K-Shell Auger Rates, Transition Energies, and Fluorescence Yields of Variously Ionized States of Argon*

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Theoretical K-shell Auger groups rates, $K\alpha$ and $K\beta$ x-ray rates, and fluorescence yields are presented for 47 defect electronic configurations of argon. Energy shifts from the normal x rays and the Auger-electron energies are also given for these defect configurations. These theoretical results can be conveniently used in the analysis of experiments involving heavy-ion–argon collisions.

I. INTRODUCTION

Several investigators[1-6] have reported on the x-ray production cross section $\sigma_x(E)$ in heavy-ion–atom collisions. The relative population of defect electronic configurations produced in ion-atom collisions depends upon the energy and charge state of the incident ion. The experimental data, in particular the high-resolution studies, show directly the production of multiple inner-shell vacancies in ion-atom collisions at bombarding energies ≈ 1 MeV/amu. The x-ray energies, for example, of the $K\alpha$ x ray, are observed to be higher than the normal values for the $[1s]$ defect configuration[7] in these experiments. This change in the x-ray transition energies is due to multiple vacancies in addition to a K-shell vacancy. Theoretical transition energies and K-shell fluorescences ω_k for the defect configurations are needed to identify the x-ray lines and to obtain the ionization cross section from $\sigma_x(E)$.

There are only few Auger electron measurements relevant to the heavy-ion–atom collisions.[8,9] Theoretical Auger-electron energies and the relative intensities are again needed for the analyses of data.

There have been relatively few calculations[10-12] of Auger rates, fluorescence yields, and transition energies for defect electronic configurations. Recently Macdonald *et al.*[13] have reported low-resolution measurements of K-shell x rays produced in heavy-ion–argon collisions. Both the Auger-electron measurements and high-resolution experiments for argon are feasible, and these should be valuable. We present the theoretical Auger-electron rates, x-ray rates, K-shell fluorescence yields, and transition energies of variously ionized states of argon. These theoretical results are applicable to the analysis of defect electronic configurations which may be produced in heavy-ion–argon collisions.

Section II contains a brief description of theory, followed by numerical results in Sec. III. Comparisons with experimental data and the statistical scaling procedure are presented in Sec. IV.

II. THEORY

The detailed theoretical development and calculational procedure have been described elsewhere.[10,14] We summarize the essential aspects of the calculations here.

The Hartree-Fock-Slater (HFS) atomic model with the exchange approximation[15] of Herman, Van Dyke, and Ortenburger was used in the calculations of appropriate bound-state wave functions. The continuum-state wave functions, needed to calculate the Auger rates, were obtained by numerical integration of the Schrödinger equation for the central field potential. The Auger group rate, in atomic units, involving two electrons initially described by quantum numbers n_1l_1 and n_2l_2, filling a vacancy (n_3l_3), and resulting in one electron in the continuum El_4 is

$$T_A(n_3l_3 - n_1l_1, n_2l_2) = 2\pi N_{12}\sum|M|^2,$$
$$M \equiv \langle \phi(n_2l_3, El_4)|(1/r_{12})|\,\phi(n_1l_1, n_2l_2)\rangle. \tag{1}$$

The initial and final states are represented by an antisymmetrized product wave function, whose components can be separated into the radial part P_{nl}/r and an angular part $Y_l^m(\Theta,\Psi)$. The weighing factor N_{12} is given in terms of the electron occupation numbers.[10] The integration over the radial parts can conveniently be expressed in terms of matrix elements of the following form:

$$R_K(1,2,3,4) \equiv \int_0^\infty\int_0^\infty P_{n_1l_1}(i)P_{n_2l_2}(j) \times (r_<^K/r_>^{K+1})P_{n_3l_3}(i)P_{El_4}(j)\,dr_i\,dr_j. \tag{2}$$

Equation (1) represents the Auger rate averaged

TABLE I. Calculated $K-LL$ Auger rates, total Auger rates, and total x-ray rates (in a.u.) for various defect electronic configuration $[1s, 2p^m, 3p^n]$ of argon.

Defect configuration		1000× $T_A(1s\text{-}2s\text{-}2s)$	1000× $T_A(1s\text{-}2s\text{-}2p)$	1000× $T_A(1s\text{-}2p\text{-}2p)$	1000× total Auger rate	10 000× total x-ray rate
m	n					
0	0	1.372	4.574	11.75	20.83	28.43
1	0	1.477	4.125	8.550	17.67	25.79
2	0	1.585	3.562	5.589	14.51	22.75
3	0	1.698	2.879	3.035	11.40	19.30
4	0	1.815	2.059	1.09	8.685	15.40
5	0	1.935	1.101	···	6.396	11.02
1	1	1.481	4.136	8.588	17.51	25.58
2	1	1.591	3.577	5.615	14.28	22.46
3	1	1.706	2.891	3.052	11.19	18.90
4	1	1.825	2.071	1.02	8.396	14.89
5	1	1.945	1.108	···	6.105	10.38
6	1	2.063	···	···	4.543	5.386
1	2	1.487	4.154	8.632	17.28	25.3
2	2	1.599	3.594	5.650	14.01	22.10
3	2	1.716	2.908	3.070	10.87	18.43
4	2	1.836	2.085	1.1094	8.060	14.30
5	2	1.956	1.115	···	5.780	9.657
6	2	2.075	···	···	4.268	4.513
1	3	1.494	4.174	8.690	17.00	24.98
2	3	1.609	3.616	5.687	13.66	21.65
3	3	1.727	2.929	3.093	10.50	17.88
4	3	1.848	2.099	1.118	7.680	13.61
5	3	1.971	1.123	···	5.427	8.833
6	3	2.088	···	···	3.979	3.537
1	4	1.503	4.201	8.754	16.66	24.59
2	4	1.619	3.642	5.734	13.28	21.16
3	4	1.741	2.950	3.120	10.08	17.25
4	4	1.864	2.117	1.127	7.265	12.84
5	4	1.986	1.133	···	5.052	7.915
6	4	2.100	···	···	3.685	2.459
1	5	1.514	4.232	8.832	16.28	24.13
2	5	1.633	3.672	5.787	12.84	20.58
3	5	1.756	2.977	3.148	9.632	16.54
4	5	1.880	2.137	1.137	6.817	11.99
5	5	2.000	1.144	···	4.658	6.897
6	5	2.115	···	···		

TABLE II. Calculated $K-LL$ Auger rates, total Auger rates, and total x-ray rates (in a.u.) for various defect configurations $[1s^1, 2s^q, 2p^m, 3s^2, 3p^6]$ of argon.

Defect configuration		1000× $T_A(1s\text{-}2s\text{-}2s)$	1000× $T_A(1s\text{-}2s\text{-}2p)$	1000× $T_A(1s\text{-}2p\text{-}2p)$	1000× total Auger rate	1000× total x-ray rate
q	m					
0	0	1.398	4.681	12.14	18.22	2.684
0	1	1.508	4.233	8.865	14.61	2.363
0	2	1.622	3.663	5.794	11.08	1.994
0	3	1.736	2.961	3.138	7.836	1.575
0	4	1.848	2.117	1.127	5.091	1.103
0	5	1.951	1.125	···	3.076	0.577
1	0	···	2.498	13.01	15.51	2.811
1	1	···	2.254	9.456	11.71	2.472
1	2	···	1.945	6.156	8.101	2.083
1	3	···	1.566	3.324	4.890	1.643
1	4	···	1.112	1.189	2.301	1.149
1	5	···	0.588	···	0.588	0.600

TABLE III. Calculated $K\alpha$ and $K\beta$ x-ray energy shifts,[a] ratio of $K\beta$ and $K\alpha$ intensities, and K-shell fluorescence yields for various defect configurations of argon.

Defect configuration $[1s, 2p^m, 3p^n]$		$\Delta E(K\alpha)$	$\Delta E(K\beta)$	$\frac{I(K\beta)}{I(K\alpha)}$	
m	n	(eV)	(eV)		ω_K
0	0	...	...	0.084	0.120
1	0	15.7	43.6	0.121	0.126
2	0	32.9	89.8	0.176	0.136
3	0	51.2	138.4	0.266	0.145
4	0	71.3	189.4	0.443	0.151
5	0	91.9	242.8	0.971	0.147
1	1	16.8	48.1	0.110	0.127
2	1	34.2	95.3	0.157	0.136
3	1	53.0	145.4	0.236	0.145
4	1	73.3	196.9	0.390	0.151
5	1	94.7	251.3	0.849	0.145
6	1	...	308.2	...	0.106
1	2	18.0	53.4	0.095	0.128
2	2	36.0	101.7	0.134	0.136
3	2	55.2	152.3	0.200	0.145
4	2	75.9	205.4	0.328	0.151
5	2	97.8	260.8	0.705	0.143
6	2	...	318.7	...	0.096
1	3	19.8	59.8	0.076	0.128
2	3	38.0	108.9	0.106	0.137
3	3	57.8	160.6	0.158	0.146
4	3	78.9	214.7	0.258	0.151
5	3	101.3	271.2	0.556	0.140
6	3	...	330.1	...	0.082
1	4	21.7	67.0	0.054	0.129
2	4	40.5	117.2	0.075	0.137
3	4	60.7	170.0	0.110	0.146
4	4	82.3	225.0	0.180	0.150
5	4	105.3	282.6	0.386	0.135
6	4	...	342.4	...	0.063
1	5	24.2	74.4	0.029	0.129
2	5	43.4	126.6	0.040	0.138
3	5	64.1	180.2	0.058	0.147
4	5	86.2	236.4	0.093	0.149
5	5	109.7	294.8	0.200	0.129
6	5	...	355.8	...	0.036

[a] Energies of the normal $K\alpha$ and $K\beta$ x rays are 2957.01 and 3190.5 eV, respectively.

TABLE IV. Calculated $K\alpha$ x-ray energy shifts[a] and K-shell fluorescence yields for various electronic configurations of argon.

Electronic configuration	$\Delta E(K\alpha)$	ω_K
$(1s)^1(2s)^2(2p)^6$	13.5	0.128
$(1s)^1(2s)^2(2p)^5$	32.4	0.139
$(1s)^1(2s)^2(2p)^4$	52.8	0.153
$(1s)^1(2s)^2(2p)^3$	74.8	0.167
$(1s)^1(2s)^2(2p)^2$	98.1	0.178
$(1s)^1(2s)^2(2p)^1$	122.8	0.158
$(1s)^1(2s)^1(2p)^6$	30.9	0.153
$(1s)^1(2s)^1(2p)^5$	50.9	0.174
$(1s)^1(2s)^1(2p)^4$	72.4	0.205
$(1s)^1(2s)^1(2p)^3$	95.33	0.252
$(1s)^1(2s)^1(2p)^2$	119.8	0.333
$(1s)^1(2s)^1(2p)^1$	145.8	0.505

[a] Energy of the normal $K\alpha$ x ray is 2957.01 eV.

over all multiplet states of a defect configuration.

The x-ray transition rates were obtained in the electric dipole approximation using the calculated wave functions for the defect configurations.

The transition energies of Auger electrons and of x rays were calculated by computing the appropriate differences of the total energy of the atom in the initial and final states. The expressions for the total energy of different electronic configurations are listed by Slater.[16]

TABLE V. $K-LL$ Auger radial matrix elements[a] $\times 100$ for various defect electronic configurations $[1s, 2p^m, 3p^n]$ of argon.

Configuration m	n	A	B	C	D	F
0	0	1.478	1.271	2.031	−2.033	5.097
1	0	1.533	1.322	2.123	−2.130	5.324
2	0	1.588	1.373	2.218	−2.229	5.556
3	0	1.644	1.425	2.315	−2.239	5.789
4	0	1.700	1.476	2.412	−2.426	6.015
5	0	1.755	1.526	2.509	...	...
1	1	1.535	1.324	2.128	−2.135	5.336
2	1	1.591	1.376	2.225	−2.235	5.569
3	1	1.648	1.429	2.322	−2.336	5.805
4	1	1.704	1.480	2.421	−2.438	6.041
5	1	1.759	1.531	2.519	...	...
6	1	1.812	...	...	...	...
1	2	1.538	1.327	2.135	−2.414	5.350
2	2	1.595	1.380	2.232	−2.242	5.586
3	2	1.653	1.433	2.332	−2.344	5.823
4	2	1.709	1.485	2.432	−2.447	6.061
5	2	1.765	1.536	2.530	...	...
6	2	1.817	...	...	...	...
1	3	1.542	1.330	2.142	−2.147	5.368
2	3	1.600	1.384	2.242	−2.250	5.605
3	3	1.658	1.438	2.343	−2.353	5.844
4	3	1.715	1.490	2.443	−2.456	6.085
5	3	1.771	1.541	2.542	...	...
6	3	1.823	...	...	...	...
1	4	1.547	1.334	2.152	−2.156	5.387
2	4	1.605	1.389	2.252	−2.260	5.628
3	4	1.664	1.443	2.354	−2.364	5.869
4	4	1.722	1.497	2.457	−2.468	6.108
5	4	1.778	1.548	2.558	...	...
6	4	1.828	...	...	...	...
1	5	1.552	1.339	2.162	−2.166	5.412
2	5	1.612	1.394	2.264	−2.271	5.653
3	5	1.672	1.449	2.368	−2.376	5.896
4	5	1.730	1.504	2.472	−2.480	6.135
5	5	1.785	1.555	2.573	...	...
6	5	1.835	...	...	...	...

[a] $A = R_0(20, 20, 10, k\,0)$, $B = R_0(20, 21, 10, k\,1)$, $C = R_1(21, 20, 10, k\,1)$, $D = R_1(21, 21, 10, k\,0)$, and $F = (21, 21, 10, k\,2)$.

TABLE VI. $K-LL$ Auger radial matrix elements [a] $\times 100$ for various defect electronic configurations $[1s, 2s^l, 2p^m, 3s^2, 3p^6]$ of argon.

Configuration						
l	m	A	B	C	D	F
0	0	1.492	1.286	2.062	−2.067	5.181
0	1	1.549	1.339	2.161	−2.170	5.422
0	2	1.607	1.392	2.262	−2.272	5.657
0	3	1.662	1.445	2.364	−2.374	5.886
0	4	1.715	1.496	2.465	−2.470	6.107
0	5	1.762	1.542	2.560	···	···
1	0	···	1.328	2.140	−2.144	5.363
1	1	···	1.382	2.241	−2.247	5.598
1	2	···	1.435	2.343	−2.348	5.830
1	3	···	1.486	2.445	−2.446	6.057
1	4	···	1.533	2.544	−2.537	6.275
1	5	···	1.576	2.638	···	···

[a] Matrix elements are defined in the footnote of Table V.

TABLE VIII. Calculated $K-LL$ Auger-electron energy shifts [a] for various defect electronic configurations $[1s^1, 2s^q, 2p^m, 3s^2, 3p^6]$ of argon.

q	m	$2s$-$2s$	$2s$-$2p$	$2p$-$2p$
0	0	−172	−175	−177
0	1	−200	−211	−221
0	2	−229	−248	−267
0	3	−257	−285	−314
0	4	−285	−323	−363
0	5	−313	−362	···
1	0	···	−215	−214
1	1	···	−252	−260
1	2	···	−290	−307
1	3	···	−328	−355
1	4	···	−367	−405
1	5	···	−406	···

[a] Auger energies for the $[1s]$ defect configurations are $E_A(2s\text{-}2s) = 2505$ eV, $E_A(2s\text{-}2p) = 2584$ eV, and $E_A(2p\text{-}2p) = 2654$ eV.

III. NUMERICAL RESULTS

The defect electronic configuration is denoted by square brackets in which the number of electrons missing in each orbital of argon are listed. For example, the *defect* electronic configuration $[1s, 2p^2, 3p^3]$ is equivalent to an electronic configuration $(1s)^1(2s)^2(2p)^4(3s)^2(3p)^3$ of argon. Tables I and II contain K-LL Auger group rates, total Auger rates, and total x-ray rates for 35 different defect configurations. The energy shifts of $K\alpha$ and $K\beta$ x rays from the normal values (2957.01 and 3190.5 eV) of the $[1s]$ defect configuration,[7] intensity ratios of $K\beta$ and $K\alpha$ x rays, and K-shell fluorescence yields are given in Tables III and IV.

The Auger radial matrix elements defined in Eq. (2) are presented in Tables V and VI so that high-resolution Auger-electron data could be analyzed with the inclusion of configuration interaction.[17,18] The shifts in the Auger-electron energies from their normal values for the $[1s]$ defect configuration are listed in Tables VII and VIII.

The high-resolution studies of x-ray spectra and the Auger-electron measurements are feasible for

TABLE VII. Calculated $K-LL$ Auger-electron energy shifts [a] for various defect electronic configurations $[1s, 2p^m, 3p^n]$ of argon.

m	n	$2s$-$2s$	$2s$-$2p$	$2p$-$2p$	m	n	$2s$-$2s$	$2s$-$2p$	$2p$-$2p$
0	0	0.0	0.0	0.0	1	3	−78.7	−86	−94
1	0	−16.7	−23.9	−21.4	2	3	−101	−117	−133
2	0	−34.5	−49.5	−65.1	3	3	−124	−148	−173
3	0	−52.9	−76.3	−100	4	3	−147	−181	−216
4	0	−72.0	−104	−131	5	3	−171	−214	···
5	0	−91.9	−134	···	6	3	−195	···	···
1	1	−36.2	−43.4	−51.0	1	4	−102	−109	−117
2	1	−55.6	−70.7	−84.5	2	4	−126	−141	−158
3	1	−81.6	−99.2	−124	3	4	−150	−174	−200
4	1	−96.2	−129	−163	4	4	−174	−208	−243
5	1	−117	−157	···	5	4	−199	−242	···
6	1	−139	···	···	6	4	−224	···	···
1	2	−56.9	−64.2	−71.8	1	5	−126	−133	−142
2	2	−77.8	−93.1	−109	2	5	−151	−167	−184
3	2	−99.3	−123	−148	3	5	−176	−201	−227
4	2	−121	−154	−189	4	5	−202	−236	−272
5	2	−144	−187	···	5	5	−253	···	···
6	2	−167	···	···					

[a] Auger-electron energies for the $[1s]$ defect configuration are $E_A(2s\text{-}2s) = 2505$ eV, $E_A(2s\text{-}2p) = 2584$ eV, and $E_A(2p\text{-}2p) = 2654$ eV.

TABLE IX. Comparison of total K-shell Auger rates, x-ray rates and fluorescence yields of argon obtained with the statistical scaling procedure and HFS calculations. The values of Larkins are shown in the last column.

$[1s, 2p^m, 3p^n]$		Total Auger rate/10^{-4} a.u.		Total x-ray rate/10^{-4} a.u.		ω_k		
m	n	Statistical scaling	HFS	Statistical scaling	HFS	Statistical scaling	HFS	Larkins (statistical scaling)
1	0	15.76	17.67	2.41	2.58	0.132	0.126	0.143
2	0	11.48	14.51	1.97	2.28	0.146	0.136	0.158
3	0	7.98	11.40	1.53	1.93	0.161	0.145	0.174
4	0	5.25	8.69	1.09	1.54	0.172	0.151	0.187
5	0	3.01	6.40	0.657	1.10	0.179	0.147	0.183
1	6	13.7	14.61	2.19	2.68	0.138	0.139	0.147
2	6	9.73	11.08	1.75	2.36	0.152	0.153	0.162
3	6	6.55	7.84	1.31	1.99	0.167	0.167	0.177
4	6	4.13	5.09	0.874	1.58	0.175	0.178	0.184
5	6	2.52	3.08	0.437	1.10	0.148	0.158	0.157

heavy-ion–argon collisions. The numerical results presented presented in this paper are applicable to the analyses of such data as well as low-resolution x-ray measurements.[13]

IV. COMPARISONS

A. Experimental Data

Bailey and Swedlund,[19] and more recently Pahor *et al.*[20] report ω_k for the [1s] defect configuration of argon as 0.119 ± 0.007 and 0.121 ± 0.003, respectively. These experimental data are to be compared with our calculated value of 0.12. Similarly, the total K-shell width equal to 0.68 ± 0.03 eV, as reported by Watanabe,[21] compares favorably with the calculated width of 0.644 eV.

It is reasonable to assume $\approx 5\%$ uncertainty in the absolute total rates presented in this paper since effects arising from electron correlation[22] have been ignored in this work.

B. Statistical Scaling Procedure

Larkins[12] proposed a very simple procedure for estimating ω_k for different defect configurations. The technique is simply to scale the individual Auger and x-ray rates calculated only for the [1s] defect configuration with weighting factors that depend upon the number of electrons participating in the process. The approximations inherent in this simple procedure are the ignoring of changes in both transition energies and wave functions for electron defect configurations.

Table IX contains a comparison of total Auger and x-ray rates obtained with the statistical scaling procedure and those obtained with the HFS model. The calculated values of ω_k using the scaling procedure, HFS model, and the values Larkins are given in the last three columns of this table. It should be noted that the statistical scaling procedure leads to significantly lower Auger and x-ray rates for most of the defect configurations. Some of these errors, however, cancel in obtaining ω_k. It is not possible to make a general observation regarding the applicability of this approximate model.

Finally, we comment on the calculations of $K\alpha$ energies reported by House[23] with the Hartree-Fock atomic model. These calculations[23] involve no approximations to the exchange contribution. This is in contrast to our work wherein the exchange approximation[15] of Herman, Van Dyke, and Ortenburger has been used. In all cases, where the two theoretical calculations overlap, there is an excellent agreement, as it is evident from Table X.

TABLE X. Comparison of theoretical $K\alpha$ adjusted transition energies (in eV) obtained in this work (HFS) and those of House (HF) for various defect configurations of argon $[1s^1, 2p^m, 3s^2, 3p^6]$.

m	Present work	House
0	2971	2970
1	2989	2990
2	3000	3000
3	3032	3032
4	3055	3056
5	3080	3080

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[1]F. W. Saris, in *Proceedings of the Seventh International Conference on the Physics of Electronic and Atomic Collisions, Amsterdam, 1971,* edited by L. M. Branscomb *et al.* (North-Holland, Amsterdam, 1972), p. 181. This paper contains an excellent review of the subject and references to work as of 1971 are given.

[2]See invited papers by W. Brandt, P. Richard, T. M. Kavanagh, D. J. Nagel, and F. W. Saris, U.S. Atomic Energy Commission Report No. CONF-720404, 1973 (unpublished). There are also many contributed papers in this report.

[3]P. Richard, U.S. Atomic Energy Commission Report No. CONF-720669, 1973 (unpublished).

[4]W. Brandt, in *Atomic Physics 3,* edited by S. S. Smith, G. K. Walters, and L. M. Volsky (Plenum, New York, 1973), p. 155.

[5]J. D. Garcia, R. J. Fortner and T. M. Kavanagh, Rev. Mod. Phys. 45, 111 (1973).

[6]Q. C. Kessel and B. Fastrup, *Case Studies in Atomic Physics 3,* (North-Holland, Amsterdam, 1973). This excellent review contains extensive references to the experimental work.

[7]J. A. Bearden and A. F. Burr, Rev. Mod. Phys. 31, 1 (1967).

[8]M. E. Rudd, in *Proceedings of the Seventh International Conference on the Physics of Electronic and Atomic Collisions,* edited by L. M. Branscomb *et al.* (North-Holland, Amsterdam, 1972), p. 107; also see M. E. Rudd in Ref. 2.

[9]D. Burch, W. B. Ingalls, J. S. Risley, and R. H. Heffner, Phys. Rev. Lett. 29, 1719 (1972).

[10]C. P. Bhalla, N. O. Folland, and M. A. Hein, Phys. Rev. A 2, 649 (1973); C. P. Bhalla and M. Hein, Phys. Rev. Lett. 30, 39 (1973).

[11]See C. P. Bhalla and D. L. Walters, in Ref. 2.

[12]F. P. Larkins, J. Phys. B 9, L29 (1971); R. J. Fortner, R. C. Der, T. M. Kavanagh, and J. D. Garcia, J. Phys. B 5, L73 (1972). The effects on fluorescence yields were calculated by an approximate (statistical scaling) procedure.

[13]J. R. Macdonald, L. M. Winters, M. D. Brown, L. D. Ellsworth, T. Chiao, and E. W. Pettus, Phys. Rev. Lett. 30, 251 (1973).

[14]D. L. Walters and C. P. Bhalla, Phys. Rev. A 3, 1919 (1971).

[15]F. Herman and K. Schwarz, *Computational Solid State Physics* (Plenum, New York, 1972).

[16]J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill, New York, 1960), Vols. I and II.

[17]W. Mehlhorn and W. N. Asaad, Z. Phys. 191, 231 (1966).

[18]C. P. Bhalla, Phys. Lett. A 44, 103 (1973).

[19]L. E. Bailey and U. B. Swedlund, Phys. Rev. 158, 6 (1967).

[20]J. Pahor, A. Moljk, A. Kodre, and T. Rupnik (private communication to W. Bambynek Ref. 2).

[21]T. Watanabe, Phys. Rev. 139, A1747 (1965).

[22]R. L. Chase, H. P. Kelley, and H. S. Köhler, Phys. Rev. A 3, 1550 (1971). The correlation effects are discussed for neon in this paper.

[23]L. H. House, Astrophys. J. Suppl. Ser. 18, 21 (1969).