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# Photoabsorption of Alkali and Alkaline Earth Elements Calculated by the Scaled Thomas Fermi Method

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Photoionization cross sections have been calculated by means of the Scaled-Thomas-Fermi method for the alkali metals and the alkaline earths. Using these results the absorption coefficients for bound-free transitions have been obtained for thermal plasmas of 6000 to 20,000 K and wavelengths from 500 to 10,000 Å. In addition the oscillator strengths are given for the principal series of the alkali metals.

## I. Introduction

For the calculation of continuous absorption coefficients $\kappa(\lambda, T)$ one needs photoionization cross sections of a large number of terms, many of them having high energies relative to the ground state of the atom. Application of Hartree-Fock procedures (HF) are laborious and need much computing time, especially for heavy atoms. For an $N$-electron atom, the photoionization cross section is given by the expression:

$$\sigma(v) = \frac{2 \cdot \pi \cdot e^2 h^2}{m^2 \cdot c \cdot v} \cdot \int d\Omega_v \left|\sum \int \psi_i^*(N) \cdot \exp(-k_v \cdot r_i) \cdot p_i \cdot \psi(N)\, dr_N\right|^2 \tag{1}$$

where $e$, $c$, $h$ and $m$ are the known atomic constants, $v$ is the frequency of the incident photon, with momentum $k_v$; $p_i$ and $r_i$ are the momentum and position of the $i$-th electron respectively. The integration is performed over all directions of ejection. $\psi_i(N)$ and $\psi_f(N)$ are the initial and final wave functions of the atomic system respectively. If more than one final state is possible one has to sum over these states suitably weighted. The exponential may be replaced by unity, because $k_v \cdot r_i$ is of the order $10^{-3}$ in the range of the atom for photons of the visible and neighbouring regions respectively. This formula can be simplified to:

$$\sigma_L(v) = \frac{4 \cdot \pi}{3} \cdot \alpha \cdot a_0^2 \cdot \frac{(I+\varepsilon)}{g_i \cdot \sqrt{\varepsilon}} \cdot |M_{i,f}|_L^2 \tag{2}$$

where $I$ is the ionization potential of the atom, $\alpha$ is the fine structure constant and $a_0$ the Bohr radius; $g_i$ is the statistical weight of the bound state and $\varepsilon$ is the energy of the free electron. The index $L$ at the matrix element indicates, that we use in the sequel the dipol length formulation. In using the central field approximation the wave functions $\psi_i$ and $\psi_f$ may represented by products of one electron eigenfunctions. In the following we consider only those transitions where one of the outer electrons, the active electron, is removed from its bound state into the continuum. This gives us the simple formula for the cross section

$$\sigma_L(v) = \frac{4\pi}{3} \alpha \cdot a_0^2 \cdot \frac{(I+\varepsilon)}{g_i \cdot \sqrt{\varepsilon}} \cdot C_p \cdot \sum_{l' = l \pm 1} C_{l'} |P_{nl}(r) \cdot r \cdot P_{\varepsilon l'}(r)\, dr|^2. \tag{3}$$

If the electrons of the core, the passive electrons, remain unchanged, $C_p$ is equal unity. HF-calculations have shown that this condition is approximately fulfilled. The factors $C_{l'}$ are constants, previously tabulated by Bates [1]. The functions $P_{n,l}(r)$ and $P_{n,l'}(r)$ are solutions of the Schrödinger equation

$$\frac{d^2 P(r)}{dr^2} + \left[V(r) + \varepsilon - \frac{l \cdot (l+1)}{r^2}\right] \cdot P(r) = O \tag{4}$$

where $\varepsilon$ is the energy of the electron in Rydberg units and $l$ its angular momentum; $r$ is measured in Bohr radii and $V(r)$ is the potential of the ion. The largest contributions to the integral in (3) are given by the regions with $r$ large, where the effective field may be assumed to be hydrogenic. Bates and Damgaard [2] used this fact to solve Equation (4), using for the bound states the experimental values of the term energies $\varepsilon_{nl}$ determined from atomic spectra. The deviation from a pure Coulomb potential was taken into account by the quantum defect $\mu = n - n^*$, $n^*$ is the effective main quantum number. $\varepsilon_{nl}$ is related to the experimental observed Rydberg series by the relation $\varepsilon_{nl} = C^2/n_l^{*2}$. Here $C = Z - N + 1$, $Z$ is the nuclear charge number and $N$ the number of electrons. Seaton [3] has extented this Coulomb approximation (CA) to free electron states ($\varepsilon = k^2 \geqq 0$). For these continuum states the wave function is given by the expression

$$P_{k,l}(r) \sim \sin(x + \delta_l(\mathrm{k})). \tag{5}$$

$x$ is a function of $k, r$ and $l$, and $\delta_l(k)$ is the phase of the free wave function, which is zero for a pure Coulomb field, and which can be related to the quantum defect by a simple relation. The quantum defects can be extrapolated into the region of positive energies. This Quantum-Defect-Method (QDM) has been applied by Burgess and Seaton [4], Peach [5], Schlüter [6] and Hofsaess [7] for a large number of elements. Many calculated photoionization cross sections agree satisfactorily with the few experimental results. The best agreement is obtained for light elements and for atoms with one electron outside of closed shells. However the method cannot be applied for terms with effective main quantum numbers, which do not satisfy the relation $n^* > l + 1$, e.g. for the ground state of C I, N I, O I, Ne I, Ar I etc. and especially heavy atoms or ions. For Fe I, this relation is not fulfilled for most of the $np$ and $nd$ levels, only the $ns$ levels satisfy this condition.

Further, the QDM is not applicable for terms which have a negative quantum defect, e.g. the $np\,^1P$ series of He I. There are further reasons why QDM may give bad results, so for terms where we have strong cancellation of the integrand in Equation (4). In this case the contributions to the matrix element from small radii becomes more important and here we need more precise wave functions than we can get from QDM.

## II. The Scaled-Thomas-Fermi Potential

We have used for our calculations a method which gives better wave functions for small radii than CA does. It employs in Equation (6) a Thomas-Fermi (TF) potential $V(r)$ modified in such a way, that the experimental energy values $\varepsilon_{n,l}$ are reproduced, Stewart and Rotenberg [8]. For an atom or ion with $N$ electrons and nuclear charge $Z$, this potential is given by

$$-V(r) = \begin{cases} \dfrac{2Z}{r}\left(\varphi(x) + q \cdot \dfrac{x}{x_0}\right) & x \leqq x_0 \\ \dfrac{2Z}{r} \cdot q & x \geqq x_0 \end{cases} \tag{6}$$

where $x = r/\mu$, $\mu = 0.8853\,Z^{-1/3}$. $\varphi(x)$ is the TF-function of the ion and $x_0$ the corresponding ionic radius, determined by the equation

$$\frac{d^2\varphi(x)}{dx^2} = \varphi(x)^{3/2} \cdot x^{-1/2} \tag{7}$$

with boundary conditions

$$\varphi(0) = 1, \qquad \varphi(x_0) = 0, \qquad \left.\frac{d\varphi(x)}{dx}\right|_{x_0} = q, \tag{8}$$

$q = (Z - N)/Z$ determines the ionization degree. $V(x)$ is altered by introducing a scaling parameter $\alpha$ and putting $x = r/\mu\alpha$. By this scaling, all effects, which are not explicitly accounted for, e.g. exchange effects, first and higher correlation effects, relativistic corrections etc. are incorporated approximately in $V(x)$. The results show that $\alpha$ depends on the quantum numbers $n$ and $l$, and is close to unity.

Figure 1 shows the ground state wave function of potassium, calculated with QDM, STF (STFP) and HFS (Hartree-Fock-Slater, Hermann and Skillman [9]). We can see from Figure 1, that STF is a more realistic approximation than QDM. The determination of the free electron wave function can be done in a similar way as with the QDM, by extrapolation of the $\alpha_{n,l}(\varepsilon)$-values into the region of positive energy values. For many atoms $\alpha_{n,l}(\varepsilon)$ varies smoothly with $n$ and $l$ and a linear extrapolation is possible, Kähler [10], see Figure 2.

It can be shown, that the STF-potential overestimates the electron density near the origin, i.e. for $r \leqq \mu/Z^{2/3}$, and also in the asymptotic region; for small $r$ the electron density $\rho(r)$ diverges like $r^{-3/2}$; for large values of $r$, i.e. $r > \mu/Z^{1/3}$ the convergence of $\rho(r)$ to zero is proportional to $r^{-6}$ instead of $e^{-r}$; the mean part of the function $\rho(r)$ is underestimated. A further problem is the core polarization of some atoms, which may not be neglected. According to these facts, we have used for the potential in Equation (4) the expression $V(r) = V_0 + V_p + V_{SO}$, where $V_0$ is a scaled TF-potential (STF), $V_p$ is a polarization potential and $V_{SO}$ is a spin-orbit potential. Instead of using for $V_p$ the Bethe-potential [11], we took a simpler modification of it:

$$V_p(r) = \frac{\alpha_d}{(r^2 + r_0^2)^2} + \frac{\alpha_q - 3 \cdot \beta \cdot a_0}{(r^2 + r_0^2)^3} \tag{9}$$

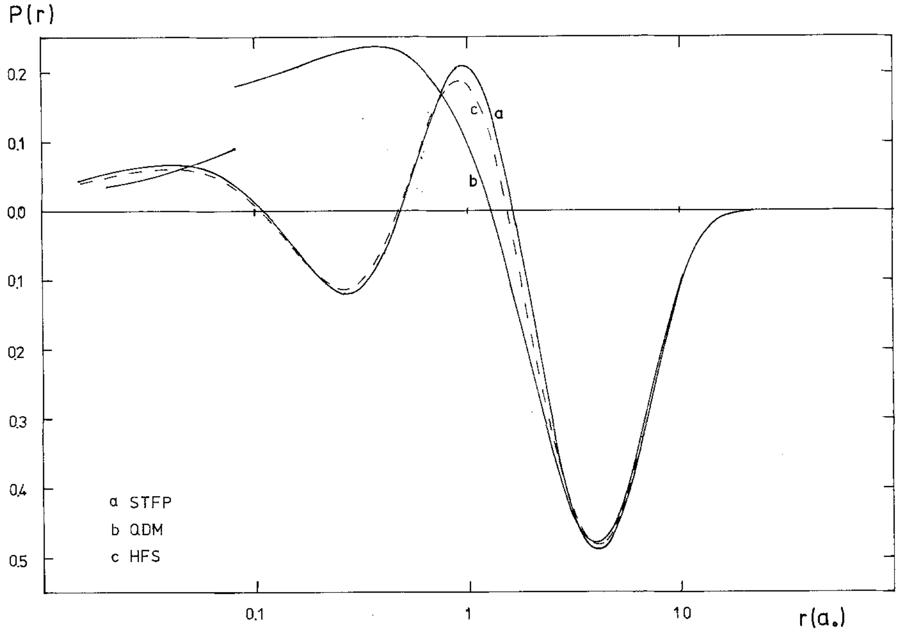

**Fig. 1.** Wave function of the ground state of potassium. The jump of the QDM wave function near $r=0.1\ a_0$ is due to a semiconvergent series

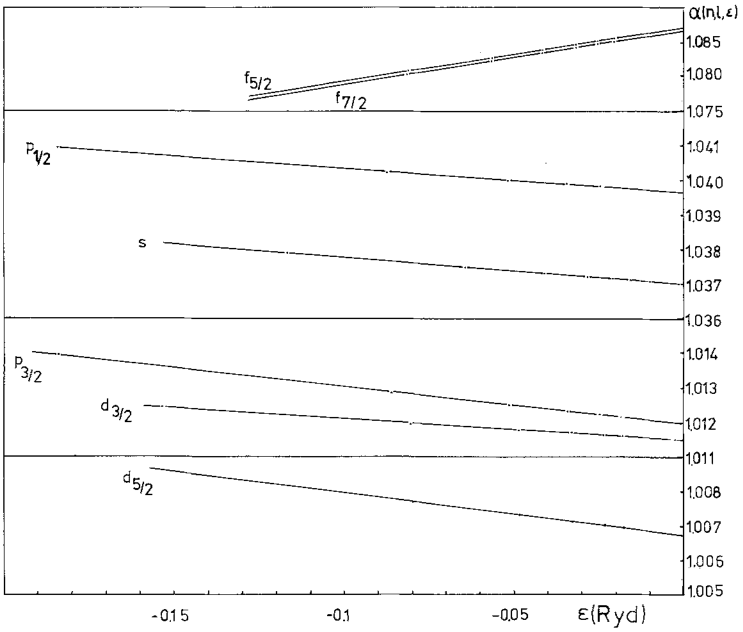

**Fig. 2.** Scaling parameter $\alpha_{n,l}(\varepsilon)$ for the cesium atom

$\alpha_d$ and $\alpha_q$ are the static dipol and quadrupol polarizabilities; $\beta$ determines the leading nonadiabatic correction to the polarizability of the core [12]. Values of $\alpha_d$ and $\alpha_q$ have been given by Lahiri and Mujkeri [15] and Dalgarno [14], they agree with the results of Edlén [13], who used the spectroscopically determined term values of *nf*, *ng*, and *nh*. For $r_0$ we used the mean radius of the ion, calculated with STF wave functions. These values for $r_0$ agree well with other calculations done with HF-methods. Our values of $r_0$ do not depend on $l$, they agree satisfactorily with the mean values of $r_0(l)$ of Parson and Weiskopf [16]. The wave functions depend only weak on $r_0$ and a small change in $r_0$ affects a small change of the cross sections and oscillator strength. The used values of $\beta$ have been calculated using the formulas of Kleinmann et al. [17] for the upper and lower bound of $\beta$, containing sums, involving oscillator strengths

**Table 1**

| | $\alpha_d$ | $\alpha_q$ | $\beta$ | $r_0$ | $r_c$ | $\lambda_{\min}$ |
|---|---|---|---|---|---|---|
| Li I | 0.193 | 0.112 | 0.024 | 0.75 | 2.0 | – |
| Na I | 0.945 | 1.52 | 0.355 | 0.99 | 3.4 | 1945 |
| K I | 5.325 | 17.6 | 3.59 | 1.50 | 1.94 | 2730 |
| Rb I | 9.80 | 70.7 | 7.25 | 1.76 | 2.79 | 2502 |
| Cs I | 19.03 | 118.26 | 19.4 | 2.01 | 3.72 | 2795 |
| Mg II | 0.471 | 0.529 | – | 0.68 | 1.37 | – |
| Ca II | 1.96 | 11.46 | – | 1.27 | 1.57 | – |

of the corresponding alkali ions, which may be replaced by $\alpha_d$, i.e. only the first term of the sum is used. The used values of $\alpha_d$, $\alpha_q$, $\beta$ and $r_0$ are given in Table 1.

For the spin-orbit potential we have taken the expression of Dirac [18]:

$$V_{SO}(r)=\frac{\alpha^2}{2}\cdot\frac{1}{r}\frac{dV(r)}{dr}\cdot\left(1+\frac{\alpha^2}{4}(\varepsilon-V(r))\right)^{-2}\cdot\mathbf{l}\cdot\mathbf{s}. \tag{10}$$

Here $V(r)=V_0+V_p$ and $\varepsilon$ is the energy of the electron state. In this case, the cross section depends on the quantum number $j$ too, and is given by the equation

$$\sigma_j(v)=\text{const.}\cdot\sum_{l'}\sum_{j'}\frac{\max(l,l')}{(2\cdot j+1)}\cdot C(l,j;l'j')\cdot\left|\int P_{nlj}(r)\cdot\mathbf{r}\cdot P_{\varepsilon l'j'}(r)\,dr\right|^2 \tag{11}$$

with

$$C(l,j;l',j')=(2j+1)\cdot(2j'+1)\cdot\begin{Bmatrix} l & j & 1/2\\ j' & l' & 1\end{Bmatrix}. \tag{12}$$

The third factor is a $6j$-symbol. These coefficients are well known and have been tabulated, e.g. Shore and Menzel [19]. A similar formula is used for the $gf$-values.

For the calculation of transition probabilities, using wave functions calculated with a potential involving a polarization potential, we have to use a modified matrix element $M_{if}$, see Bersuker [20]. Here we applied a simplified form of this, following Hameed [21] and Norcross [22]:

$$M_{if}=\int P_i(r)\cdot\mathbf{r}\cdot\left[1-\frac{\alpha_d}{r^3}(1-\exp(-r/r_c)^3)\right]\cdot P_f(r)\cdot dr. \tag{13}$$

Here $r_c$ is a cut-off radius, comparable with the *TF*-radius of the ion. $\sigma(\lambda)$ and $gf$ depend strongly on $r_c$, and it is necessary to determine this parameter as well as possible. This point will be discussed at the end of this paper (Appendix II). The used values of $r_c$ are tabulated on Table 1.

## III. Absorption Cross Section

1. We have calculated $gf$-values for the alkali elements Li I to Cs I. In Table 2 are listed the results for the principal series $n_0s\ ^2S_{1/2}\rightarrow np\ ^2P_{3/2}$, $n_0$ stands for the main quantum number of the ground state. For our calculation we have used the term values given in

**Table 2**

| | Li I | | Na I | | K I | | Rb I | | Cs I | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | $f_{3/2}$ | $\rho$ | $f_{3/2}$ | $\rho$ | $f_{3/2}$ | $\rho$ | $f_{3/2}$ | $\rho$ | $f_{3/2}$ | $\rho$ |
| 2 | 4.95(−1) | 2.00 | – | – | – | – | – | – | – | – |
| 3 | 3.10(−3) | 2.00 | 6.40(−1) | 2.00 | – | – | – | – | – | – |
| 4 | 2.82(−3) | 2.00 | 8.78(−3) | 2.03 | 6.58(−1) | 2.01 | – | – | – | – |
| 5 | 1.68(−3) | 2.00 | 1.28(−3) | 2.06 | 5.72(−3) | 2.18 | 6.82(−1) | 2.03 | – | – |
| 6 | 1.04(−3) | 2.00 | 3.82(−4) | 2.07 | 6.07(−4) | 2.35 | 9.47(−3) | 2.68 | 6.89(−1) | 2.08 |
| 7 | 6.74(−4) | 2.00 | 1.62(−4) | 2.08 | 1.39(−4) | 2.55 | 1.44(−3) | 3.27 | 1.05(−2) | 4.40 |
| 8 | 4.70(−4) | 2.00 | 8.32(−5) | 2.09 | 4.65(−5) | 2.76 | 4.38(−4) | 3.79 | 1.63(−3) | 7.97 |
| 9 | 3.22(−4) | 2.00 | 4.87(−5) | 2.14 | 2.05(−5) | 2.95 | 1.86(−4) | 4.27 | 5.33(−4) | 13.64 |
| 10 | 2.43(−4) | 2.00 | 3.11(−5) | 2.00 | 1.06(−5) | 3.15 | 9.65(−5) | 4.70 | 2.34(−4) | 22.16 |
| 11 | 2.45(−4) | 2.00 | 2.04(−5) | 2.00 | 6.07(−6) | 3.30 | 5.62(−5) | 5.04 | 1.24(−4) | 34.53 |
| 12 | 1.38(−4) | 2.00 | 1.46(−5) | 2.00 | 3.92(−6) | 3.35 | 3.60(−5) | 5.32 | 7.54(−5) | 46.65 |
| 13 | 1.13(−4) | 2.00 | 1.14(−5) | 2.00 | 2.76(−6) | 3.54 | 2.42(−5) | 5.58 | 4.88(−5) | 67.64 |
| 14 | 8.98(−5) | 2.00 | 8.08(−6) | 2.00 | 2.02(−6) | 3.64 | 1.73(−5) | 5.88 | 3.38(−5) | 95.72 |
| 15 | 8.78(−5) | 2.00 | 6.26(−6) | 2.00 | 1.60(−6) | 3.63 | 1.25(−5) | 6.04 | 2.42(−5) | 100.19 |
| 16 | 7.10(−5) | 2.00 | 4.95(−6) | 2.00 | 1.32(−6) | 3.63 | 9.55(−6) | 6.42 | 1.85(−5) | 154.83 |
| 17 | 4.77(−5) | 2.00 | 4.41(−6) | 2.00 | 1.06(−6) | 3.77 | 7.28(−6) | 6.70 | 1.40(−5) | 174.17 |
| 18 | 3.68(−5) | 2.00 | – | – | – | – | 5.96(−6) | 6.99 | 1.10(−5) | 218.46 |
| 19 | 3.22(−5) | 2.00 | – | – | – | – | 4.65(−6) | 7.07 | 8.75(−6) | 253.16 |
| 20 | 3.27(−5) | 2.00 | – | – | – | – | 3.67(−6) | 7.45 | 7.13(−6) | 302.58 |
| 21 | – | – | – | – | – | – | 2.88(−6) | 7.92 | 5.93(−6) | 337.05 |

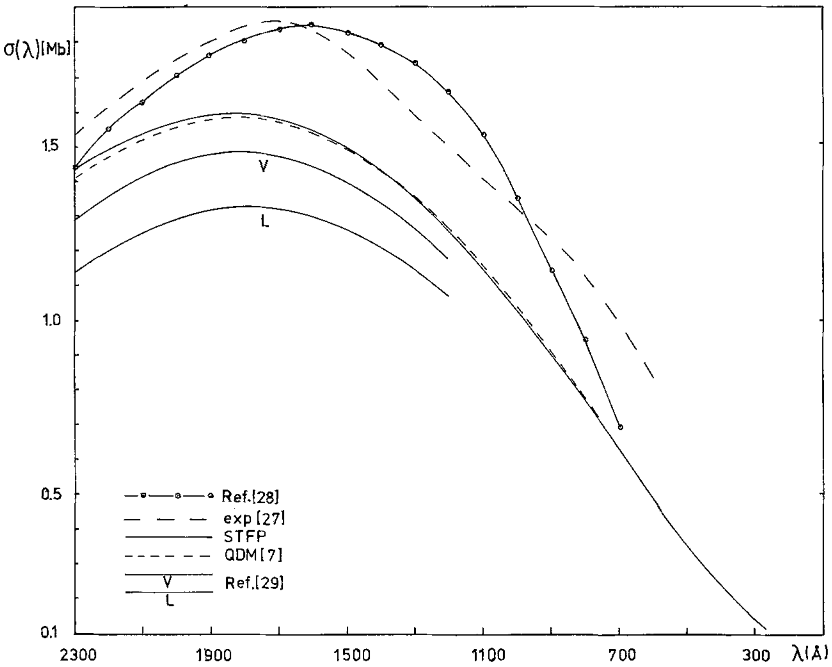

**Fig. 3.** Photoionization cross section of the $2s\,^2S$ state of Li I

AEL by Moore [23]. Because the data of term values are incorrect for large $n$ numbers, we can not conclude that there exists a maximum of the ratio $\rho = f_{3/2}/f_{1/2}$ for the Cs atom in the region $18 \leqq n \leqq 20$. If we correct these data to linearity by extrapolation of the quantum defect, we get a monotonically increasing ratio $\rho$. If there really exists a maximum, this theory would be too simple to get such results. Experimental results of Sambursky [24] and Fulop and Stroke [25] show maxima for $n=10$ and $n=11$ respectively. Recent measurements of Pichler [26] show no maximum up to $n=18$. Our data for $f_{1/2}$, $f_{3/2}$ and $\rho$ are in good argeement with the latter one.

2. Photoionization cross sections have been calculated for the alkali elements Li I to Cs I and for the alkaline earths Mg I, Mg II, Ca I and Ca II, for the ground states and all excited states up to $n=10$ and $l=3$. Besides some exceptions we only have experimental measurements of $\sigma(\lambda)$ for the ground states. In general we can say, that we get better results with a STF-potential corrected for polarization which takes account of the spin-orbit interaction in a direct way (STFP+SO), as given by formula (10), than STFP wich takes account of this interaction indirectly by the scaling parameters $\alpha_{n,l}$. So, the value of the minimum of the cross section of the alkali elements calculated with STFP is nearly zero, but with STFP+SO, the result of our calculation agrees well with the experimental value which is not zero. For excited states, the difference between STFP and STFP+SO is very small, concerning the cross sections. The $\alpha_{n,l}$-values of the latter lie closer to unity than those of the former. In the following the results of our calculations will be discussed and compared with the experiments.

Li I—Figure 3 shows the calculated cross section for the ground state of lithium. For energies larger than the ionization potential, $\sigma(\lambda)$ is fairly smaller than the experimental data of Hudson and Carter [27]. This may be due to the strong absorption of the $Li_2$-molecules, which is difficult to determine. The dipol length result of the HF-calculation of Sewell [28] is in close agreement with the experiment; however these calculations are probably in error, because Sewells results for $\sigma_L(\lambda)$ and $\sigma_V(\lambda)$ violate the first Chang-McDowell theorem [29], which states, that the two curves are not independent quantities within the context of HF-calculation. The exited states differ from the results of QDM more than the ground state does. Figure 4 shows the cross section for the $2p\,^2P$ state, measured by Rothe [30] and calculated with STFP+SO; other calculations give similar results (Ya'akobi [31], Moskvin [32]). A large difference is seen for terms with $l=3$; so for $\varepsilon=0$ the cross section differs from QDM by a factor 2 and for $\varepsilon=1$ Ryd by about a factor 10 to 20. For energies larger than 1 Ryd, $\sigma(\lambda)$ depends strongly on the extrapolated scaling factor $\alpha_{n,l}(\varepsilon)$, and in some cases, no linear extrapolation is possible, because the derivative $d\alpha/d\varepsilon$ has a large negative value. We used therefore a quadratic extrapolation to an asymptotic value, which has been arbitrarily determined.

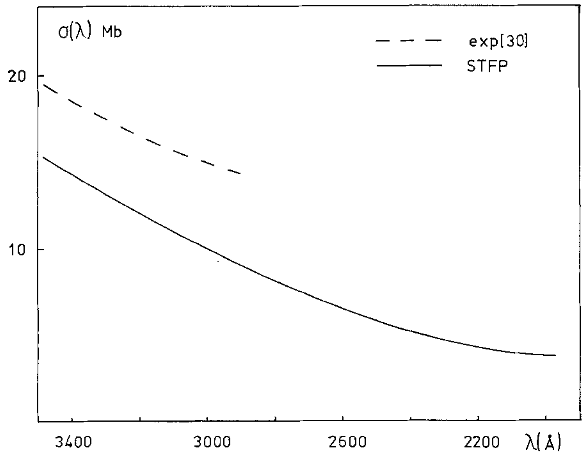

**Fig. 4.** Photoionization cross section of the $2p\,^2P$ state of Li I

Na I – For sodium we get with STFP+SO a cross section which differs for energies larger than 0.2 Ryd by a large amount from QDM. At the spectral head, the value of $\sigma(\lambda)$ is 0.119 Mb and lies near to the experimental value 0.13 Mb of Hudson and Carter [27]. With STF we get the value 0.16 Mb. Towards shorter wavelengths the experimental data depart considerably from the theoretical results; other calculations show the same behaviour for large energies, see Figure 5. The cross section of sodium depends sensitive on the values $\alpha_d$, $r_0$ and $r_c$. The latter constant can be determined only approximately, see Appendix II.

K I – Our result of the cross section of the ground state of potassium lies close to the experimental values of Marr and Creek [33], see Figure 6. The measurements of Hudson and Carter [34] show a large discrepancy to the results of Marr and Creek for $\lambda < 2400$ Å. The minimum value of our result lies at 2750 Å and is in good agreement with the experimental one. Concerning the excited states, a comparison with QDM shows, that STFP+SO values are always lower by a factor 2 to 3 for all angular momenta considered and for the energy $\varepsilon = 1$ Ryd. For larger energies, the discrepancy becomes still larger.

Rb I – The results with STFP+SO agree well with the measurements of Marr and Creek [33], Figure 7. The results of Mohler and Boeckner [35] are also consistent with our calculation, but they are only available up to 2300 Å. The values of STF and QDM are seen to be far away from the experimental curves. The shape of $\sigma(\lambda)$ for excited states calculated with STF or STFP+SO often differ strongly from that calculated with QDM, owing to the fact, that the QDM wave function for the bound states have wrong behaviour for small radii.

Cs I – The photoionization cross section of the ground state of cesium has a minimum at 2595 Å and this point agrees well with the experimentally determined energy of the minimum, see Figure 8. That the value of the measurements of Marr and Creek and Mohler and Boeckner are larger than the theoretical results is due to the difficult determination of the $Cs_2$-molecule absorption. The excited states remain nearly unaffected by the radius $r_c$. In Figure 9 is shown the cross section for the $6p\,^2P$ state, calculated with QDM, STFP+SO, theoretical results of Weisheit [36] and experimental results of Mohler [37]. Our results agree well with the experimental data.

Mg II – Ca II – No experimental data of cross sections and $gf$-values are available for Mg II and Ca II. First calculations with HF were done by Bates and Massey [38] for the spectral head of Ca II. Because the determination of $r_c$ can not be done very exact, we have used their result $\sigma(\varepsilon = 0) = 0.236$ Mb to determine $r_c$ (see Appendix II). With STF we get for the cross section at the spectral head the value 0.0667 Mb and with QDM the value 0.175 Mb. The shapes of these curves differ strongly from each other (Fig. 10). The wave function of the ground state and of the excited states $4p$ and $3d$ agree well with those of the HF-calculation of Trefftz [39].

For Mg II a HF-calculation has been done by Biermann and Lübeck [40]; they have calculated transitions from the ground state and from excited states $3p$, $3d$ and $4f$. Their results for the excited states agree well with our STFP results. Figure 11 shows the cross section for the ground state of Mg II.

Mg I – For the alkaline earths we have performed our calculations without an additional polarization potential though $\alpha_d$ and $\alpha_q$ are well known, because a comparison of the ground state wave function of Mg with HF-calculation of Trefftz [41] shows, that the wave function of STFP deviates more from her result and from HFS calculations than STF does. By introduction of an exchange potential STFD (Scaled Thomas-Fermi-Dirac), Gombás [43], Hofsaess [42] we obtain results similar to STFP. Though the result for the cross section of the ground state, calculated with STFD gives better agreement with the experiment of Ditchburn and Marr [44], we have used for the calculation of all cross sections a STF potential. Probably, for Mg I and Ca I, it is not sufficient to correct the potential for polarization or exchange; other effects are of the same magnitude and should be taken into account too.

The term system of Mg I is disturbed, so the $3snd\,^1D$ series is disturbed by the $3p^2\,^1D$ term, and the function $\alpha_{n,l}(\varepsilon)$ increases with $n$ in a nonlinear form for this series, so an extrapolation is difficult and un-

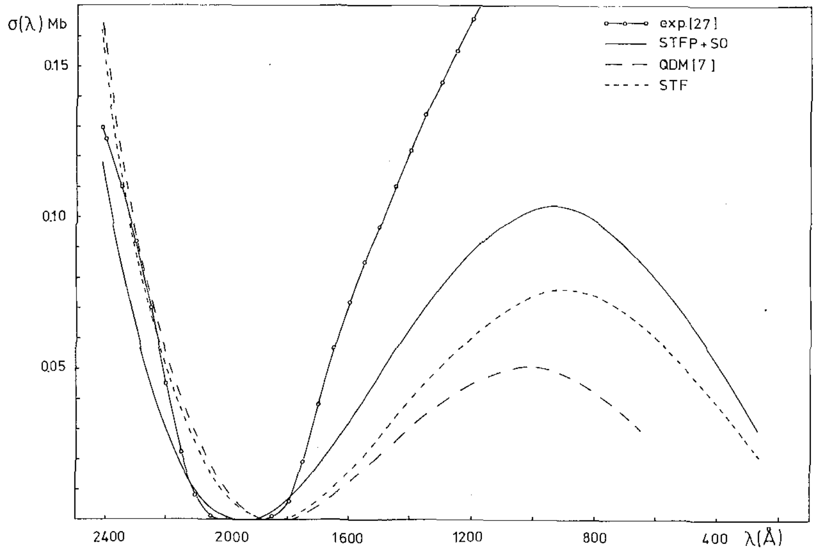

Fig. 5. Photoionization cross section of the $3s\,^2S$ state of Na I

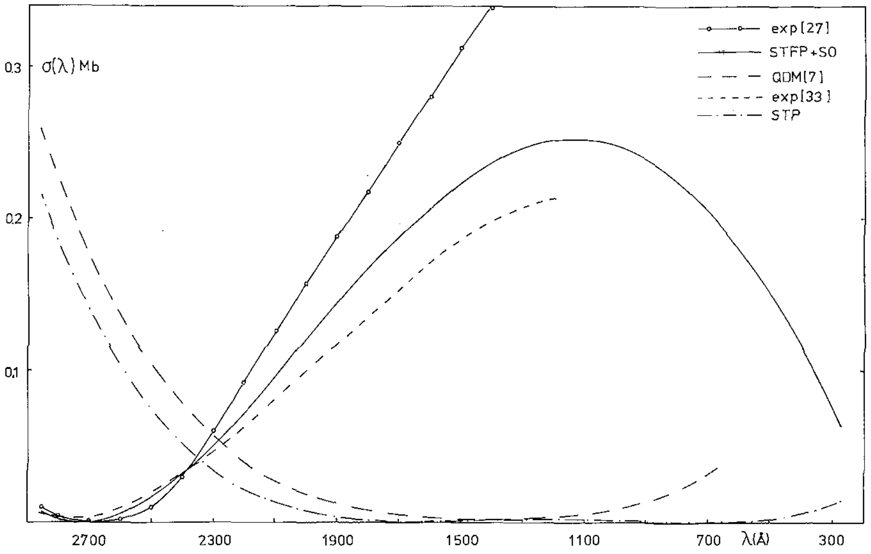

Fig. 6. Photoionization cross section of the $4s\,^2S$ state of K I

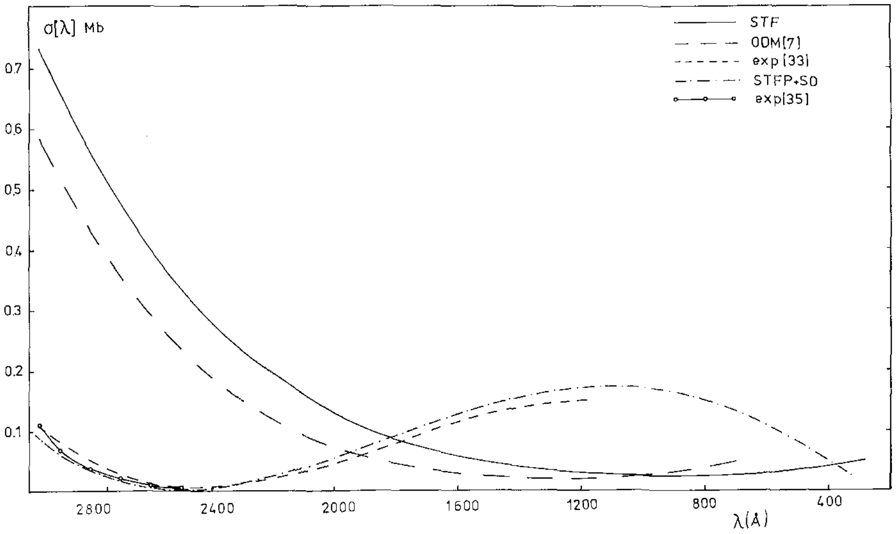

Fig. 7. Photoionization cross section of the $5s\,^2S$ state of Rb I

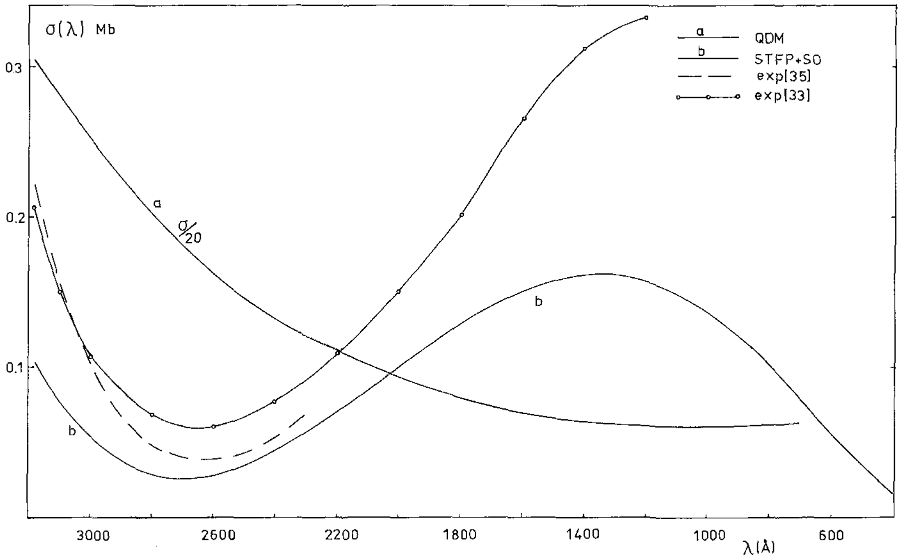

Fig. 8. Photoionization cross section of the $6s\,^2S$ state of Cs I

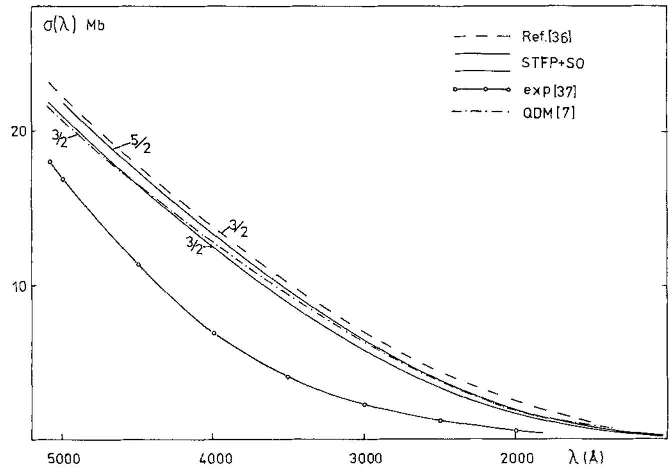

**Fig. 9.** Photoionization cross sections of the $6p\,^2P_{1/2,\,3/2}$ states of Cs I

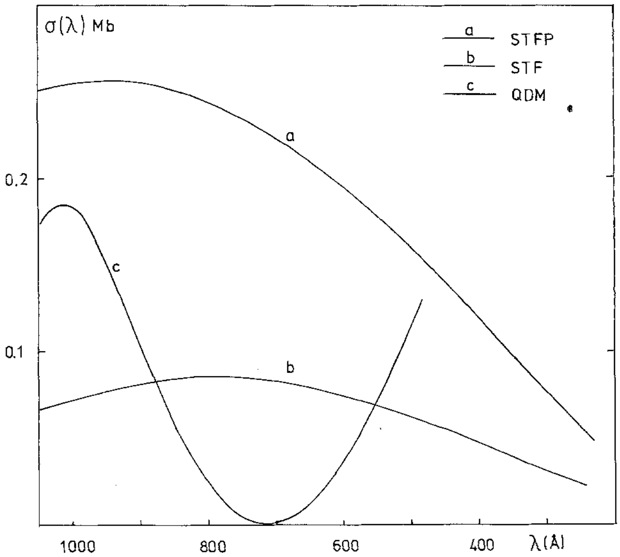

**Fig. 10.** Photoionization cross section of the $4s\,^2S$ state of Ca II

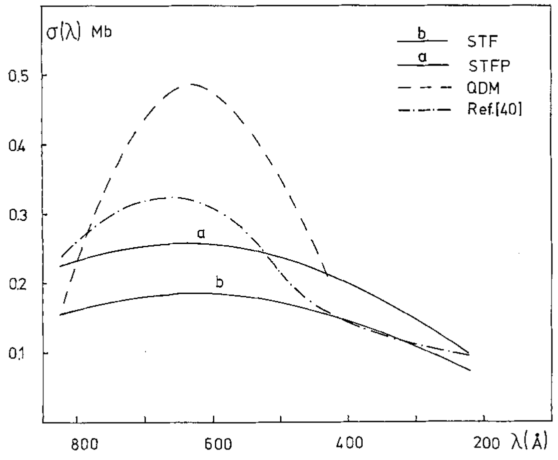

**Fig. 11.** Photoionization cross section of the $3s\,^2S$ state of Mg II

exact. The other series give good linear functions for the scaling parameter. The cross section for the ground state is given in Figure 12 calculated with STF, STFP and QDM [7]. The QDM results of Peach [5] are probably in error by a factor 2; we have calculated $\sigma(\lambda)$ with the same formula as that used by Peach and get nearly the same result as with the QDM formulas of Schlüter [6].

Ca I – The term system of calcium is strongly disturbed, especially the series $d\,^1P$, $p\,^3P$, $d\,^3D$ and $s\,^1S$ have nonlinear functions $\alpha_{n,\,l}(\varepsilon)$. Figure 13 shows $\alpha_{n,\,l}(\varepsilon)$ for the series $np\,^1P$ and $nd\,^3D$; the latter is disturbed by the doubly excited level $3d5s\,^3D_3$. For the determination of $\alpha_{n,\,l}(0)$ and $d\alpha_l(\varepsilon)/d\varepsilon$ the highly excited levels, i.e. $n > 10$ have to be taken into account. The solution of Equation (6) for these levels was done

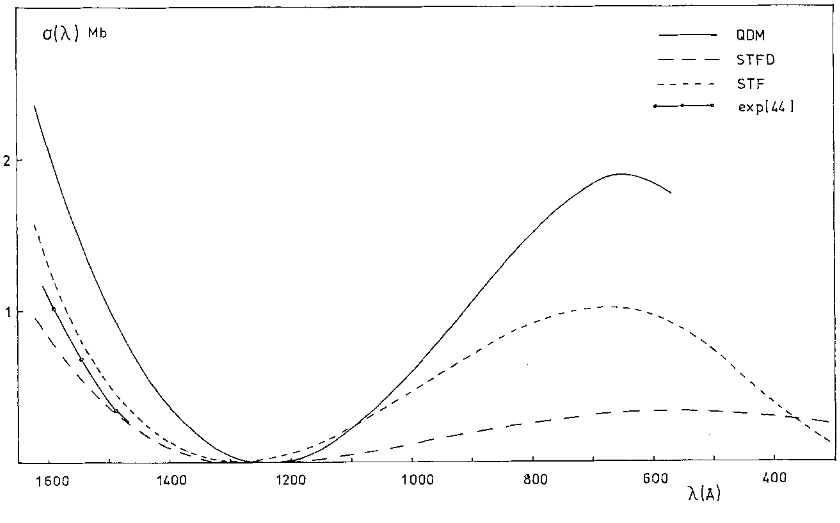

**Fig. 12.** Photoionization cross section of the $3s^2\,^1S$ state of Mg I

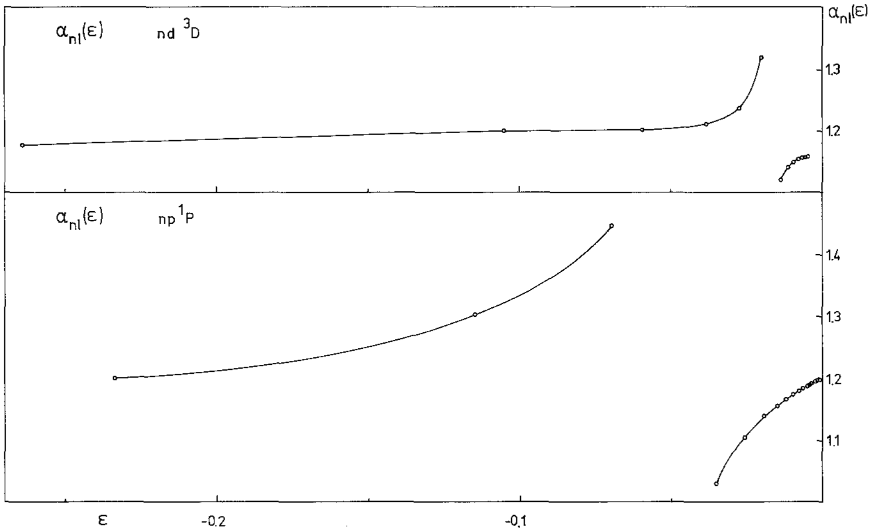

**Fig. 13.** Scaling parameter $\alpha_{n,l}(\varepsilon)$ of the $nd\,^3D$ and the $np\,^1P$ series of Calcium

with Numerovs procedure including the correction of Olver [45]. Figure 14 shows the cross section for the ground state of Ca I calculated with STF, STFP and QDM and the experimental results of Hudson and Ditchburn [46]. The large differences between the various results are striking. For energies between 0.02 and 0.15 Ryd strong autoionization lines are dominating the experimental cross section. We can not take into account this phenomenon with a simple method like STF. By means of new data, Brown and Tilford [47], for the second term system $3dnl$ a two channel STF method would certainly yield better results for the cross section of the ground state of calcium.

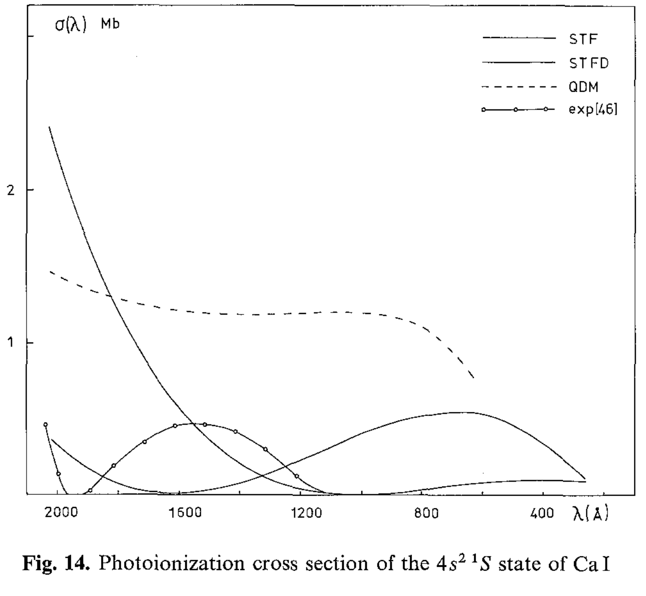

**Fig. 14.** Photoionization cross section of the $4s^2\,^1S$ state of Ca I

## IV. Absorption Coefficients of Thermal Plasmas

The absorption coefficient of an atom is given by the expression:

$$\kappa(\lambda, T) = \sum_i w_i \cdot \sigma_i(\lambda) \tag{14}$$

where the $w_i$ are weights according to the Boltzmann law; the sum is extended over all states with $n_i^* \geqq R \cdot \lambda$ ($R$ = Rydberg constant). According to Unsöld [48] and Schlüter [49]; this expression can be written as

$$\kappa(\lambda, T) = B \cdot T \cdot \lambda^3 \cdot \exp(-I/kT) \cdot [\exp(hc/\lambda kT) - 1] \cdot \gamma \cdot \xi(\lambda, T)/Z_0 \tag{15}$$

where $B = 6.62 \cdot 10^{-8}$ [cm$^{-1}$ $K^{-1}$]. $\xi(\lambda, T)$ denotes a dimensionless function according to Bibermann et al. [50], which depends only weak from temperature and is of the order 1. The factor $\gamma$ is the statistical weight of the ground state of the parent ion. $Z_0$ is the partition function of the atom.

The calculations of $\xi(\lambda, T)$-factors were performed in two parts. First we have calculated the sum for all states with $n \leqq 10$, the rest of the sum was obtained by integration, because the states lie very close together. The numerical calculation of states with $n > 10$ is often a difficult problem. Owing to the fact, that the ionization energy of an atom in a plasma is smaller than in the case of a free atom, the summation should be extended only over a finite number of states. We can however see, that the sum over the different states in the expression for the $\xi(\lambda, T)$-factor includes factors $1/n^{*5}$, and the contributions of these highly excited states are very small.

We have calculated tables of $\xi(\lambda, T)$-factors for the above mentioned atoms, for a wavelength intervall [300, 10,000] Å and a temperature intervall [4,000, 20,000] K. The results are shown in the Figures 15–23 for some temperatures.

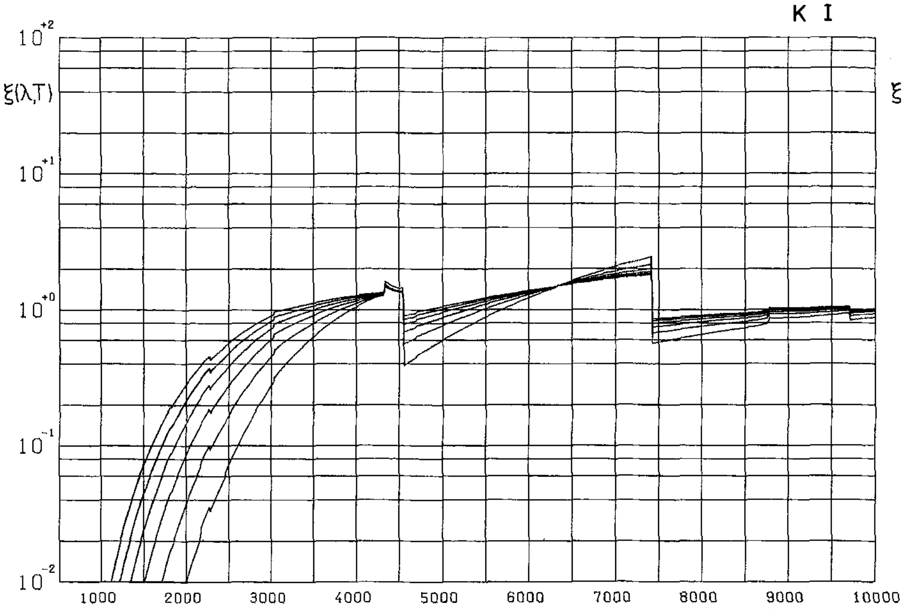

Fig. 15. $\xi(\lambda, T)$-factor for Lithium

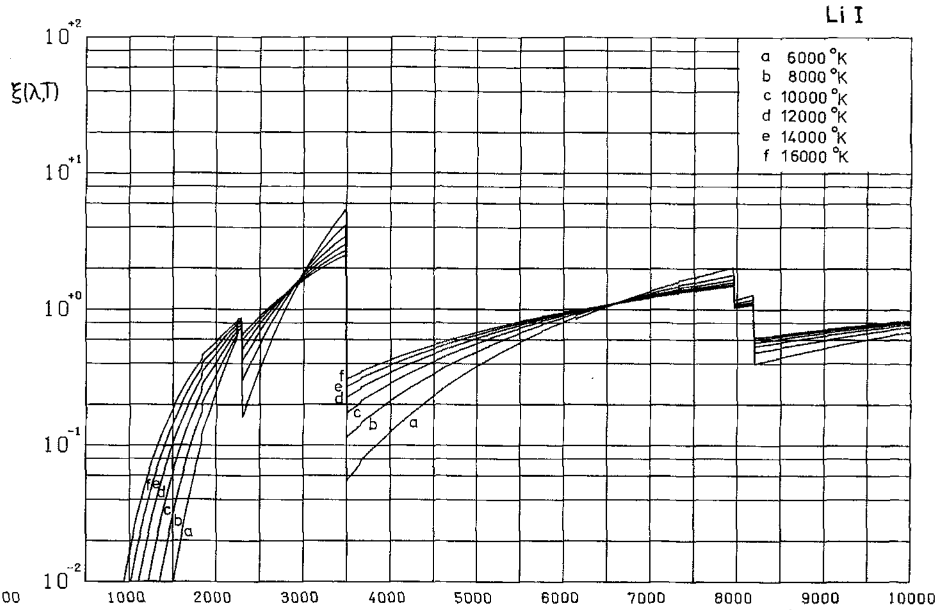

Fig. 16. $\xi(\lambda, T)$-factor for Sodium

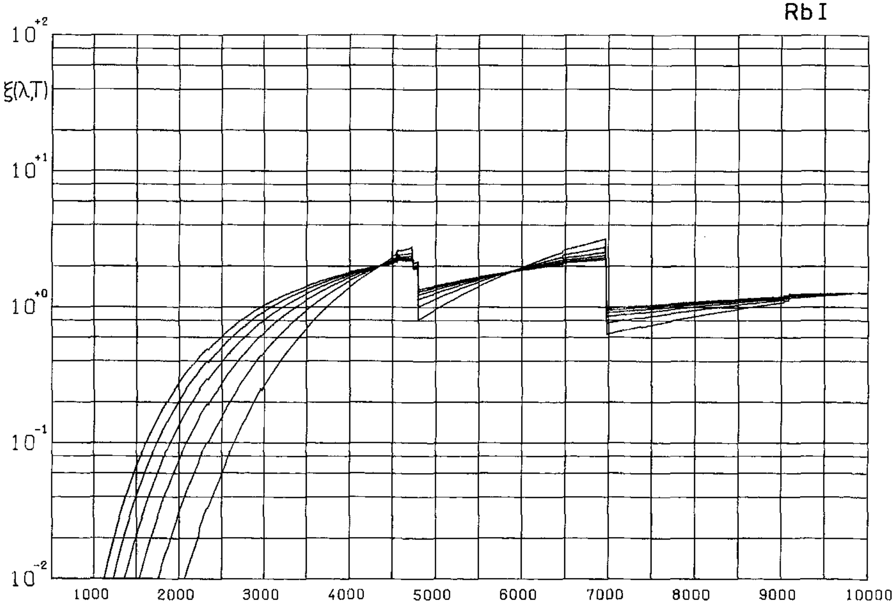

Fig. 17. $\xi(\lambda, T)$-factor for Pottasium

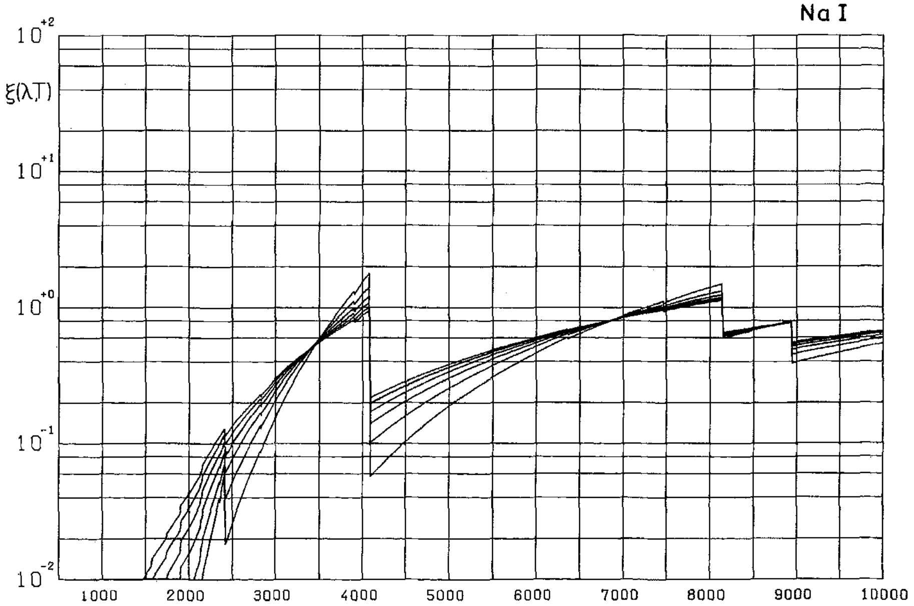

Fig. 18. $\xi(\lambda, T)$-factor for Rubidium

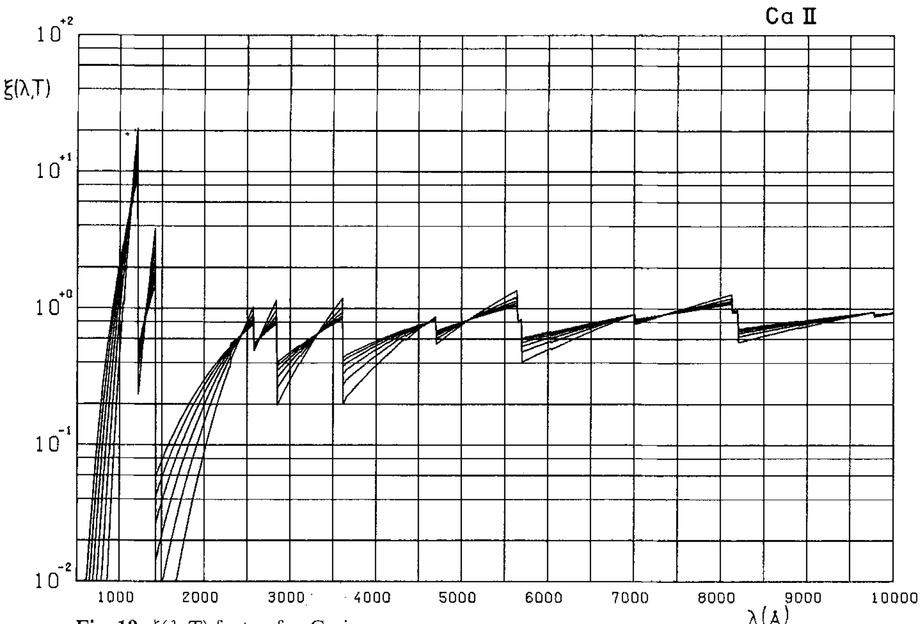

**Fig. 19.** $\xi(\lambda, T)$-factor for Cesium

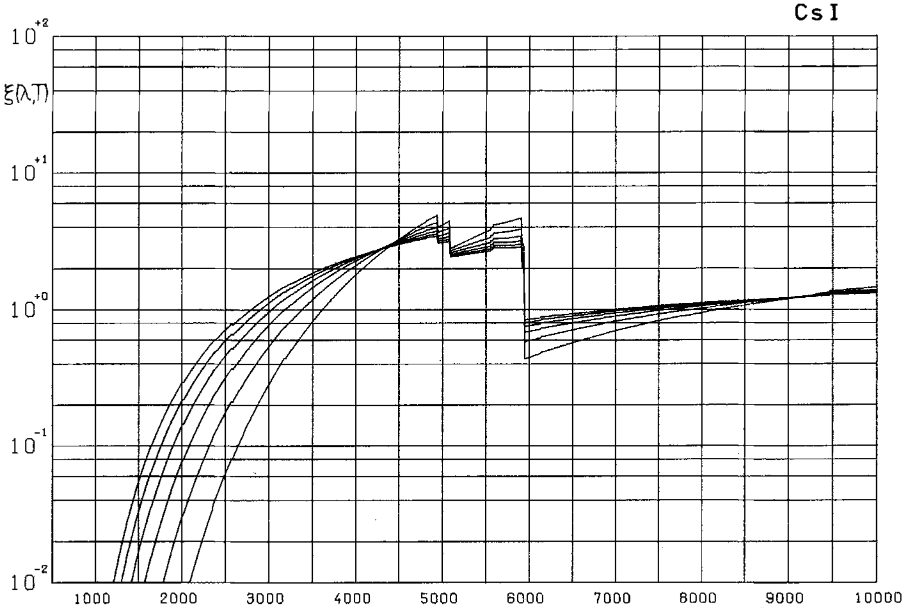

**Fig. 20.** $\xi(\lambda, T)$-factor for Magnesium II

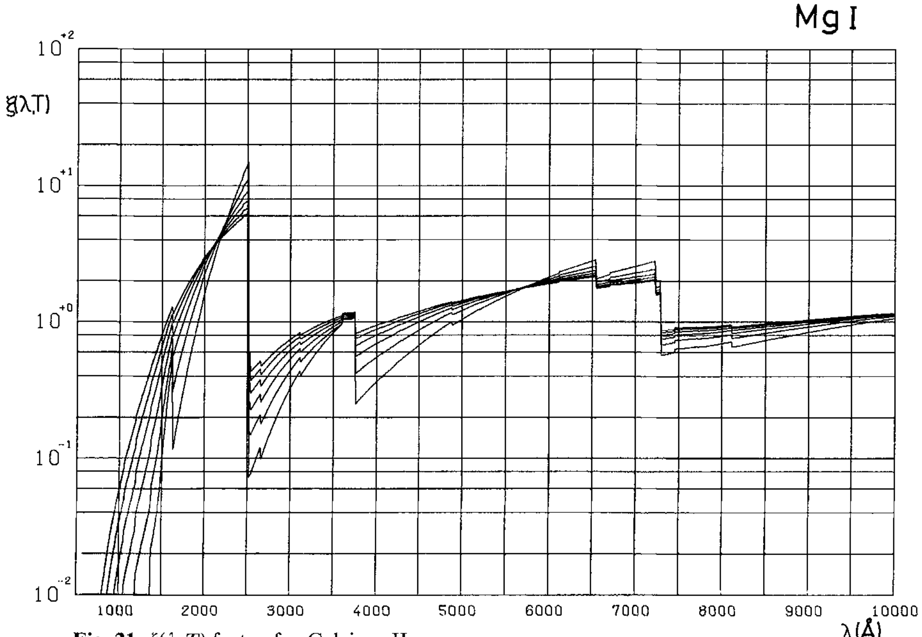

**Fig. 21.** $\xi(\lambda, T)$-factor for Calcium II

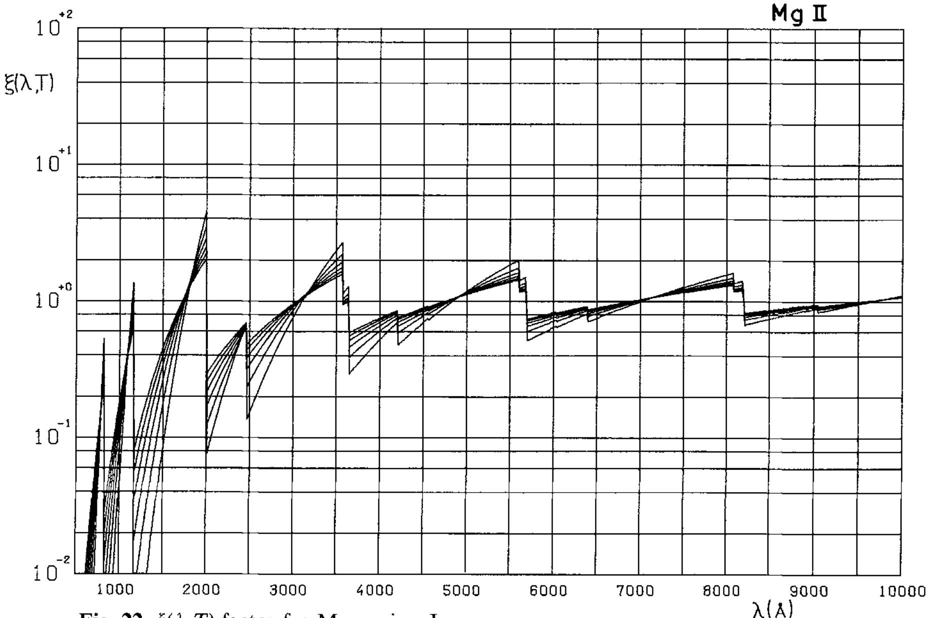

**Fig. 22.** $\xi(\lambda, T)$-factor for Magnesium I

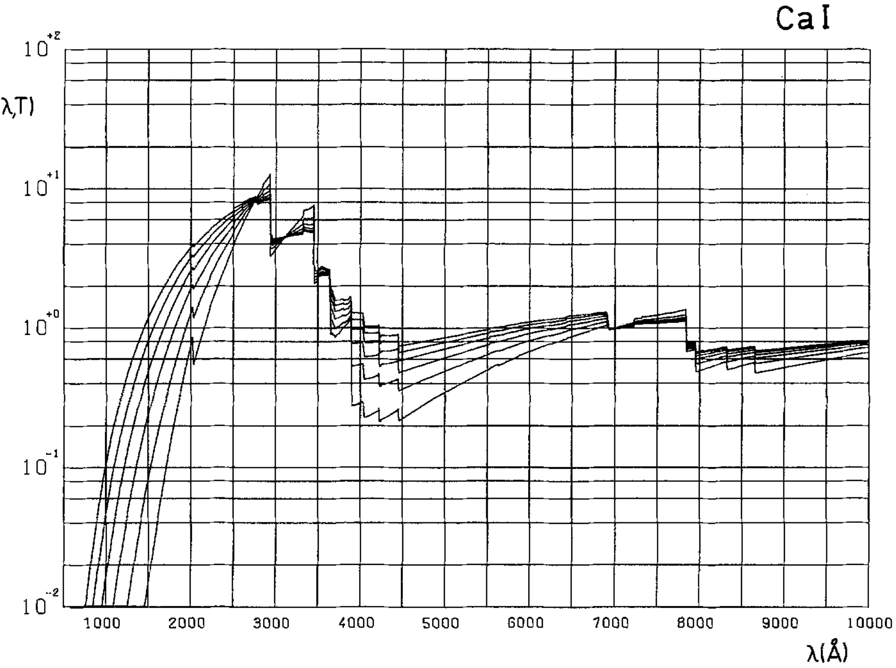

**Fig. 23.** $\xi(\lambda, T)$-factor for Calcium I

## Appendix I

Tables with $gf$-values and $\xi(\lambda, T)$ factors are available on request.

## Appendix II

The unknown parameter $r_c$ used in formula (13) must be determined by comparison with experimental data, because up to now no theoretical calculations are available.

a) If experimental oscillator strengths $f_{n,m}$ for a transition $m, l \rightarrow n, l'$ are available, we can calculate the function $df_{n,l'}/d\varepsilon_{n,l'} = 0.5 \cdot n^{*3} \cdot f_{n,l'}$, and have to compare this with the function calculated with theoretical determined $f_{n,l'}$-values depending on $r_c$. Varying $r_c$ to get accordance between theory and experiment for the two curves $df/d\varepsilon$ we get an $r_c$-value which can be used for the calculation of photoionization cross sections. This procedure can only be done for K I (Weisheit and Dalgarno [51]), because for this element we have a large number of experimentally determined oscillator strengths (Mazing and Serapinas [52]). By this procedure we obtain for K I $r_c = 1.95$.

b) The parameter $r_c$ can be determined much more exact by means of the experimentally determined Fano-function $x(\varepsilon)$, Fano [53]. For transitions from the ground state $ns$ of the alkali atoms to states $np_j$ we define

$$x(\varepsilon) = \frac{(2M_3 + M_1)}{(M_3 + M_1)} \tag{16}$$

where $M_1$ and $M_3$ are matrix elements which differ by the quantum number $j$

$$\begin{aligned} M_1 &= \int P_{ms}(r) \cdot Q(r) \cdot P_{np}^{1/2}(r)\, dr \\ M_3 &= \int P_{ms}(r) \cdot Q(r) \cdot P_{np}^{3/2}(r)\, dr. \end{aligned} \tag{17}$$

For transitions from the ground state to the continuum states, $P_{np}^{j}(r)$ has to be replaced in Equation (17) by $P_{\varepsilon p}^{j}(r)$. For $\varepsilon \leq I$ (ionization potential) $x(\varepsilon)$ is defined only for discrete energy states of the valence electron. For $\varepsilon > I$, $x(\varepsilon)$ is a continuous function. We define the ratio of the doublet line strength by the Fano function

$$\rho = \frac{S(n^2P_{3/2})}{S(n^2P_{1/2})} = \frac{2 \cdot M_3^2}{M_1^2} = \frac{2 \cdot (x+1)^2}{(x-2)^2}. \tag{18}$$

Baum et al. [55] have measured $x(\varepsilon)$ using the function

$$Q(\varepsilon) = \frac{(2x-1)}{(x^2+2)} \tag{19}$$

defining the counting rate asymmetry for ionization of spin-polarized atoms by alternately left- and right circularly polarized light. For $\varepsilon > 0$, $x(\varepsilon)$ has a minimum which lies near the minimum of $\sigma(\lambda)$. The zero point of $x(\varepsilon)$ can be determined very precisely; using this fact we can now determine our parameter $r_c$ by varying this value until the calculated function $x(\varepsilon, r_c)$ has the same zero point as the experimental one.

For K I, Rb I and Cs I we have performed this calculation using the measurements of Baum et al. and Lorenz and Kessler [54]. The results are shown in Table 1. For Na I no experimental values for $x(\varepsilon)$ are available. Here we have used the fact, that the theoretical cross section $\sigma(\lambda)$ reaches its minimum at nearly the same point $\lambda_{\min}$ as the measured cross section. This holds for K I, Rb I and Cs I. The value $\lambda_{\min}$ is tabulated in Table 1. The value of $r_c$ for K I agrees well with the result described in a). For Li I the dependence of $\sigma(\lambda)$ on $r_c$ is very small and may be neglected. We have used the value $r_c = 2.0$, because no experimental data are available and probably not measurable either. The determination of $r_c$ for Mg II and Ca II was done by means of the relation

$$\frac{r_c(\mathrm{Ca\,II})}{r_c(\mathrm{K\,I})} = \left[\frac{I(\mathrm{K\,I})}{I(\mathrm{Ca\,II})}\right]^n .$$

The exponent $n$ was determined by using this relation for the core radius $r_0$ instead $r_c$. The values for $n$ lie between 1/3 and 1/4. For Mg II we get for $r_c = 1.31$ and for Ca II $r_c = 1.57$. The dependence of the cross sections of these ions from $r_c$ is smaller than it is for the isoelectronic atoms.

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