LIFETIME AND TRANSITION PROBABILITIES OF np^4 - (n + 1) p STATES OF Ne II, A II AND Kr II

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ABSTRACT

Life time as well as transition probabilities of the first p-excited states of neon$^+$, argon$^+$, and krypton$^+$ have been calculated.

LIFETIME AND TRANSITION PROBABILITIES OF np^4 - (n + 1) p STATES OF NeII, AII AND KrII

Lifetime and transition probabilities of some of the first excited "p" states of neon II, argon II and krypton II[1,2,3] for the configuration of np^4 - (n + 1)p, have been calculated. This information is needed to determine the possible efficiencies of current and proposed laser systems and to aid in the identification of the energy levels involved.

The exact mixed wave functions $\Psi_i(E_i)$ corresponding to the experimentally found energy levels E_i can be expressed in terms of purely LS coupled wave functions ϕ_i, with ϕ_i corresponding to the LS coupled states of the form $|p^4 \overline{L}\overline{S};\ \ell_{ex} s;\ L_i S_i J_i M_i>$, i.e.,

$$(1) \qquad \Psi_i(E_i) = \sum_j a_{ij}\, \phi_j .$$

where $\overline{L}\,\overline{S}$ are the orbital and spin angular momentum of the p^4 core electrons while L_j S_j are the total orbital and spin angular moments. $\underline{J} = \underline{L} + \underline{S}$ and M is the projection of J on the z-axis. ℓ_{ex} is the excited p electron with its spin s. The functions $\Psi_i(E_i)$ were found by treating the radial integrals as adjustable parameters so as to obtain the best fit with the experimentally found energy levels. This was done by choosing arbitrarily close test values for the parameters $[^1D]$, $[^3P]$ core energy states, F_2, G_0, G_2 direct and exchange integrals and ζ_{np} and $\zeta_{\ell\, ex}$ corresponding to the spin orbit interaction terms of the np^4 core and (n + 1)p excited electron.

With the inititially chosen test parameters $[^1D]_0$, $[^3P]_0$ . . . etc. and the Hamiltonian

$$(2) \qquad H = -\sum \frac{h^2}{2m}\nabla^2 - \sum_i \frac{e^2}{r_i} + \sum_{i>j} \frac{e^2}{r_{ij}} + \sum_i \xi(r)\, \ell_i, S_i ,$$

the matrix $[H_0]$ was constructed having elements $[H_0]_{ij}$ where

$$(3) \qquad [H_0]_{ij} = <\phi_i\, |H'|\phi_j>_0$$

In Eq. (3), the subscript naught designated that in the calculation of the elements $[H_0]_{ij}$ the first set of test parameters are used.

A matrix $[M_0]$ is found such that,

(4) $$[M_0]^{-1}\,[H_0]\,[M_0] = [D_0]$$

with $[D_0]$ being a diagonal matrix. If the choice of the parameters were appropriate $[D_0]$ will differ little from the experimentally found energy levels. If not, a new matrix equation is constructed having the form,

(5) $$[M_0^{-1}]\,[H]\,[M_0] = [E]$$

where $[E]$ is again a diagonal matrix having for its diagonal elements the experimental energy levels E_i, $[M_0]$ is the matrix which was used to diagonalize $[H_0]$, and $[H]$ is the Hamiltonian matrix with its elements expressed in terms of the radial parameters[4], i.e.,

(6) $$[H]_{ij} = \langle \phi_i | H | \phi_j \rangle = a_{ij}[^1D] + b_{ij}[^3P] + C_{ij}F_2 + d_{ij}G_0 + \ldots$$

Multiplying out $[M_0]^{-1}\,[H]\,[M]$ and equating it to $[E]$ one obtains, taking the diagonal terms only, a linear set of nineteen simultaneous equations in terms of the seven parameters $[^1D]$, $[^3P]$, F_2, G_0, G_2, ζ_{np} and $\zeta_{\ell ex}$. Solving the equations and least-square-fitting the results, we obtain a new set of parameters $[^1D]_1$ $[^3P]_1$ . . . etc. These parameters are now used to obtain the matrix $[H_1]$, with matrix elements $[H_1]_{ij}$ in which the set of the newly found values of the radial parameters have been substituted, i. e.,

$$[H_1]_{ij} = a_{ij}[^1D]_1 + b_{ij}[^3P]_1 + C_{ij}(F_2)_1 + d_{ij}(G_0)_1 + \ldots$$

Once again we find a matrix $[M_1]$ which diagonalizes $[H_1]$ giving the diagonal matrix $[D_1]$ i. e.,

(7) $$[M_1]^{-1}[H_1]\,[M_1] = [D_1]$$

If again the elements $[D_1]$ would differ much from the experimentally found energy levels E_i the process is repeated by solving the simultaneous equation obtained from the matrix equation,

(8) $$[M_1]^{-1}[H]\,[M_1] = [E]$$

where again the elements of the matrix H are given by Eq. 6. A new set

of parameters $[^1D]_2$, $[^3P]_2$ . . . etc., are found. The process is repeated until the parameters $[^1D]_n$ $[^3P]_n$ . . . etc. converge and the matrix equation $[M_n]^{-1}[H_n][M_n] = [D_n] \simeq [E]$.

If the initial set of test parameters are close to the actual values, the process would terminate after a few cycles, and the parameters would converge to fixed values. If not, the convergence is not easily attained. In the above calculations the states arising from the ^1S core were not taken into consideration. However, their contribution to the states $^2P_{\frac{1}{2}}$, $^2P_{\frac{3}{2}}$, $^2P'_{\frac{1}{2}}$ and $^2P'_{\frac{3}{2}}$ can be calculated by perturbation theory. The shift in energy would be $\Delta E = -\frac{H^2_{ij}}{E_i - E_j}$. Table one gives the values of the parameters ^1D, ^3P, F_2, G_0, . . . etc. using Hartree Fock[6] wavefunctions and also the values which were obtained by the above fitting techniques. The two sets of values are more or less very close. Table II gives the theoretical and experimentally found energy levels and the mixing coefficients a_{ij}. Table III gives the transition probabilities for the states arising from the $np^4 - (n+1)p$ configuration of neon, argon, and krypton to the lower states of $np^4 - (n+1)s$ configuration. Finally Table IV gives the lifetimes of some of the higher states of interest.

TABLE I

	Ne		Ar		Kr	
	Calculated Cm^{-1}	Fitting Cm^{-1}	Calculate Cm^{-1}	Fitting Cm^{-1}	Calculate Cm^{-1}	Fitting Cm^{-1}
$F_2(p_{core}-p_{ex})$	422.	433	424	365	415	397
$G_0(p_{core}-p_{ex})$	4166.	2452	2614	1752	2176	1802
$G_2(p_{core}-p_{ex})$	160.	167	122.5	86	111	171
$\zeta_{p_{core}}$	1104	790	1198	1075	2593	2929
ζ'_{p-ex}	63	-33	107	187	251	570
$[^3P]$	—	252853	—	159918	—	140669
$[^1D]$	—	278205	—	173491	—	152937
$F_2(p_{core}-p_{core})$	4757	4225	2827	2262	2488	2044

TABLE II-a

Experimental and theoretical energy levels of Ne II taken from Moore[7], tables of atomic energy levels and this calculation. The mixing coefficients a_{ij} are those given in Eq. (1).

Ne II States	E_{exp} Cm^{-1}	E_{theor} Cm^{-1}	^4D	^4P	^4S	^2D	^2P	^2S	$^2P'$	$^2D'$	$^2F'$
$^4D_{\frac{7}{2}}$	249110.8	248652.5	0.99976								0.21956
$^2F_{\frac{7}{2}}$	274411.3	274228.2	0.21956								-0.99976
$^4P_{\frac{5}{2}}$	246194.8	246314.4	0.10198	0.99415		0.03104				0.01720	0.00042
$^4D_{\frac{5}{2}}$	249448.0	249217.8	0.98594	-0.09696		-0.13543				0.00271	0.01307
$^2D_{\frac{5}{2}}$	251013.3	251158.4	-0.13166	0.04497		-0.98950				-0.03385	0.01966
$^2F'_{\frac{5}{2}}$	274366.9	274229.0	0.01038	0.00010		-0.02106				-0.00511	-0.99971
$^2D'_{\frac{5}{2}}$	277346.1	277407.1	-0.00883	-0.01525		-0.03379				0.99926	-0.00449
$^4P_{\frac{3}{2}}$	246417.4	246617.2	0.09174	0.99253	0.06423	0.00625	-0.04273		0.02033	0.00773	
$^4D_{\frac{3}{2}}$	249697.7	249553.3	-0.99010	0.09102	0.01201	0.09658	0.04061		-0.00908	-0.00448	
$^2D_{\frac{3}{2}}$	251524.7	251713.3	0.10309	-0.00654	0.01349	0.97118	0.20859		-0.04265	0.02494	
$^2P_{\frac{3}{2}}$	254167.0	253922.7	0.02353	0.05218	-0.11802	-0.21197	0.94040		-0.23011	-0.02373	
$^4S_{\frac{3}{2}}$	252956.0	253072.9	-0.00743	0.05933	-0.99058	0.04020	-0.11599		0.00933	0.00375	
$^2P'_{\frac{3}{2}}$	276278.6	276396.3	-0.00025	-0.00729	-0.01897	-0.00409	0.23087		0.96654	-0.10978	
$^2D'_{\frac{3}{2}}$	277327.6	277411.8	0.00721	0.00697	0.00196	0.02967	-0.04370		-0.10217	-0.99331	
$^4P_{\frac{1}{2}}$	246599.9	246861.7	0.05282	0.99729			-0.02210	-0.04454	-0.01249		
$^4D_{\frac{1}{2}}$	249841.8	249749.7	0.99720	-0.05422			-0.04947	-0.00301	0.01401		
$^2P_{\frac{1}{2}}$	254294.0	254197.1	0.04669	0.00333			0.89586	-0.37847	-0.22804		
$^2S_{\frac{1}{2}}$	252800.8	252885.9	0.02493	0.04932			0.36197	0.92444	-0.10641		
$^2P'_{\frac{1}{2}}$	276514.1	276598.9	0.00137	0.00587			-0.25193	-0.01308	-0.96764		

TABLE II-b

Experimental and theoretical energy levels of Ar II taken from Minnhagen[8] and from this calculation. The mixing coefficients of a_{ij} are those given in Eq. (1).

Ar II States	E_{exp} Cm^{-1}	E_{theor} Cm^{-1}	^4D	^4P	^4S	^2D	^2P	^2S	$^2P'$	$^2D'$	$^2F'$
$^4D_{\frac{7}{2}}$	157233.93	157176.6	0.99839								0.05680
$^2F'_{\frac{7}{2}}$	170530.31	170582.7	0.05680								-0.99839
$^4P_{\frac{5}{2}}$	155043.07	155128.2	0.18291	0.98216		0.02312				0.03949	0.00299
$^4D_{\frac{5}{2}}$	157673.32	157556.9	0.86726	-0.15036		-0.47202				-0.00525	0.04919
$^2D_{\frac{5}{2}}$	158730.21	158710.3	-0.46181	0.10820		-0.87867				-0.04014	0.03689
$^2F'_{\frac{5}{2}}$	170400.94	170364.6	-0.02553	0.00160		0.05688				-0.03043	0.99759
$^2D'_{\frac{5}{2}}$	173393.38	173432.7	0.02203	0.03525		0.03701				-0.99794	-0.03204
$^4P_{\frac{3}{2}}$	155351.03	155383.5	0.16724	0.96996	0.11854	-0.1561	-0.11366		0.05959	0.02102	
$^4D_{\frac{3}{2}}$	158167.71	158007.6	0.91426	-0.18070	-0.04193	-0.31306	-0.17205		0.04422	0.01261	
$^2D_{\frac{3}{2}}$	159393.31	159244.3	0.36791	0.00919	0.00421	0.80472	0.44766		-0.12847	0.00763	
$^2P_{\frac{3}{2}}$	160239.35	160354.7	0.01598	0.09361	0.06872	-0.50253	0.81016		-0.27314	-0.05244	
$^4S_{\frac{3}{2}}$	161048.64	161012.7	0.01607	-0.13135	0.98834	0.01899	-0.03572		0.06355	0.00052	
$^2P'_{\frac{3}{2}}$	172213.80	172213.8	-0.00095	0.01493	0.05133	0.0218	-0.30918		-0.94747	0.05873	
$^2D'_{\frac{3}{2}}$	173347.83	173349.9	0.01702	0.01413	0.00192	0.02951	-0.06202		-0.04059	-0.99657	
$^4P_{\frac{1}{2}}$	155708.02	155781.9	0.09789	0.99105			-0.06195	-0.05442	0.03795		
$^4D_{\frac{1}{2}}$	158428.03	158331.0	-0.98840	0.10630			0.09918	0.01678	-0.04050		
$^2P_{\frac{1}{2}}$	159706.46	159869.7	-0.11005	-0.07824			-0.80018	-0.49034	0.31788		
$^2S_{\frac{1}{2}}$	161089.31	161306.5	-0.03676	0.01627			-0.46980	0.86912	0.14933		
$^2P'_{\frac{1}{2}}$	172816.21	172726.4	-0.00350	-0.01162			0.35401	0.03085	0.93465		

TABLE II-c

Experimental and theoretical energy levels of Kr II taken from Moore[7], tables of atomic energy levels and this calculation. The mixing coefficients a_{ij} are those given in Eq. (1).

	E_{exp} Cm^{-1}	E_{theor} Cm^{-1}	^4D	^4P	^4S	^2D	^2P	^2S	$^2P'$	$^2D'$	$^2F'$
$^4D_{\frac{7}{2}}$	135783.18	136046.4	0.98818								0.15329
$^2F'_{\frac{7}{2}}$	149704.55	149720.5	0.15329								-0.98818
$^4P_{\frac{5}{2}}$	133925.65	133855.3	0.35157	0.92956		-0.00191				0.10898	0.02069
$^4D_{\frac{5}{2}}$	136071.00	136913.7	0.69899	-0.26376		-0.64380				-0.04663	0.15873
$^2D_{\frac{5}{2}}$	140118.99	139794.1	-0.61630	0.24015		-0.73946				-0.08975	0.08744
$^2F'_{\frac{5}{2}}$	149173.42	149096.5	-0.06087	0.00875		0.17647				-0.05814	0.98066
$^2D'_{\frac{5}{2}}$	152316.26	152377.9	0.06542	0.09275		0.08704				-0.98717	-0.07092
$^4P_{\frac{3}{2}}$	134288.44	134032.7	0.29227	0.86841	0.24557	-0.06918	-0.25507		0.15819	0.07257	
$^4D_{\frac{3}{2}}$	138381.35	138171.7	0.70387	-0.33387	-0.23513	-0.42128	-0.39352		0.05687	-0.04741	
$^2D_{\frac{3}{2}}$	141995.68	142424.3	0.15404	-0.21173	0.13765	0.80116	-0.43082		0.25429	0.14271	
$^2P_{\frac{3}{2}}$	140137.15	140117.4	0.62449	0.04557	0.03686	0.32338	0.67428		-0.21368	-0.04111	
$^4S_{\frac{3}{2}}$	141722.72	141508.3	0.05458	-0.29324	0.91550	-0.23728	0.06388		0.10487	-0.03901	
$^2P'_{\frac{3}{2}}$	150203.48	150519.5	-0.00713	0.02327	0.16055	0.07215	-0.32003		-0.91809	0.15208	
$^2D'_{\frac{3}{2}}$	152191.86	152172.6	0.04903	0.03093	0.01389	0.09900	-0.18255		-0.08685	-0.97251	
$^4P_{\frac{1}{2}}$	135783.03	135638.4	0.20533	0.92476			-0.20833	-0.19012	0.15203		
$^4D_{\frac{1}{2}}$	140163.25	139549.3	-0.85103	0.01265			-0.28601	-0.40360	0.17577		
$^2P_{\frac{1}{2}}$	139103.36	139042.2	-0.47019	0.37937			0.56136	0.46584	-0.32072		
$^4S_{\frac{1}{2}}$	142363.55	142592.5	-0.11170	0.00795			-0.59032	0.76087	0.24507		
$^2P'_{\frac{1}{2}}$	152240.97	152094.4	-0.00571	-0.02610			0.45955	0.07095	0.88491		

TABLE III

Transition probabilities between 3p-3s levels of Ne II, 4p-4s levels of Ar II and 5p-5s levels of Kr II, each with a $p^4\,[^3P]$ core. A in sec^{-1}.

	Neon II		Argon II		Krypton II	
	Pure L's	Mixed	Pure L's	Mixed	Pure L's	Mixed
$^4D_{\frac{7}{2}} - {}^4P_{\frac{5}{2}}$	197.81×10^6	197.71×10^6	146.53×10^6	146.06×10^6	168.15×10^6	164×10^6
$^2D_{\frac{5}{2}} - {}^4P_{\frac{5}{2}}$	0	0.28	0	4.67	0	5.28
$- {}^4P_{\frac{3}{2}}$	0	4.12	0	31.65	0	91.27
$- {}^2P_{\frac{3}{2}}$	143.30	140.31	103.65	80.03	140.97	77.08
$^4D_{\frac{5}{2}} - {}^4P_{\frac{5}{2}}$	61.37	43.08	46.53	18.91	52.37	4.59
$^4P_{\frac{3}{2}}$	135.98	149.75	97.25	90.69	89.85	68.27
$^2P_{\frac{3}{2}}$	0	2.20	0	19.70	0	31.39
$^4P_{\frac{5}{2}} - {}^4P_{\frac{5}{2}}$	101.86	114.65	79.28	96.24	91.38	122.90
$^4P_{\frac{3}{2}}$	41.20	28.96	30.06	14.84	27.86	4.29
$^4S_{\frac{3}{2}}$ $^4P_{\frac{5}{2}}$	142.05	124.62	116.11	87.65	167.69	71.85
$^4P_{\frac{3}{2}}$	90.42	93.83	70.32	77.64	87.52	93.20
$^4P_{\frac{1}{2}}$	44.00	52.87	33.11	49.39	32.51	69.82
$^2P_{\frac{3}{2}}$	0	1.41	0	0.088	0	0.26
$^2P_{\frac{1}{2}}$	0	1.17	0	0.13	0	7.28
$^2P_{\frac{3}{2}}$ $^4P_{\frac{5}{2}}$	0	0.59	0	2.80	0	10.91
$^4P_{\frac{3}{2}}$	0	3.29	0	0.0073	0	44.51
$^4P_{\frac{1}{2}}$	0	1.31	0	0.088	0	24.04
$^2P_{\frac{3}{2}}$	166.49	119.05	106.91	36.64	117.77	78.98
$^2P_{\frac{1}{2}}$	31.30	62.62	18.56	69.40	16.23	0.039
$^2D_{\frac{3}{2}}$ $^4P_{\frac{5}{2}}$	0	0.20	0	1.60	0	0.036
$^4P_{\frac{3}{2}}$	0	1.00	0	12.59	0	0.53
$^4P_{\frac{1}{2}}$	0	1.35	0	8.83	0	17.24
$^2P_{\frac{3}{2}}$	25.27	52.23	19.01	61.98	30.15	0.74
$^2P_{\frac{1}{2}}$	118.08	91.00	82.01	29.97	107.19	105.87

		Neon II con't.		Argon II con't.		Krypton II con't.	
		Pure L's	Mixed	Pure L's	Mixed	Pure L's	Mixed
$^4D_{\frac{3}{2}}$	$^4P_{\frac{5}{2}}$	10.48×10^6	4.97×10^6	8.26×10^6	0.47×10^6	11.60×10^6	12.58×10^6
	$^4P_{\frac{3}{2}}$	106.23	96.59	79.06	58.08	93.66	48.93
	$^4P_{\frac{1}{2}}$	80.54	93.00	57.72	65.89	51.96	41.17
	$^2P_{\frac{3}{2}}$	0	0.72	0	7.74	0	30.95
	$^2P_{\frac{1}{2}}$	0	0.58	0	3.79	0	3.66
$^4P_{\frac{3}{2}}$	$^4P_{\frac{5}{2}}$	67.11	79.86	51.03	67.56	61.83	92.73
	$^4P_{\frac{3}{2}}$	18.77	21.67	13.38	16.69	13.11	14.86
	$^4P_{\frac{1}{2}}$	56.72	41.97	38.69	20.49	26.90	4.76
	$^2P_{\frac{3}{2}}$	0	0.11	0	0.73	0	3.75
	$^2P_{\frac{1}{2}}$	0	0.040	0	0.052	0	0.055
$^2S_{\frac{1}{2}}$	$^4P_{\frac{3}{2}}$	0	0.82	0	0.0000053	0	0.41
	$^4P_{\frac{1}{2}}$	0	0.0018	0	0.32	0	2.34
	$^2P_{\frac{3}{2}}$	115.86	161.43	95.83	27.63	126.35	14.90
	$^2P_{\frac{1}{2}}$	54.30	9.24	41.81	98.32	45.17	115.01
$^4D_{\frac{1}{2}}$	$^4P_{\frac{3}{2}}$	33.68	25.84	25.55	14.40	36.51	24.72
	$^4P_{\frac{1}{2}}$	163.34	170.51	119.48	128.23	133.01	97.63
	$^2P_{\frac{3}{2}}$	0	0.12	0	0.50	0	34.71
	$^2P_{\frac{1}{2}}$	0	0.17	0	0.43	0	0.000026
$^4P_{\frac{1}{2}}$	$^4P_{\frac{3}{2}}$	119.75	124.82	88.10	94.35	102.62	106.05
	$^4P_{\frac{1}{2}}$	23.162	17.90	16.33	9.74	13.92	3.02
	$^2P_{\frac{3}{2}}$	0	0.20	0	0.41	0	5.47
	$^2P_{\frac{1}{2}}$	0	0.0045	0	0.020	0	0.16

TABLE IV

Lifetimes of some of the 3p of Ne II, 4p of A II and 5p of Kr II (in nanoseconds)

	Ne II	A II	Kr II
$^4D_{\frac{7}{2}}$	5.0579	6.8457	6.0841
$^4D_{\frac{5}{2}}$	5.1276	7.7325	9.5710
$^2D_{\frac{5}{2}}$	6.9104	8.5926	5.7454
$^4P_{\frac{5}{2}}$	6.9598	8.9995	7.8594
$^4D_{\frac{3}{2}}$	5.1102	7.3537	7.2848
$^2D_{\frac{3}{2}}$	6.8593	8.6801	7.8240
$^4P_{\frac{3}{2}}$	6.9615	9.4748	8.6004
$^2P_{\frac{3}{2}}$	5.3463	9.0649	6.2623
$^4S_{\frac{3}{2}}$	3.6508	4.6504	4.1172
$^4D_{\frac{1}{2}}$	5.0853	6.9650	6.3331
$^4P_{\frac{1}{2}}$	6.9967	9.5673	8.7047
$^2S_{\frac{1}{2}}$	5.8307	7.8869	7.3880
$^2P_{\frac{1}{2}}$	5.5149	9.2892	8.5162
$^2F'_{\frac{7}{2}}$	6.1745	8.0360	6.3348
$^2F'_{\frac{5}{2}}$	6.2084	7.9657	6.7005
$^2D'_{\frac{5}{2}}$	4.5647	5.5537	4.6621
$^2D'_{\frac{3}{2}}$	4.5505	5.4526	4.5695
$^2P'_{\frac{3}{2}}$	4.1451	5.3876	5.0771
$^2P'_{\frac{1}{2}}$	3.9419	4.7836	3.7494

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