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LITHIUMLIKE-IONS (Al^{10+} TO Ti^{19+}) CALCULATED DATA FOR X-UV LASERS

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Résumé. Dans le cadre des recherches sur les lasers à rayons X utilisant la recombinaison d'ions héliumoides en ions lithiunoides (par captures d'électrons libres) au sein d'un plasma chaud qui se détend en se refroidissant, nous présentons un ensemble de données spectroscopiques nécessaires pour mettre en œuvre une modélisation des populations des états excités. Des estimations de gain de rayonnement pour des transitions 3-4, 3-5 et 4-5 d'ions lithiunoides, selon les conditions de température et de densité du plasma, sont aussi présentées.

Abstract. Within the framework of X-ray laser research using the recombination of heliumlike ions with free electrons to produce lithiumlike ions in expanding and cooling hot plasmas, we present a set of spectroscopic data required to achieve a modelling of the excited-states populations. Estimates of radiation gain for 3-4, 3-5 and 4-5 transitions of lithiumlike ions, according to the plasma temperature- and density-conditions, are also presented.

1-INTRODUCTION:

During the cooling phase of a laser-produced plasma, the recombination of He-like ions with free electrons producing Li-like ions is mainly achieved by two ways: the radiative recombination to the low-lying levels, essentially those of the $1s^2 2s$ and $1s^2 2p$ configurations, and the (three-body) collisional recombination to the highly excited $1s^2 n_l$ Rydberg levels. At the same time, radiative and collisionally-induced transitions between all the levels occur. In this complex process, transient population inversions appear between $n=3$, $n=4$, and $n=5$ levels of Li-like ions. Both observed and predicted results have been reported (see for example ref./1/ and references in it). The wavelengths of the corresponding transitions, such as 3d-4f, 3d-5f, or 4f-5g, are situated in the X-UV range for the elements considered in this work.

The story of the population densities of the different ionic levels, in the plasma, can be estimated using a collisional-radiative model /2/ coupled with a simulation of the plasma hydrodynamics /3/. A lot of atomic data are required for this: wavelengths, radiative transitions probabilities, collisional rates, ionisation and recombination coefficients.

In this work, we present the most recent results that we have obtained in this way. In addition, we compare the evolution through the isoelectronic series with hydrogenic scaling laws. Actually, apart from the autoionising levels which are not concerned here, the lithiumlike states present some features which correspond to hydrogenic systems but two principal differences occur: the levels of a same configuration are separated not only by the relativistic interactions (mainly spin-orbit) but also by the Coulomb interactions between the electrons, and the n principal quantum number sequence

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begins at $n = 2$, the corresponding "ground" level being rendered inaccessible by the presence of the closed K shell.

II-ATOMIC DATA:

Energies and wavefunctions of atomic (ionic) states are calculated by a direct SCF method of numerical multiconfigurational Hartree-Fock type including the spin-orbit term of the Pauli approximation, allowing a direct calculation in the intermediate coupling scheme /4/. For the ions studied in this work, as it has been shown in ref. /1/ for the Cu^{26+} ion, the electric-dipole transitions are sufficiently dominant above other transition types as long as processes involving K shell vacancies are not considered. So, non electric-dipole transitions between Li-like levels are not considered hereafter.

The line strength S_{ij} of a transition is given by the square of the reduced matrix-element $\langle i||er||j \rangle$ easily obtained from the wavefunctions. The absorption oscillator strength f_{ji} is given by the relation

$$f_{ji} = (2/3)h\nu S_{ij}/g_j$$

where $h\nu$ and S_{ij} are expressed in atomic units; $h\nu$ is equal to $E_i - E_j$, the energy difference between the upper level i and the lower level j , and g_j is the statistical weight of the level j . The probability of spontaneous emission A_{ij} is

$$A_{ij} = (S_{ij}/g_i)64\pi^4/(3h\lambda^3)$$

λ being the wavelength of the transition. If S_{ij} is expressed in atomic unit, λ in \AA , and A_{ij} in s^{-1} , this becomes

$$A_{ij} = 2.026 \times 10^{18} S_{ij} / (g_i \lambda^3)$$

The collisional rates (excitations and de-excitations) are calculated from the f_{ji} 's by the Van Regemorter formula /5/. The ionisation and recombination coefficients are given by the formulae of Seaton /6/.

Table I shows wavelengths and transition probabilities for radiative spontaneous emission in the X-UV range from $n = 5$ to $n = 3$, $n = 4$ to $n = 3$, and $n = 5$ to $n = 4$ between the $1s^2n_l$ levels of the Cl^{14+} , K^{16+} , Ca^{17+} and Ti^{19+} ions. Analogous data for Al^{10+} and S^{13+} are reported in ref. /2/. In Table I, the wavelengths are presented in the increasing order for K^{16+} . This introduces a few inversions in the lists of the other ions.

In Tables II and III, a limited number of transitions are selected to analyse the dependance of their wavelengths and probabilities with respect to the atomic number Z (i.e. the nuclear charge) and compare it with hydrogenic laws relative to a $(Z-\sigma)$ nuclear charge where σ is a screening parameter:

$$\lambda \text{ (in } \text{\AA}) = 911.267 (1/n^2 - 1/n'^2)^{-1} (Z-\sigma)^{-2}$$

$$A/(Z-\sigma)^4 = \text{constant}$$

III-POPULATION DENSITIES IN PLASMAS:

The population densities of the excited levels of Li-like ions are calculated by the method already used in previous works /1,2/. Plasma density and temperature, and ionic fractions, can be taken as parameters or given by a hydrodynamics simulation code. N_i being the population density of the level i , the reduced population is N_i/g_i and the density of inversion between an upper level u and a lower level l is $\Delta n_{ul} = N_u/g_u - N_l/g_l$. The values of the inversion densities are provided by the collisional-radiative model. In case of positive inversion density, a gain G (>0) of radiation is obtained at the wavelength of the corresponding transition. Expressing the inversion density Δn in cm^{-3} , the product kT (where T is the temperature) in eV, the line strength S in atomic unit, and the

Table I: Calculated wavelengths λ (in Å) and spontaneous emission probabilities A (in $(\text{ns})^{-1}$) for transitions from $1s^2n'l'J'$ to $1s^2n_lJ$ in the Cl^{14+} , K^{16+} , Ca^{17+} and Tl^{19+} ions. The wavelengths are accurate to within a few per thousand.

		Cl^{14+}		K^{16+}		Ca^{17+}		Tl^{19+}	
$n_l J$	$n'l'J'$	λ	A	λ	A	λ	A	λ	A
3s1/2	5p3/2	54.28	78	42.48	131	37.98	165	30.88	252
"	1/2	54.32	79	42.52	133	38.02	168	30.92	257
3p1/2	5d3/2	56.01	145	43.65	239	38.94	300	31.56	458
3/2	5/2	56.20	174	43.83	286	39.13	359	31.74	547
"	3/2	56.21	29	43.84	48	39.14	60	31.75	91
1/2	5s1/2	56.61	20	44.05	31	39.29	39	31.80	58
3/2	"	56.81	40	44.25	64	39.49	80	32.00	120
3d3/2	5f5/2	56.89	216	44.29	356	39.50	448	31.99	682
5/2	7/2	56.94	231	44.34	380	39.55	477	32.04	727
"	5/2	56.95	15	44.35	25	39.56	32	32.05	48
3/2	5p3/2	57.05	.9	44.39	1.4	39.59	1.7	32.05	2.6
"	1/2	57.10	9	44.44	15	39.63	18	32.09	28
5/2	3/2	57.11	8	44.45	13	39.65	16	32.11	24
3s1/2	4p3/2	78.02	142	61.17	236	54.72	298	44.55	457
"	1/2	78.18	144	61.33	241	54.89	305	44.71	470
3p1/2	4d3/2	81.35	295	63.42	486	56.59	612	45.87	933
3/2	5/2	81.72	354	63.78	584	56.95	734	46.23	1119
"	3/2	81.76	59	63.83	98	57.01	123	46.28	187
3d3/2	4f5/2	83.19	653	64.76	1077	57.76	1354	46.77	2065
5/2	7/2	83.29	698	64.86	1152	57.86	1448	46.87	2206
"	5/2	83.32	47	64.88	77	57.88	96	46.90	147
3p1/2	4s1/2	83.87	41	65.14	65	58.04	81	46.92	120
3d3/2	4p3/2	83.87	2	65.21	3.2	58.13	4	47.03	6
5/2	"	84.00	18	65.34	30	58.26	37	47.16	55
3/2	1/2	84.05	21	65.39	34	58.31	42	47.21	64
3p3/2	4s1/2	84.31	84	65.58	134	58.48	166	47.35	249
4s1/2	5p3/2	169.97	33	133.14	55	119.06	70	96.86	107
"	1/2	170.36	34	133.53	57	119.45	72	97.25	111
4p1/2	5d3/2	176.17	61	137.32	101	122.54	127	99.31	194
3/2	5/2	176.88	74	138.02	122	123.23	153	100.00	234
"	3/2	177.00	12	138.14	20	123.36	26	100.13	39
4d3/2	5f5/2	179.72	122	139.90	202	124.78	253	101.06	386
4f5/2	5d5/2	179.97	.1	140.08	.2	124.93	.3	101.17	.4
"	5g7/2	179.95	208	140.09	343	124.95	431	101.20	657
4d5/2	5f7/2	179.91	131	140.09	216	124.97	271	101.25	414
"	5/2	179.97	9	140.16	14	125.03	18	101.31	28
4f7/2	5g9/2	180.04	215	140.17	355	125.03	447	101.29	681
"	5d5/2	180.09	2.5	140.21	4	125.06	5	101.30	8
5/2	3/2	180.10	2.6	140.21	4	125.06	5	101.30	8
7/2	5g7/2	180.07	8	140.21	13	125.08	16	101.32	24
4d3/2	5p3/2	181.34	1.1	140.98	1.7	125.67	2	101.67	3
5/2	"	181.60	10	141.24	16	125.92	20	101.92	30
3/2	1/2	181.78	11	141.42	18	126.11	23	102.10	34
4p1/2	5s1/2	182.17	14	141.43	22	125.99	28	101.82	41
3/2	"	183.05	29	142.30	46	126.86	57	102.67	86

Table II: Z-dependence analysis of wavelengths λ (in Å) of some transitions in Li-like ions. Within four per thousand, listed values coincide with λ (in Å) = 911 (1/n²-1/n'²)⁻¹ (Z- σ)⁻².

nl J	n'l' J'	Al10+	S13+	Cl14+	K16+	Ca17+	Ti19+	σ
3p1/2	5d3/2	103.83	64.26	56.01	43.65	38.94	31.56	1.875
3/2	5/2	104.02	64.45	56.20	43.83	39.13	31.74	1.903
3d3/2	5f5/2	105.81	65.31	56.89	44.29	39.50	31.99	1.990
5/2	7/2	105.86	65.37	56.94	44.34	39.55	32.04	1.999
3p1/2	4d3/2	150.56	93.31	81.35	63.42	56.59	45.87	1.820
3/2	5/2	150.95	93.68	81.72	63.78	56.95	46.23	1.859
3d3/2	4f5/2	154.72	95.50	83.19	64.76	57.76	46.77	1.986
5/2	7/2	154.82	95.60	83.29	64.86	57.86	46.87	1.999
4d3/2	5f5/2	334.23	206.32	179.72	139.90	124.78	101.06	1.986
5/2	7/2	334.42	206.51	179.91	140.09	124.97	101.25	1.997
4f5/2	5g7/2	334.67	206.58	179.95	140.09	124.95	101.20	1.997
7/2	9/2	334.74	206.67	180.04	140.18	125.03	101.29	2.000

Table III: Z-dependence analysis of probabilities A (in (ns)⁻¹) of some transitions in Li-like ions. Within two per cent, listed values coincide with A/(Z- σ)⁴ = constant, where σ is taken from Table II.

nl J	n'l' J'	Al10+	S13+	Cl14+	K16+	Ca17+	Ti19+	A/(Z- σ) ⁴
3p1/2	5d3/2	42	110	145	239	300	458	2.77x10 ⁻³
3/2	5/2	50	132	174	286	359	547	3.35 "
3d3/2	5f5/2	62	164	216	356	448	682	4.26 "
5/2	7/2	66	175	231	380	477	727	4.55 "
3p1/2	4d3/2	85	223	295	486	612	933	5.55 "
3/2	5/2	102	268	354	584	734	1119	6.71 "
3d3/2	4f5/2	189	495	653	1077	1354	2065	1.29x10 ⁻²
5/2	7/2	202	530	698	1152	1448	2206	1.38 "
4d3/2	5f5/2	35	93	122	202	253	386	2.40x10 ⁻³
5/2	7/2	38	99	131	216	271	414	2.58 "
4f5/2	5g7/2	60	158	208	343	431	657	4.10 "
7/2	9/2	62	164	215	355	447	681	4.26 "

gain Θ in cm⁻¹, one obtains

$$\Theta_{ul} = 3.274 \times 10^{-14} S_{ul} M^{1/2} (kT)^{-1/2} \Delta n_{ul}$$

where M is the *atomic weight* (12 for carbon 12). An equivalent expression is

$$\Theta_{ul} = 1.616 \times 10^{-23} g_{ul} A_{ul} \lambda^3 M^{1/2} (kT)^{-1/2} \Delta n_{ul}$$

where A_{ul} is in (ns)⁻¹ and λ in Å (Θ , M, kT and Δn as above). The hydrodynamical simulation coupled with the collisional-radiative model for Al¹⁰⁺ predicts that a plasma produced by a Nd-glass-laser Gaussian pulse of 2.55x10¹² W/cm² (2ns duration) gives a maximum gain of 0.6 cm⁻¹ for the 3d-5f line at 105.8 Å, of 2 cm⁻¹ for the 3d-4f line at 154.8 Å, and of 6.5 cm⁻¹ for the 4f-5g line at 334.7 Å. This can be compared with experimental results of Carillon et al. /7/. They have observed a gain of 0.8 cm⁻¹ for the 3d-5f line and 1.5 cm⁻¹ for the 3d-4f line. However, it must be noted that the calculated maximum gains occur farther from the initial target position, and later after the laser pulse, than observed. This is due to the fact that the simulation does not reproduce faithfully the plasma global recombination (the hydrodynamics code is well suited for hot and dense regions of the plasma but not so well otherwise, and the atomic model must also be improved for low-temperature and-density conditions). If this is not too critical for the aluminium case, it becomes definitely worse for the sulphur. Indeed, a similar work has been undertaken on sulphur. The input laser

intensity has been increased to 5.25×10^{12} W/cm² to account for the higher ionisation potentials, but the results of the complete simulation appear deceiving : all predicted gains fall down dramatically unless the simulation be extended beyond realistic limits of duration and distance from the initial target position. Nevertheless, starting with Al¹⁰⁺ results and considering simple Z-scaling laws leads to predicted values for S¹³⁺ which seem in reasonable agreement with experiment /8/. We are thence now working to improve our models for the next applications.

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