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EXCITATION OF DOUBLY-CHARGED YTTRIUM IONS IN ELECTRON-ATOM COLLISIONS

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***Abstract**: Excitation of a doubly-charged yttrium ion in e–Y collisions has been studied using the method of extended crossing beams. Forty-one YIII excitation cross-sections have been measured at exciting electron energy of 50 eV. Three optical excitation functions (OEFs) have been recorded in the electron energy range of 0…200 eV.*

***Keywords**: inelastic collisions, excitation, cross-sections, yttrium ion, energy levels, spectral lines*

I. Introduction

Excitation with simultaneous double ionization is an elementary process that has so far received little attention both by theoretical and experimental researchers. However, studies of such processes are of much interest not only for fundamental science but for today's practical problems. The threshold energy of excitation with simultaneous double ionization is in tens of electron volts range; the chance for electrons with such energies to occur in regular gas-discharge plasma is hardly probable. However, the recent decades have seen increased use of electron-beam plasma devices that may use primary electrons with velocities ranging from only slightly suprathermal to relativistic. The range of cascade electron velocities is similarly broad. Electron velocities are also large in magnetron sputtering and in plasma chemical reactors. However, only limited information is available on properties of collisions occurring in beam plasma specifically. In particular, as far as inelastic collisions of electrons with metal atoms are concerned, the process of excitation accompanied with double ionization has so far been studied for two subjects only: yttrium [1] and ytterbium [2]. In addition, the work cited in [1] has been performed in suboptimal conditions and its results call for extension and refinement. A doubly-charged yttrium ion is isoelectronic with a rubidium atom. However, in contrast with rubidium atom's ground term of $4s^24p^65s\ ^2S$, the doubly-charged yttrium atom has $4s^24p^64d\ ^2D$ as its ground term while the term $4s^24p^65s\ ^2S$ is by 7467 cm^{-1} above the ground level $4s^24p^64d\ ^2D_{3/2}$. Nevertheless, in all other aspects the energy structure of YIII electron shell is similar to that of alkali metal atoms where all states resulting from excitation of a single valence electron belong to the doublet term system. The most extensive study of YIII spectrum and energy levels is provided in [3], with a total of 113 spectral lines identified and classified within a wavelength range stretching from vacuum UV (λ = 64.3 nm) to near IR (λ = 911.6 nm). 50 energy levels belonging to *ns* (n = 5…9), *np* (n = 5…9), *nd* (n = 4…8), *nf* (n = 4…10), *ng* (n = 5…8), *nh* (n = 6…8) sequences have been located and interpreted. Our work is focused on studying collisions of electrons with yttrium atoms resulting in doubly-charged yttrium ions in excited states as follows:

$$\mathrm{Y} + \mathrm{e} \rightarrow \mathrm{Y}^{++*} + \mathrm{e}' + \mathrm{e}'' + \mathrm{e}''' , \qquad (1)$$

where e and e′ are the incident and scattered electrons, respectively; e″ and e‴ are electrons knocked out yttrium atom as a result of its ionization. Asterisk denote excited particle. The experiment was carried out using the method of extended crossing beams described in detail in several papers [4]–[6]. Therefore, in the present paper, we will only note experiment conditions relevant to the yttrium experiment directly.

II. Main Experimental Conditions

ITM-2 brand of metallic yttrium with total impurities content of 0.18% (mainly comprised by Ta, Mo, Cu, Gd, Tb) was evaporated to produce atomic beam by heating the metal surface with electronic beam to 1870 K. Atom concentration within intersection zone of atomic and electronic beams was 4.3×10^9 cm^{-3}. Electron beam current densities inside the entire range of electron energies of 0…200 eV stood below 1.0 mA/cm^2. The real spectral resolution of the optical system was about 0.1 nm within the short-wavelength part of the spectrum ($\lambda < 600$ nm) but was successfully reduced to 0.05 nm in individual cases. It degraded to 0.2 nm for wavelengths $\lambda > 600$ nm as monochromator diffraction grating had to be replaced (a resolution of about 0.1 nm was still achieved for some lines in this part of the spectrum). Unlike the case in [1], spectral lines emitted by helium atoms were used as reference for scaling absolute cross-section values. For these spectral lines, cross-section values at electron energy of 50 eV have been determined with outstandingly low error in [7]. The ground term of yttrium atom, $4d5s^2\ a^2D$, has a J-splitting ΔE = 530.5 cm^{-1}; for the ground level, $J = 3/2$, and for a higher-lying level, $J = 5/2$.

With evaporation temperature indicated above the concentration ratio is $n(5/2)/n(3/2) = 1.00$; therefore, the effect of Boltzmann exponent is precisely compensated for by the relationship between statistical weights of these levels. Higher-lying excited levels are populated to a negligible extent, as the nearest of these, $5s^25p$ $z^2P^\circ_{1/2}$, is separated from the ground state by a gap greater than 10000 cm^{-1}. Therefore, when process (1) is accomplished to our experimental setup, we only considered two levels of the ground state of yttrium atoms as initial states. Inasmuch that excitation cross-sections of YIII spectral lines are, on average, much smaller than those of YI, relative values of excitation cross-sections of YIII have been measured with a margin of error ranging between 8% and 15%. Absolute excitation cross-section values have been determined with a margin of error within 23…30%.

III. Results and Discussion

The optical emission spectrum resulting from bombardment of yttrium atoms with electrons at the energy of 50 eV has been recorded within a spectral range of 190 to 850 nm. At this energy, YI, YII and YIII spectra are excited simultaneously. Of the 41 YIII excitation cross-sections measured in our work, 9 are related to blends which, with only a single exception, also belong to the YIII spectrum. These blends occur inevitably owing to the available spectral resolution of our equipment, as the splitting of ng^2G and nh^2H terms is quite narrow (0.1 cm^{-1} and less). The results of measurements supplemented with necessary spectroscopic data are summarized in Tables I, II. Table I lists spectral lines for which optical excitation functions have been recorded in the exciting electron energy range of 0…200 eV. This table includes wavelengths λ, transitions, quantum numbers of total electron shell momenta for the lower J_{low} and upper J_{up} levels, the energies of the lower E_{low} and upper E_{up} levels (relative to the YIII ground level), excitation cross-sections at exciting electron energy of 50 eV Q_{50} and in the OEF maximum $Q_{\max}$, and the location of OEF maximum $E(Q_{\max})$. Numbers in the OEF column correspond to curve numbers in Fig. 1. Table II contains similar data on lines for which reliable recording of OEF has proved impossible; the difference with Table I is that the last three columns have been omitted.

Table I Excitation Cross-Sections of Two-Charged Yttrium Ion (with OEFs Recorded)

λ (nm)	Transition	J_{low}–J_{up}	E_{low} (cm^{-1})	E_{up} (cm^{-1})	Q_{50} (10^{-18} cm^2)	$Q_{\max}$ (10^{-18} cm^2)	$E(Q_{\max})$ (eV)	OEF
232.731	$4d^2D$–$5p^2P^\circ$	3/2–3/2	0	42954	1.01	1.65	75	*2*
236.723	$4d^2D$–$5p^2P^\circ$	5/2–3/2	724	42954	4.81	7.87	75	*2*
241.464	$4d^2D$–$5p^2P^\circ$	3/2–1/2	0	41401	3.23	4.25	65	*1*
281.704	$5s^2S$–$5p^2P^\circ$	1/2–3/2	7467	42954	5.93	9.71	75	*2*
294.601	$5s^2S$–$5p^2P^\circ$	1/2–1/2	7467	41401	2.89	3.80	65	*1*
403.960	$4f^2F^\circ$–$5g^2G$	7/2–9/2	101088	125836	} 1.41	2.83	75	*3*
404.011	$4f^2F^\circ$–$5g^2G$	5/2–7/2	101091	125836				

Information on wavelengths, transitions, J values and energy levels has been provided per [3]. It should be noted that [3] indicates a transition $5s^2S_{1/2}$–$5p^2P^\circ_{5/2}$ for λ = 294.601 nm, however the only valid J values for term $5p^2P^\circ$ are 1/2 and 3/2. Based on transition energy, the upper level $5p^2P^\circ_{1/2}$ should be indicated here. It should also be noted that, among above-mentioned blends associated with relatively narrowly split terms ng^2G and nh^2H, there is a close pair of YIII lines, λ = 403.960 and 404.011 nm, that is superimposed spectrally with an YI line, λ = 403.983 nm. Absolute values of excitation cross-sections turned out to be numerically close for these YI and YIII lines, even though their threshold excitation energies differ considerably (by more than 31 eV). This has provided an opportunity for separating YI and YIII graphically, as the above-mentioned YI line participate in branching and shares a common upper level with another line, λ = 412.831 nm, for which an OEF has also been recorded. And besides, a line pair was discussed in paper [1], comprised by an YII line of λ = 241.393 nm

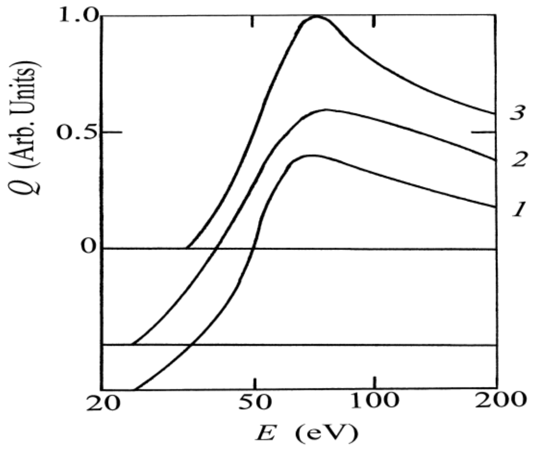
Table II Excitation Cross-Sections of Two-Charged Yttrium Ion (without OEFs Recorded)

λ (nm)	Transition	J_{low}–J_{up}	E_{low} (cm^{-1})	E_{up} (cm^{-1})	Q_{50} (10^{-18} cm^2)
206.058	$5d^2D$–$6f^2F^\circ$	3/2–5/2	88379	136894	0.85
206.898	$5d^2D$–$6f^2F^\circ$	5/2–7/2	88578	136895	1.48
212.798	$5p^2P^\circ$–$5d^2D$	1/2–3/2	41401	88379	3.02
219.116	$5p^2P^\circ$–$5d^2D$	3/2–5/2	42954	88578	4.68
220.076	$5p^2P^\circ$–$5d^2D$	3/2–3/2	42954	88379	0.72
220.603	$5p^2P^\circ$–$6s^2S$	1/2–1/2	41401	86717	0.87
226.141	$4f^2F^\circ$–$7g^2G$	7/2–9/2	101088	145294	} 0.61
226.157	$4f^2F^\circ$–$7g^2G$	5/2–7/2	101091	145294	
228.434	$5p^2P^\circ$–$6s^2S$	3/2–1/2	42954	86717	1.37
231.992	$6p^2P^\circ$–$8d^2D$	3/2–5/2	99943	143035	0.23
271.030	$4f^2F^\circ$–$6g^2G$	7/2–9/2	101088	137973	} 0.92
271.053	$4f^2F^\circ$–$6g^2G$	5/2–7/2	101091	137973	
280.327	$5d^2D$–$7p^2P^\circ$	3/2–1/2	88379	124041	0.17
286.767	$6p^2P^\circ$–$7d^2D$	1/2–3/2	99345	134206	0.22
291.341	$6p^2P^\circ$–$7d^2D$	3/2–5/2	99943	134257	0.39
291.856	$6p^2P^\circ$–$8s^2S$	1/2–1/2	99345	133599	0.25
297.042	$6p^2P^\circ$–$8s^2S$	3/2–1/2	99943	133599	0.53
301.393	$4f^2F^\circ$–$7d^2D$	7/2–5/2	101088	134257	0.28

301.885	$4f\,^2F^\circ–7d\,^2D$	5/2–3/2	101091	134206	0.19
412.161	$5g\,^2G–8h\,^2H^\circ$	7/2,9/2–9/2,11/2	125836	150091	0.32
473.762	$5f\,^2F^\circ–7g\,^2G$	5/2–7/2	123192	145294	0.28
	$5f\,^2F^\circ–7g\,^2G$	7/2–9/2	123193	145294	
510.288	$6p\,^2P^\circ–6d\,^2D$	1/2–3/2	99345	118936	0.37
512.040	$5g\,^2G–7h\,^2H^\circ$	7/2,9/2–9/2,11/2	125836	145360	0.44
523.810	$6p\,^2P^\circ–6d\,^2D$	3/2–5/2	99943	119029	0.54
526.358	$6p\,^2P^\circ–6d\,^2D$	3/2–3/2	99943	118936	0.063
538.364	$6p\,^2P^\circ–7s\,^2S$	1/2–1/2	99345	117915	0.41
556.281	$6p\,^2P^\circ–7s\,^2S$	3/2–1/2	99943	117915	0.73
556.727	$6d\,^2D–6f\,^2F^\circ$	3/2–5/2	118936	136894	0.49
557.224	$4f\,^2F^\circ–6d\,^2D$	7/2–5/2	101088	119029	0.57
559.548	$6d\,^2D–6f\,^2F^\circ$	5/2–7/2	119029	136895	0.78
560.208	$4f\,^2F^\circ–6d\,^2D$	5/2–3/2	101091	118936	0.39
725.458	$5f\,^2F^\circ–6g\,^2G$	5/2–7/2	123192	137973	0.41
	$5f\,^2F^\circ–6g\,^2G$	7/2–9/2	123193	137973	
755.871	$6s\,^2S–6p\,^2P^\circ$	1/2–3/2	86717	99943	0.47
786.453	$5d\,^2D–4f\,^2F^\circ$	3/2–5/2	88379	101091	0.58
791.671	$6s\,^2S–6p\,^2P^\circ$	1/2–1/2	86717	99345	0.47
798.941	$5d\,^2D–4f\,^2F^\circ$	5/2–5/2	88578	101091	0.91
799.143	$5d\,^2D–4f\,^2F^\circ$	5/2–7/2	88578	101088	
817.141	$5g\,^2G–6h\,^2H^\circ$	7/2,9/2–9/2,11/2	125836	138070	0.59

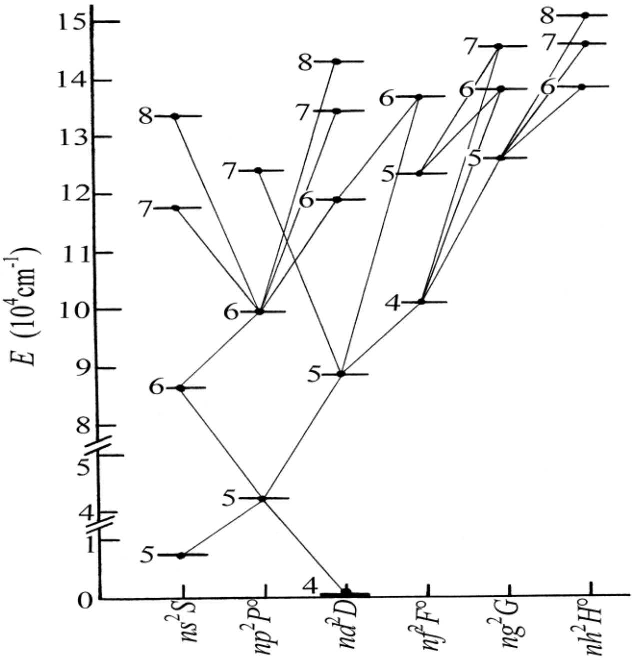
and an YIII line of $\lambda = 241.464$ nm; this pair was not resolved in [1]. Now we have been able to resolve this pair instrumentally by optimizing recording conditions despite atom concentration being just one-third of that in [1] at an equal electron beam current density. Fig. 2 shows a state diagram for a doubly-charged yttrium ion with transitions investigated. *J*-splitting of terms above $\Delta E = 100$ cm^{-1} in the case of YIII only has place for $np\,^2P^\circ$ terms. For known terms $nd\,^2D$ ($n = 4…8$), it stays within 30…100 cm^{-1}, decreasing to 1 cm^{-1} or less for all other terms. Therefore, for the sake of visual simplicity, Fig. 2 shows all terms without *J*-splitting; naturally, any transitions between terms correspond to multiplets, but not to individual lines. All state properties with the exception of principal quantum number are indicated below the horizontal axis; principal quantum number values are indicated next to levels on the chart. All YIII levels known from [3] correspond to excitation of the only valence electron, while the closed shell $4p^6$ is not affected by excitation. Hence, all YIII terms being discussed are displaced doublets.

Figure 1 Optical Excitation Functions of YIII.



Resonant YIII transitions, as well as transitions to the low-lying $5s\,^2S_{1/2}$ metastable level are almost exclusively located within the vacuum UV area of spectrum and are beyond the possibilities of our equipment. The only exception is provided by five primary (series head) transitions in $5s\,^2S_{1/2}–np\,^2P^\circ$ and $4d\,^2D–np\,^2P^\circ$ series located within 232…295 nm wavelength range and corresponding to $n = 5$. Excitation cross-sections measured by us have been the highest for these five transitions, their values being within the range $Q_{50} = (1.0…5.9) \times 10^{-18}$ cm^2. OEFs recorded have been identified for them. Transitions ending in $5p\,^2P^\circ$ levels are, too, almost exclusively located in the vacuum UV range, the exception being head multiplets $5p\,^2P^\circ–6s\,^2S_{1/2}$ and $5p\,^2P^\circ–5d\,^2D$. Notably, $5d\,^2D–5f\,^2F^\circ$ transitions are absent while $5d\,^2D–4f\,^2F^\circ$ and $5d\,^2D–6f\,^2F^\circ$ transitions have been recorded and their excitation cross-sections are far from small: $Q_{50} \sim 10^{-18}$ cm^2. However, intensities for transitions from $5f\,^2F^\circ_{5/2,7/2}$ levels have been estimated in [3] to be much less than intensities for transitions from $4,6f\,^2F^\circ_{5/2,7/2}$ levels. Moreover, in the conditions of our experiment, both transitions from $5f\,^2F^\circ_{5/2,7/2}$ levels have been blended with lines of yttrium atom and singly-charged yttrium ion. In paper [3] also notes irregular behavior of a fine structure in *nf* configurations.

Figure 2 State Diagram of Two-Charged Yttrium Ion with Transition Studied.



As indicated in the previous section, initial states for YIII excitation correspond to two levels of yttrium atom's ground term, $4d5s^2\ ^2D_{3/2,5/2}$; they are populated identically in the conditions of our experiment. When the process (1) is put in place, two outer electrons are removed while the remaining valence electron transfers to either of excited states of a doubly-charged yttrium ion. Considering that the ground state of an yttrium atom is even and removal of any pair of outer electrons ($5s^2$ or $4d5s$) does not alter parity, the excitation of the remaining valence electron into odd states of YIII is more likely. Thus, excitation cross-sections of $np^2F°$, $nf^2F°$, $nh^2H°$ levels should be on average greater than those of ns^2S, nd^2D, ng^2G levels. The data from Table I generally agree with this assumption, however information on YIII transitions in VUV range would be necessary to confirm such a conclusion. The same is true for both transitions from levels with energy $E < 100000$ cm^{-1} and transitions from high-lying levels with $E > 130000$ cm^{-1}. It would be possible to clarify the matter if additional data on transition probabilities or branching factors were available, however the data on YIII is quite scarce at present. Only recently were A_{ki} values reported for ten transitions between low-lying levels of doubly-charged yttrium ion and compared with previous researchers' data in [8]. All these results have been obtained computationally, relying on various theoretical schemes. No experimental data whatsoever is available on transition probabilities or branching factors for YIII. Somewhat earlier, theoretical evaluations of radiative lifetimes of energy levels for ScIII and YIII doubly-charged ions have been presented in [9] but these belong to the lowest-lying metastable levels of the two ions. The circumstances cited made impossible more detailed analysis of our results.

IV. Conclusion

The excitation of YIII spectral lines in the wavelength range of 190 to 850 nm by collisions of electrons with yttrium atoms has been studied in detail. Forty-one excitation cross-sections have been measured at electron energy of 50 eV. Even though our results cover transitions from the majority of known YIII energy levels, a similar experiment in vacuum UV range would still be relevant.

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