e+01	1.5481e+00 -2.8790e+01 2.4240e+02 *
7	2.0000e+00	7.5697e-04	1.4050e+00 -2.1230e+01	1.2357e+02 -2.7867e+02	1.6305e+00 -3.2543e+01 2.5456e+02 *
		b = -.000547 kev	c = .000556 kev	z1 = 26	
1	7.8387e-02	3.6237e-09	5.0095e-01 3.6788e-01	2.5392e+01 -5.7801e+01	4.4220e-01 3.5083e+00 -1.8769e+01
2	1.0000e-01	1.2769e-08	9.1027e-01 -9.9639e-01	2.8028e+01 -1.1452e+02	1.0923e+00 -1.0293e+01 1.4227e+02
3	2.0000e-01	1.2904e-07	1.2715e+00 -1.1980e+01	8.3218e+01 -2.9935e+02	1.0583e+00 -4.4918e-01 -8.3949e+01
4	4.0000e-01	1.9844e-06	1.3588e+00 -1.6548e+01	8.7895e+01 -2.1710e+02	1.2706e+00 -1.1643e+01 1.1617e+01 *
5	7.0000e-01	2.6123e-05	1.4480e+00 -2.2475e+01	1.3985e+02 -3.4095e+02	1.5216e+00 -2.5798e+01 1.6339e+02 *
6	1.0000e+00	1.6159e-04	1.5536e+00 -2.7618e+01	1.9056e+02 -4.8394e+02	1.5535e+00 -2.6898e+01 1.5328e+02 *
7	2.0000e+00	7.8790e-03	1.4975e+00 -2.3832e+01	1.3232e+02 -2.5931e+02	1.4775e+00 -2.2408e+01 9.8839e+01 *
		b = -.000545 kev	c = .000549 kev	z1 = 26	
1	7.8383e-02	8.7473e-09	4.2710e-01 2.3718e+00	-4.5230e+00 6.5499e+01	4.4004e-01 1.6022e+00 9.2613e+00
2	1.0000e-01	2.1330e-08	1.0317e+00 -3.3028e+00	5.3397e+01 -2.3200e+02	1.1349e+00 -8.3292e+00 1.0536e+02
3	2.0000e-01	3.0397e-07	1.638e+00 -8.8180e+00	3.7946e+01 -1.3316e+02	1.3415e+00 -1.7864e+01 1.3787e+02
4	4.0000e-01	7.9185e-06	1.4694e+00 -2.0390e+01	1.0959e+02 -2.3492e+02	1.1655e+00 -4.2372e+00 -1.1395e+02 *
5	7.0000e-01	1.6547e-05	1.8428e+00 -3.8536e+01	2.9666e+02 -7.8881e+02	1.2468e+00 -6.3973e+00 -1.6664e+02 *
6	1.0000e+00	1.3753e-03	1.9297e+00 -4.3437e+01	3.5070e+02 -9.5641e+02	1.3354e+00 -1.1118e+01 -1.2462e+02 *
		b = -.000546 kev	c = .000551 kev	z1 = 26	
1	7.8383e-02	8.0350e-09	3.7599e-01 3.8189e+00	-2.5830e+01 1.5229e+02	4.4754e-01 -1.2711e-01 3.4253e+01
2	1.0000e-01	4.3866e-08	1.0946e+00 -5.2835e+00	7.3235e+01 -3.3092e+02	1.0428e+00 -2.1648e+00 1.2820e+01
3	2.0000e-01	1.0339e-06	9.9500e-01 -2.4003e+00	-5.5237e+01 2.4102e+02	1.6251e+00 -3.5533e+01 3.8926e+02
4	4.0000e-01	4.7600e-05	1.3696e+00 -1.8076e+01	7.3631e+01 -4.8230e+01	1.5039e+00 -2.4989e+01 1.6071e+02
5	7.0000e-01	1.5660e-03	1.5765e+00 -2.4908e+01	1.0452e+02 1.8671e+00	1.2822e+00 -9.6097e+00 -9.4245e+01
6	1.0000e+00	1.6909e-02	1.5388e+00 -2.1074e+01	1.4658e+01 4.7262e+02	1.1990e+00 -4.1058e+00 -1.7866e+02
		b = -.000546 kev	c = .000549 kev	z1 = 26	
1	7.8383e-02	2.0091e-08	3.6944e-01 4.0106e+00	-2.8829e+01 1.6479e+02	4.5892e-01 -8.8594e-01 4.4333e+01
2	1.0000e-01	1.3378e-07	1.0440e+00 -1.9324e+00	1.9873e+01 -1.3354e+02	9.8795e-01 1.1794e+00 -2.8285e+01
3	2.0000e-01	5.7385e-06	9.5707e-01 -1.3405e-01	-1.0946e+02 5.0729e+02	1.6731e+00 -3.8119e+01 4.1361e+02
4	4.0000e-01	4.8485e-04	1.1561e+00 -1.5615e+01	6.1159e+01 0.	2.4034e+00 -8.0475e+01 9.0434e+02 *
5	7.0000e-01	7.9153e-03	3.2718e-01 -2.3805e+00	1.5695e-01 0.	6.3930e-01 -1.8613e+01 2.1118e+02 *
		b = -.000545 kev	c = .000549 kev	z1 = 26	
1	7.8383e-02	9.8193e-08	4.1995e-01 2.2522e+00	-5.0891e+00 7.4747e+01	4.5976e-01 7.1895e-02 2.7567e+01
2	1.0000e-01	7.9555e-07	9.4424e-01 2.6547e+00	-5.3953e+01 1.6856e+02	1.0939e+00 -5.3781e+00 6.0197e+01
3	2.0000e-01	6.8587e-05	1.3833e+00 -1.5725e+01	4.1821e+01 5.0985e+01	1.1559e+00 -3.9797e+00 -1.0793e+02
4	4.0000e-01	1.0702e-02	1.5231e+00 -2.9597e+01	1.9469e+02 -4.0271e+02	2.0369e+00 -5.5716e+01 5.1101e+02 *

For these cases the polynomial fits should not be used for z < 8.

Table II - Screening parameters (s_{nl}) and coefficients for Eq. (3) of text.

$\langle x_0 \rangle$ = Z-average of x corresponding to edge.

Table II

$\langle x_0 \rangle$	s_{nl}	a_0	a_1	a_2	a_3
2s-5.598	2.218e+00	1.16579e+00-3.17450e+00-3.15840e-02	9.40884e-03		
2p-5.665	2.022e+00-4.02684e+00-4.06600e+00-3.96844e-02	6.98789e-03			
3s-6.435	1.911e+00	7.76182e-02-3.16582e+00-5.64859e-02	4.59327e-03		
3p-6.474	2.215e+00-5.07265e+00-4.01668e+00-1.47591e-02	1.20084e-02			
3d-6.492	1.862e+00-1.17330e+01-4.77786e+00	3.23797e-02	1.42398e-02		
4s-7.023	1.806e+00-8.89286e-01-3.30874e+00-1.03454e-01-1.45335e-04				
4p-7.051	2.218e+00-6.04960e+00-4.22412e+00-8.02067e-02	6.55075e-03			
4d-7.067	1.944e+00-1.27453e+01-5.26820e+00-8.44138e-02	8.06583e-03			
4f-7.069	1.944e+00-1.20468e+01-3.48598e-01	1.19046e+00	9.38353e-02		
6s-7.848	1.634e+00-1.74529e+00-3.01248e+00-4.13482e-02	3.03871e-03			
6p-7.865	2.078e+00-6.84348e+00-4.05242e+00-6.44119e-02	6.21764e-03			
6d-7.878e+00	2.033e+00-1.20981e+01-4.25480e+00	1.11636e-01	2.09815e-02		
6f-7.880	1.893e+00-1.74456e+01-4.18441e+00	3.24881e-01	3.62043e-02		
6g-7.880	1.868e+00-2.16570e+01-3.29201e+00	6.48568e-01	5.51623e-02		
6h-7.880	1.658e+00-3.36990e+01-5.97346e+00	3.59258e-01	3.91294e-02		
10s-8.883e+00	1.481e+00-3.24171e+00-3.05652e+00-6.90098e-02-2.27880e-04				
10p-8.893e+00	2.060e+00-8.59518e+00-4.26373e+00-1.28544e-01	6.18727e-04			
10d-8.900e+00	2.178e+00-1.40716e+01-4.86570e+00-5.35682e-02	8.78834e-03			
10f-8.901e+00	2.065e+00-1.89390e+01-4.96068e+00	9.71828e-02	1.99609e-02		
10g-8.902e+00	1.975e+00-3.14063e+01-8.18898e+00-2.02690e-01	9.36665e-03			
10h-8.902e+00	1.802e+00-2.28843e+01-2.23858e+00	7.77251e-01	5.66042e-02		
10i-8.902e+00	1.664e+00-4.17646e+01-7.85724e+00	1.33549e-01	2.88400e-02		
10k-8.902e+00	1.732e+00-8.47619e+01-2.21574e+01-1.55863e+00-4.09295e-02				
10l-8.902e+00	2.011e+00-2.77855e+01	2.70676e+00	1.79394e+00	1.04086e-01	
10m-8.902e+00	2.335e+00	3.69711e+01	3.03354e+01	5.40393e+00	2.55083e-01

Table III

RATIOS OF $2 \sum_{\ell} (2\ell+1) \sigma^{n\ell}(\text{nu})$ TO BETHE-SALPETER
 HYDROGENIC VALUE (EQ. 71.20 OF [5]) WITH Z-2 FOR N=6, 10.

n	Approximate $\ell = 0$ Edge (keV)	$h\nu$ (keV)			
		.01	0.1	1.0	10.0
C^{+3}	6	.00642	.990	1.49	2.30
	10	.00226	1.19	1.65	>1.75
Al^{+10}	6	.047		.997	1.22
	10	.0167		1.054	1.23
Mo^{+39}	6	0.617		.990	1.22
	10	0.220		1.057	1.23

Table IV
COEFFICIENTS FOR FITS (EQ. 4 OF TEXT) GIVING TEMPERATURE
DEPENDENCE OF SUMMED RECOMBINATION RATE COEFFICIENTS, $\sum_{nl} \alpha^{nl}(T)$ (cm³/s),
FOR IONS THAT ARE LI-LIKE AFTER RECOMBINATION.

	kT (keV)					
	min	max	B ₀	B ₁	B ₂	B ₃
C+3	.01	1.00	1.99421e-14	-4.70848e-15	-5.16767e-15	-6.36586e-15
O+5	.01	3.00	6.57030e-14	-7.63145e-15	-1.58908e-14	-2.48969e-15
Al+10	.01	3.00	3.82161e-13	1.42036e-14	-8.89663e-14	-2.13726e-14
Fe+23	.03	10.00	3.56417e-12	9.91530e-13	-4.98071e-13	-2.42434e-13
Mo+39	.10	10.00	1.38883e-11	6.85401e-12	-9.61099e-13	-1.18680e-12

Table V
 RATIOS OF SUMMED RECOMBINATION RATE COEFFICIENTS TO
 KRAMERS MODEL VALUES. (THE ION STAGE IS THAT OF THE RECOMBINED ION.)

$kT(\text{keV})$	C^{+3}	O^{+5}	Al^{+10}	Fe^{+23}	Mo^{+39}
.01	.98	.943	.965		
.03	1.06	.984	.964	.957	
.1	1.18	1.05	.980	.961	.943
.3	1.33	1.15	1.02	.972	.962
1.0	1.53	1.29	1.08	.999	.989
3.0		1.41	1.15	1.041	1.026
10.0				1.10	1.083