

## Calculation of muonic Coulomb-capture probabilities from electron binding energies

T. von Egidy, D. H. Jakubassa-Amundsen, and F. J. Hartmann  
*Physik-Department, Technische Universität München, D-8046 Garching, Germany*  
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Muonic Coulomb-capture probabilities are calculated assuming that electrons with binding energies less than a given limit (about 80 eV) contribute with a weight which is a function of the electron binding energy, the electron quantum numbers  $n$  and  $l$ , and  $Z$ . This functional dependence is suggested by a quantum-mechanical calculation. By fitting few free parameters, good agreement with experimental capture probabilities is obtained; in particular, the periodicity with  $Z$  of these values is well reproduced.

### I. INTRODUCTION

Negative muons which are slowed down in a chemical compound or mixture of elements will be captured in one of the constituents and then cascade down to the muonic  $1s$  state by emission of characteristic x rays or Auger electrons. Muonic Coulomb-capture ratios have been measured for very many compounds. These capture ratios vary periodically with the atomic number  $Z$  of the capturing atom as was first observed by Zinov *et al.*<sup>1</sup> It has been shown recently<sup>2</sup> that per-atom capture ratios  $A(Z, Z')$  can be well reproduced by ratios of capture probabilities  $P(Z)$ ,

$$A(Z, Z') = P(Z)/P(Z'), \quad (1)$$

because the valence of the constituents plays a minor role (less than 10% variation).

A semiclassical model has been frequently applied for the theoretical description of the capture process where the capture probability is obtained from the energy loss of the muon in collision with the electrons. These calculations were pioneered by Fermi and Teller<sup>3</sup> who suggested a simple  $Z$  proportionality for the capture probabilities. However, the periodicity with  $Z$  is included only in the calculations by Daniel<sup>4</sup> and by Schneuwly, Pokrovsky, and Ponomarev<sup>5</sup> who relate the capture probabilities to the atomic radius or to the number of not too strongly bound electrons, respectively. These two theories are in good agreement with experimental results in some regions of the periodic table, but they show notable discrepancies for other regions. Therefore, a new attempt has been made to calculate muonic Coulomb-capture probabilities within a quantum-mechanical picture.

Quantum-mechanical calculations assume usually that the Coulomb capture of muons takes place via radiation or emission of an Auger electron.<sup>6-8</sup> Experiments<sup>9,10</sup> showed that the muon is predominantly captured into orbits with large principal quantum number  $n_\mu$  ( $n_\mu$  mostly  $> 20$ ). For these large- $n_\mu$  orbits Auger electron emission is the main capture mechanism.<sup>6,7</sup> Only a few authors<sup>5,11</sup> discuss the dependence of the capture probability on the characteristics of the electron orbits or their energies. We assume in a similar way as Schneuwly *et al.*<sup>5</sup> that the in-

teraction of slow muons ( $< 100$  eV) with individual electrons is responsible for the capture and that the interaction cross section  $\sigma_i$  depends mainly on the atomic binding energies  $E_i$ , the quantum numbers  $n_i, l_i$  of these electrons, and on  $Z$ . The capture probabilities  $P$  can then be calculated by the sum over all electrons weighted with the individual cross sections  $\sigma_i$ ,

$$P \propto \sum_i N_i \sigma_i(E_i, n_i, l_i, Z, k_\mu). \quad (2)$$

$N_i$  is the number of electrons in an orbit with the energy  $E_i$ .  $k_\mu$  is the average momentum of the muon to be captured. We primarily consider the dependence of  $E_i$ ,  $n_i$ ,  $l_i$ , and  $Z$  since most of the other properties such as spatial or momentum distribution of electrons, or atomic radius, are closely related with these values.

### II. DEPENDENCE OF MUON CAPTURE CROSS SECTIONS ON ATOMIC PROPERTIES

In contrast to the semiclassical picture, where an average interaction of the electrons with the  $\mu^-$  is made responsible for the capture, the quantum-mechanical description is based on the interaction of the  $\mu^-$  with a single atomic electron. Since we are looking for the general dependence of the capture probability on the electron binding energy, we apply the first-order perturbation theory where the transition amplitude for  $\mu^-$  capture with simultaneous electron ejection is given by (atomic units are used,  $e = m_e = \hbar = 1$ )

$$W_{fi} = \int d\vec{r}_\mu d\vec{r}_e \chi_f^*(\vec{r}_\mu) \psi_f^*(\vec{r}_e) \frac{e^{-\lambda |\vec{r}_e - \vec{r}_\mu|}}{|\vec{r}_e - \vec{r}_\mu|} \times \chi_i(\vec{r}_\mu) \psi_i(\vec{r}_e), \quad (3)$$

where  $\chi_{i,f}$  and  $\psi_{i,f}$  are the initial and final states of the  $\mu^-$  and electron, respectively. The screening of the  $e^-$ - $\mu^-$  interaction due to the outer electrons may be approximated by means of the constant  $\lambda = 2\sqrt{v_F}/\pi$  where  $v_F$  is the Fermi velocity.<sup>12</sup> The exact evaluation of (3) is rather

TABLE I. Comparison of different calculations of muonic capture probabilities with average experimental values from Ref. 2.

Authors	Formulas
Daniel (Ref. 4)	$P(Z) = Z^{1/3} \ln(0.57Z) / R(Z)$
Schneuwly <i>et al.</i> (Ref. 5) <sup>a</sup>	$\frac{P(Z)}{P(8)} = \frac{\sum_i N_i^Z \sigma(E_i^Z) + (2\omega_Z - 1) \nu_Z \sigma(E_\nu)}{\sum_i N_i^0 \sigma(E_i^0) + (1 - 2\omega_Z) \nu_0 \sigma(E_\nu)},$ $\sigma(E) = \begin{cases} 1, & E \leq E_0 \\ \exp[-(E - E_0)^2 / E_1^2], & E > E_0 \end{cases}$
Present work	$P(Z) = \sum_i N_i^Z \sigma(E_i^Z),$ $\sigma(E) = \begin{cases} C(1 - E/E_0)^{1/2} Z^a n^b (n - l)^c (n + l)^d, & E \leq E_0 \\ 0, & E > E_0 \end{cases}$

<sup>a</sup>See Ref. 5 for the formula  $P(Z)/P(8)$ . The binding energy  $E_\nu$  for valence electrons is about 3 eV,  $\nu_Z$  is the number of valence electrons, and  $\omega_Z$  is the distribution probability.

<sup>b</sup>The case  $E_1 = 0$  is the sharp-cut case, for which  $\sigma(E)$  is a unit step function. The cases  $E_1 > 0$  are smooth-cut cases.

<sup>c</sup>For  $Z \leq 18$ .

<sup>d</sup>For  $Z \geq 19$ .

involved<sup>6,7</sup> due to the high quantum states of the muon. In order to extract the qualitative behavior, we introduce some simplifications which lead to an analytic expression for the transition amplitude. Since the incoming muon experiences a neutral atom which is also true for the outgoing electron—because the  $\mu^-$  has been captured—the wave functions  $\chi_i$  and  $\psi_f$  will be described by plane waves. The resulting nonorthogonality between initial and final states does not lead to spurious overlap terms because the screening parameter  $\lambda$  cuts off the low components of the momentum transfer  $q$ . Actually, as  $\lambda$  is quite small and the velocity of the free particles low, the application of plane waves may be a crude approximation. When the Fourier transform of the interaction field is introduced, (3) can thus be expressed in terms of the wave functions  $\phi_\mu$  and  $\phi_e$  of the final muon and initial electron state in momentum space:

$$W_{fi} = \frac{1}{2\pi^2} \int \frac{d\vec{q}}{q^2 + \lambda^2} \phi_e(\vec{k}_e - \vec{q}) \phi_\mu^*(\vec{k}_\mu - \vec{q}), \quad (4)$$

where  $\vec{k}_\mu$  and  $\vec{k}_e$  are the momenta of the free muon and electron, respectively.

For the calculation of the total capture cross section, one has to sum over all quantum numbers of the captured muon, as well as over all quantum numbers of the atomic electrons. From this, we justify our second approximation: We replace the momentum wave functions by their corresponding densities which are averaged over the angular momentum quantum numbers  $l$  and  $m$ . Describing the atomic potential by means of an effective charge  $Z_e$ , this leads to hydrogenlike scaled  $1s$  functions,<sup>13</sup> such that

$$W_{fi} = \frac{4}{\pi^4} \left[ \frac{Z_e^2 m_\mu}{n_e n_\mu} \right]^{5/2} \times \int \frac{d\vec{q}}{q^2 + \lambda^2} \frac{1}{[(Z_e/n_e)^2 + (\vec{k}_e - \vec{q})^2]^2} \times \frac{1}{[(Z_e m_\mu/n_\mu)^2 + (\vec{k}_\mu - \vec{q})^2]^2}, \quad (5)$$

where  $m_\mu = 206.8$  is the mass of the muon, and  $n_e$  is the principal quantum number of the electron. It is shown later on that it may, nevertheless, be of some importance to retain the individual  $l$  of the electrons.

Due to the structure of the wave functions, the integrand in (5) has two maxima at  $\vec{q} = \vec{k}_e$  and  $\vec{k}_\mu$ . If we assume the orbits of the electron and muon to have about the same size, it follows that  $Z_e m_\mu / n_\mu \gg Z_e / n_e$ . Then the first maximum is much larger than the other at  $\vec{q} = \vec{k}_\mu$ . Thus, we may approximate the integral by its mean value (at  $|\vec{k}_e - \vec{q}| \approx Z_e / n_e$ ) times the width  $\Delta q \approx Z_e / n_e$ . Moreover, due to the large muon mass,  $k_\mu \gg k_e$  so that  $\vec{q}$  may be neglected in the second bracket of (5). This approximation is the better, the larger  $n_e$ , since the electronic function is sharply peaked in  $\vec{k}_e$  for large  $n_e$ .

With this approximation, the capture cross section with simultaneous ejection of an electron from the shell  $n_e$  can be expressed in terms of the properties of the atomic electrons:

TABLE I. (Continued.)

C	Parameters				$E_0$ (eV)	$E_1$ (eV)	No. of fitted parameters	$\chi^2/N$	
	a	b	c	d				Z=3,4,5	Other 62 elements
							0	634	17.8
					60 <sup>b</sup>	0 <sup>b</sup>	0	10.8	11.2
					64 ± 3 <sup>b</sup>	0 <sup>b</sup>	1	10.8	11.0
					15	70 <sup>c</sup>	0	1.9	15.5
					15	100 <sup>d</sup>			
					15	70	0	1.9	10.1
					24 ± 12	47 ± 15	2	7.2	8.8
0.0864	0.30 ± 0.03	0	0	0	75.8 ± 3.1		3	118	4.4
0.0942	0	0.74 ± 0.06	0	0	79.7 ± 3.9		3	190	4.0
0.1163	0	4.82 ± 0.71	-1.28 ± 0.22	-2.85 ± 0.57	79.4 ± 4.0		5	301	3.1
0.1151	-0.674 ± 0.020	5.90 ± 0.04	-1.54 ± 0.05	-2.10 ± 0.04	81.8 ± 4.0		6	432	2.7

$$\begin{aligned}
\sigma(k_e, k_\mu) &= \sum_{n_\mu} 2n_\mu^2 \frac{(2\pi)^4 m_\mu}{k_\mu} \\
&\quad \times \int d\vec{k}_e |W_{fi}|^2 \\
&\quad \times \delta \left[ \frac{k_\mu^2}{2m_\mu} - E_e - \frac{k_e^2}{2} + E_\mu \right] \\
&\approx c_0(\mu) k_e \left[ \frac{n_e}{Z_e} \right], \quad (6)
\end{aligned}$$

where  $E_e$  and  $E_\mu$  are the binding energies of the electron and the muon, respectively. The dependence of the cross section on the properties of the muon is incorporated in the constant  $c_0(\mu)$  which does not explicitly depend on  $n_e$  and  $k_e$ , and which is assumed to vary smoothly with the nuclear charge  $Z$ . The momentum  $k_e$  of the Auger electron is obtained from energy conservation

$$\begin{aligned}
k_e &= [2(k_\mu^2/2m_\mu + E_\mu - E_e)]^{1/2} \\
&= [2(k_\mu^2/2m_\mu + E_\mu)]^{1/2} \left[ 1 - \frac{E_e}{k_\mu^2/2m_\mu + E_\mu} \right]^{1/2} \quad (7)
\end{aligned}$$

which requires the kinetic plus binding energy of the muon to be larger than  $E_e$ . From the  $k_\mu$  dependence of (5) it follows that muons with  $k_\mu^2/2m_\mu \leq E_\mu = Z_e^2 m_\mu / 2n_\mu^2$  will be preferentially captured, since for larger  $k_\mu$ ,  $W_{fi}$  will decrease rapidly with  $k_\mu$ .

The capture probability  $P_e(Z)$  for a given electron orbit

is obtained by means of multiplying  $\sigma(k_e, k_\mu)$  with the flux density  $\rho(k_\mu)$  of the muon and integrating over  $k_\mu$ . The accurate determination of the muon capture probability would require a consistent calculation of the cross sections for the competing processes of muon slowing down by inelastic scattering and capture. However, as we are only interested in relative capture probabilities at an average muon energy, we make the assumption that the energy distribution of the muon inside the target is roughly constant in the region where the capture is likely to occur,<sup>4</sup> such that  $P_e(Z)$  is directly proportional to  $\sigma(k_e, \bar{k}_\mu)$  at the muon energy  $\bar{k}_\mu^2/2m_\mu$  where  $\sigma(k_e, k_\mu)$  has its largest value. The total capture probability  $P(Z)$  for a given atom is then obtained by summing over all electrons.

For the sake of comparison with experimental capture data<sup>2</sup> we are led from (6) and (7) to the following parametrization of the capture probability where  $i$  indicates the orbits filled with  $N_i$  electrons:

$$P(Z) = \sum_i N_i \sigma_i$$

with

$$\sigma_i = \begin{cases} C(1 - E_i/E_0)^{1/2} Z^a n_i^b, & E_i < E_0 \\ 0, & E_i \geq E_0. \end{cases} \quad (8)$$

Experimental electron binding energies<sup>14</sup>  $E_i$  are taken and  $C$ ,  $E_0$ ,  $a$ , and  $b$  are fit parameters. In contrast to the formula of Schneuwly *et al.*,<sup>5</sup> where the limitation to not too strongly bound electrons was introduced *ad hoc*, our quantum-mechanical calculation yields this cut in a natural way.

TABLE II. Experimental and calculated muonic capture probabilities or ratios.

Element	Z	Avg. expt. prob. <sup>a</sup>	Present calc. <sup>b</sup>	Daniel <sup>c</sup>	Schneuwly <i>et al.</i> <sup>d</sup>
Li	3	0.18±0.04	0.32	0.22	0.19
Be	4	0.075±0.01	0.43	0.50	0.06
B	5	0.25±0.07	0.57	0.08	0.11
N	7	1.02±0.30	0.77	1.31	0.69
O	8	0.994±0.10	0.87	1.00	1.00
F	9	0.99±0.03	0.93	1.01	1.83
Na	11	1.00±0.04	1.02	0.93	0.90
Mg	12	0.93±0.04	0.98	1.20	0.90
Al	13	0.76±0.06	0.97	1.43	0.85
Si	14	0.84±0.06	0.91	1.65	0.91
P	15	1.04±0.06	1.03	1.80	1.16
S	16	1.23±0.05	1.21	1.91	1.53
Cl	17	1.32±0.04	1.35	1.40	1.60
K	19	1.54±0.05	1.67	1.16	1.27
Ca	20	1.90±0.09	1.86	1.46	1.47
Sc	21	2.78±0.31	2.03	1.82	1.45
Ti	22	2.66±0.19	2.26	2.11	2.20
V	23	2.76±0.17	2.44	2.37	2.48
Cr	24	2.98±0.19	2.57	2.56	2.57
Mn	25	2.73±0.18	2.63	2.67	2.69
Fe	26	3.28±0.21	2.80	2.73	2.99
Co	27	2.94±0.27	2.95	2.85	3.14
Ni	28	2.88±0.22	3.00	2.94	3.19
Cu	29	3.26±0.36	3.16	2.93	3.32
Zn	30	3.20±0.19	2.98	2.75	3.16
Ga	31	2.77±0.31	2.98	2.78	3.32
Ge	32	2.90±0.33	2.96	2.93	3.65
As	33	2.89±0.26	2.88	2.95	3.60
Se	34	2.72±0.31	2.68	2.98	3.81
Br	35	2.70±0.14	2.44	2.18	3.16
Rb	37	2.39±0.19	1.98	1.74	2.01
Sr	38	2.13±0.14	2.23	2.09	2.22
Y	39	2.34±0.19	2.40	2.54	2.65
Zr	40	2.60±0.26	2.57	2.90	3.03
Nb	41	3.06±0.34	2.62	3.22	3.51

The mean dependence on the target charge  $Z$  has been explicitly included. From classical calculations, predictions for the exponent  $a$  vary from 1 to  $\frac{1}{3}$  (Refs. 3 and 4). This average  $Z$  dependence is based on the Thomas-Fermi description of the atomic potential which yields a value of  $0.885Z^{-1/3}$  for the extension  $\langle r \rangle$  of the atom. Equating this with the radius  $n_i^2/Z$  of an atomic orbital leads to an estimate for the average principal quantum number of the outermost atomic shells  $n_i \sim Z^{1/3}$ . From this one obtains the estimate (for example, by means of a variational calculation)  $Z_e/n_i \sim Z^{2/3}$  for the wave function.<sup>15</sup> This discussion shows that instead of  $Z^a$  the term  $n_i^b$  might also be introduced.

As the shell structure of the individual atoms is accounted for by means of  $E_i$  and  $N_i$ , formula (8) is able to describe the oscillatory behavior of the experimental capture probabilities. In particular, the low  $P(Z)$  values for the alkali-metal and alkaline-earth elements result from the small number  $N_i$  of loosely bound electrons in these atoms.

### III. COMPARISON WITH EXPERIMENTAL CAPTURE PROBABILITIES

Formula (8) was used to calculate relative muonic Coulomb-capture probabilities and to compare them with experimental probabilities which are given for 65 elements in Ref. 2. The electron binding energies were taken from Table II of Ref. 14 for neutral atoms. The parameters  $C$ ,  $E_0$ , and  $a$  (or  $b$ ) were determined by a least-squares fit to the experimental data with a special computer program. Sixty-two elements with  $Z > 6$  are included in the fit. The light elements Li, Be, and B were not used for the fit, because for these elements the electronic structure is strongly influenced by the chemical bond and the assumption that the atoms have  $Z$  electrons is less justified than for heavier elements. The resulting parameters are  $E_0 = (76 \pm 3)$  eV,  $a = 0.30 \pm 0.03$ , and  $C = 0.0864$  if  $b = 0$ ; or  $E_0 = (79.7 \pm 4.0)$  eV,  $b = 0.735 \pm 0.060$ , and  $C = 0.0942$  if  $a = 0$ . As absolute values of  $P(Z)$  are not known, the probabilities have been normalized to  $P(\text{oxygen}) = 1$ .

TABLE II. (Continued.)

Element	Z	Avg. expt. prob. <sup>a</sup>	Present calc. <sup>b</sup>	Daniel <sup>c</sup>	Schneuwly <i>et al.</i> <sup>d</sup>
Mo	42	3.48±0.29	2.81	3.69	4.03
Tc	43	3.30±0.50	2.93	3.58	3.87
Pd	46	3.60±0.50	3.17	3.70	4.06
Ag	47	3.14±0.19	3.33	3.57	3.86
Cd	48	3.01±0.18	3.38	3.34	4.04
In	49	2.90±0.50	3.27	3.19	4.27
Sn	50	2.54±0.18	3.19	3.47	4.54
Sb	51	3.16±0.23	3.28	3.42	4.41
Te	52	3.16±0.36	3.35	3.44	4.72
I	53	2.97±0.26	3.37	2.58	4.00
Cs	55	3.25±0.27	2.98	2.09	2.91
Ba	56	3.76±0.27	2.83	2.57	3.09
La	57	3.43±0.33	3.11	3.10	3.46
Ce	58	5.20±0.50	4.18	3.23	3.66
Nd	60	5.80±0.40	4.32	3.30	3.88
Sm	62	4.40±0.10	5.02	3.41	4.34
Eu	63	4.30±0.80	5.46	3.45	4.57
Gd	64	5.80±0.50	5.68	3.47	4.76
Dy	66	6.40±0.60	6.24	3.60	5.06
Er	68	6.80±0.80	6.93	3.70	5.53
Yb	70	6.20±0.50	7.54	3.80	6.06
Lu	71	5.30±0.90	7.64	3.84	6.26
Ta	73	6.00±0.50	7.06	4.62	7.08
W	74	6.60±0.90	6.79	4.85	7.40
Hg	80	4.80±0.50	3.52	4.55	5.06
Tl	81	5.00±0.50	3.48	4.20	4.83
Pb	82	3.69±0.24	3.42	4.15	4.95
Bi	83	3.78±0.39	3.60	4.30	4.74
Th	90	3.00±0.60	3.55	4.27	4.49
U	92	4.70±0.90	4.04	4.98	4.83

<sup>a</sup>Average experimental capture probabilities from Ref. 2, normalized to  $P(8)=1.0$ .

<sup>b</sup>Calculated with formula (8) including  $(n-l)^c(n+l)^d$  and parameters  $E_0=81.8$ ,  $a=-0.674$ ,  $b=5.90$ ,  $c=-1.54$ ,  $d=-2.10$ , and  $C=0.115$ .

<sup>c</sup>Reference 4 for oxides.

<sup>d</sup>Version (b) of Ref. 5 but with  $E_0=15$  eV and  $E_1=70$  eV for all elements; for oxides.

Table I compares the  $\chi^2/N$  values ( $N$  being the number of fitted values, which equals 62) for various calculations.

The parameter  $E_0$  reflects the order of magnitude of the kinetic energy of the muon before capture. The parameter  $a$  has a value close to  $\frac{1}{3}$ . This may be understood with the assumption that the average quantum number  $n_\mu$  of the captured  $\mu$  is proportional to  $n_i$ , i.e.,  $\sim Z^{1/3}$ , while the kinetic energy of the captured  $\mu$  is only weakly dependent on  $Z$ . The term  $n_i^b$  gives a better  $\chi^2/N$  than the term  $Z^a$ .

Several functions similar to (8) with additional free parameters have been tested if they might yield better agreement with the experimental capture probabilities. The additional terms  $(n-l)^c$  and  $(n+l)^d$  resulted in essential improvement which is definitely superior than would be expected for irrelevant additional parameters. Table I shows the  $\chi^2/N$  values and the parameters obtained with the fit. These terms  $(n-l)^c$  and  $(n+l)^d$  are reasonable because they appear in the normalization of the electronic wave functions if the averaging over  $l$  is not carried out. Table II lists for 65 elements average experimental capture prob-

abilities<sup>2</sup> and values calculated with (8) including  $(n-l)^c(n+l)^d$ . These results are also plotted in Fig. 1.

The present calculation assumes neutral atoms. The possibility was considered of also including a term which accounts for electron redistribution in an ionic bond. However, a comparison with the experimental capture probabilities (Fig. 1) shows a trend in the opposite direction. The calculated values for neutral atoms have the tendency to be too low at the beginning of the fourth and sixth periods although they are expected to be too high since the valence electrons of these elements move nearer to the other constituent. This behavior can be explained by assuming that the effect of electrons lost or gained by ionic bonding is compensated or even overcompensated by the effect of the positive or negative ionic charge, respectively, which attracts or repulses the muons. A detailed calculation of these effects would give information on the influence of the chemical bond and of the valence on capture ratios. A quantitative comparison of such calculations with the experimental results is difficult, because the

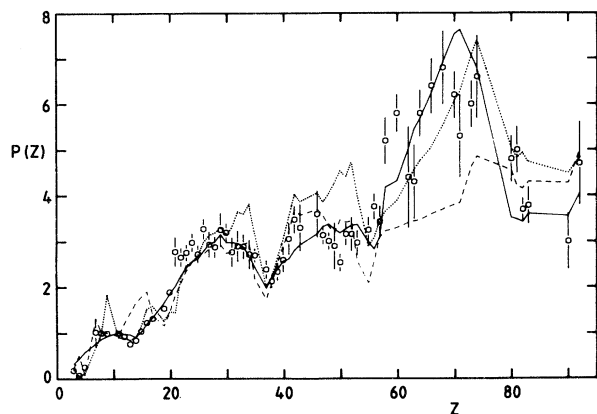


FIG. 1. Experimental (with error bars) and calculated capture probabilities. The solid, dashed, and dotted lines correspond to the present calculation (with six parameters) and to values according to Daniel (Ref. 4) and Schneuwly *et al.* (Ref. 5) ( $E_0=15$  eV,  $E_1=70$  eV), respectively.

magnitude of these effects is of the order of the experimental errors. Accordingly, these effects are not included in the present calculation.

Fig. 1 shows that there is generally good agreement between the calculated and the averaged experimental capture probabilities. The possible origins of the discrepancies of Li, Be, and B are mentioned above.

#### IV. COMPARISON WITH OTHER CALCULATIONS OF CAPTURE PROBABILITIES

The results of the present calculation are compared with the values obtained with the formulas given by Daniel<sup>4</sup> and by Schneuwly, Pokrovsky, and Ponomarev<sup>5</sup> in Table II and Fig. 1. The parameters used by Schneuwly *et al.* have also been varied in order to see if the agreement with the experimental data<sup>2</sup> could be improved. The formulas, parameters, and  $\chi^2/N$  values are given in Table I. The variation of the parameters in the formulas of Schneuwly *et al.*<sup>5</sup> does not essentially improve the agreement. It should be noted that the formula of Ref. 5 with a smooth cut gives better agreement if for all  $Z$  values  $E_0=15$  eV and  $E_1=70$  eV are used than if for  $Z \geq 19$ ,  $E_1=100$  eV is taken as prescribed in this reference. Therefore, the formula with  $E_0=15$  eV and  $E_1=70$  eV for all  $Z$  is applied for the last column in Table II and in Fig. 1.

We have also checked to see if the additional terms

$Z^a n^b (n-l)^c (n+l)^d$  used in our calculations, would improve the agreement of the formula of Schneuwly *et al.* with the experimental capture probabilities. The terms  $Z^a$  or  $n^b$  alone improve  $\chi^2/N$  only by about 1. However, these terms together with a general calibration factor  $C$  [to  $P(Z)/P(8)$ ] yield a  $\chi^2/N=3.7$  (with  $E_0=34.4$ ,  $E_1=55.3$ ,  $a=-0.616$ ,  $b=9.30$ ,  $c=-2.43$ ,  $d=-5.40$ , and  $C=0.740$ ). That means that this fit with seven parameters is about 40% worse than our approach with six parameters.

The  $\chi^2/N$  values provided in Table II show that the present calculation gives better agreement than the previous formulas. It can be concluded that (1) the consideration of the atomic radius together with a function of  $Z$  for capture probabilities is not sufficient to reproduce capture probabilities; (2) the assumption of Schneuwly *et al.*<sup>5</sup> that not too strongly bound electrons play a major role is justified and represents the basis of the periodicity of capture probabilities; and (3) the treatment of the valence electrons with the mesomolecular model<sup>16</sup> is not necessary to reproduce capture ratios, but leads to discrepancies with experimental values especially before the atomic shell closures at  $Z=36$  and 54.

The calculations of Schneuwly are much better than the other ones for the very light elements Li, Be, and B. In these cases the chemical bond plays a decisive role and the distribution of electrons and muons must be taken into account more carefully. For all heavier elements it seems sufficient to assume neutral atoms for the calculation of average capture probabilities.

In conclusion, it can be stated that muonic capture probabilities can be predicted with the assumption that muons are captured by individual electrons, and are determined by a general function involving the electron binding energy, electron quantum numbers, and  $Z$ . Theoretical and empirical considerations show that this function can be approximated by  $(1-E_i/E_0)^{1/2} Z^a n_i^b (n_i-l_i)^c (n_i+l_i)^d$  (for  $E_i < E_0$ ). It should be mentioned that already a function with two parameters ( $E_0$  and  $b$ ) in addition to the calibration constant  $C$  yields good agreement. The average kinetic energy predicted for the muons before capture is of the order of their binding energy and thus about one-half of  $E_0$  (about 40 eV). This is in agreement with recent experimental results.<sup>17</sup>

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<sup>1</sup>V. G. Zinov, A. D. Konin, and A. I. Mukhin, *Yad. Fiz.* **2**, 859 (1965) [*Sov. J. Nucl. Phys.* **2**, 613 (1966)].

<sup>2</sup>T. von Egidy and F. J. Hartmann, *Phys. Rev. A* **26**, 2355 (1982).

<sup>3</sup>E. Fermi and E. Teller, *Phys. Rev.* **72**, 399 (1947).

<sup>4</sup>H. Daniel, *Z. Phys. A* **291**, 29 (1979).

<sup>5</sup>H. Schneuwly, V. I. Pokrovsky, and V. I. Ponomarev, *Nucl.*

*Phys.* **A312**, 419 (1978).

<sup>6</sup>P. K. Haff and T. A. Tombrello, *Ann. Phys. (N.Y.)* **86**, 178 (1974).

<sup>7</sup>M. Y. Au-Yang and M. L. Cohen, *Phys. Rev.* **174**, 468 (1968).

<sup>8</sup>J. S. Cohen, R. L. Martin, and W. R. Wadt, *Phys. Rev. A* **27**, 1821 (1983).

<sup>9</sup>F. J. Hartmann, T. von Egidy, R. Bergmann, M. Kleber, H.-J.

- Pfeiffer, K. Springer, and H. Daniel, *Phys. Rev. Lett.* 37, 331 (1976).
- <sup>10</sup>F. J. Hartmann, R. Bergmann, H. Daniel, H.-J. Pfeiffer, T. von Egidy, and W. Wilhelm, *Z. Phys. A* 305, 189 (1982).
- <sup>11</sup>H. Daniel, *Radiat. Eff.* 28, 189 (1976).
- <sup>12</sup>P. Vogel, P. K. Haff, V. Akylas, and A. Winther, *Nucl. Phys. A* 254, 445 (1975).
- <sup>13</sup>V. Fock, *Z. Phys.* 98, 145 (1935).
- <sup>14</sup>K. D. Sevier, *At. Data Nucl. Data Tables* 24, 323 (1979).
- <sup>15</sup>C. A. Coulson and N. H. March, *Proc. Phys. Soc. London Ser. A* 63, 367 (1950).
- <sup>16</sup>S. S. Gershtein, V. I. Petrukhin, L. I. Ponomarev, and Yu. D. Prokoshkin, *Usp. Fiz. Nauk* 97, 3 (1969) [*Sov. Phys.—Usp.* 12, 1 (1969)].
- <sup>17</sup>G. Fottner, H. Daniel, P. Ehrhart, H. Hagn, F. J. Hartmann, E. Köhler, and W. Neumann, *Z. Phys. A* 304, 333 (1982).