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Fully relativistic calculations of cross sections for electron impact ionisation of carbon-like uranium ions

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Abstract

Cross sections for electron impact ionisation from the 2*s* and 2*p* shells of C-like U ions have been calculated by the relativistic distorted wave method at incident energies from threshold up to five times the ionisation energy. Cross sections for transitions between individual *J* states of the target U^{86+} and ionised U^{87+} ion are given. (Int J Mass Spectrom 192 (1999) 23–26) © 1999 Elsevier Science B.V.

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1. Introduction

This article is the latest in a series [1–5] reporting the results of calculations of electron impact ionisation cross sections of highly charged ions using a fully relativistic distorted wave method with exchange [6]. The treatment previously applied to hydrogenic, He-like, Li-like, and Be-like ions is here extended to carbon-like uranium ions. In these ions a new feature arises, an unfilled 2*p* shell. The processes under study are of the form

$$U^{86+}(1s^2 2s^2 2p^2 J) + e^- \rightarrow U^{87+}(1s^2 2s^2 2p J') + e^- + e^-$$

and

$$U^{86+}(1s^2 2s^2 2p^2 J) + e^- \rightarrow U^{87+}(1s^2 2s 2p^2 J'') + e^- + e^-$$

with $J = 0, 1, 2$; $J' = 1/2, 3/2$; $J'' = 1/2, 3/2, 5/2$.

2. Method

The theoretical method, in which the direct and exchange ionisation amplitudes are derived from lowest-order quantum electrodynamic (QED) theory and expressed as multiple partial-wave expansions, has been described by Pindzola et al. [6] and Moores and Pindzola [7].

Fully relativistic wave functions for the U^{86+} and U^{87+} ions were obtained from the multiconfiguration Dirac-Fock code of Grant and co-workers [8]. Only configurations belonging to the $n = 2$ complex were taken into account. For the initial states, just one nonrelativistic configuration $1s^2 2s^2 2p^2$ was included, the $2p^4$ configuration being weakly coupled to it. Similarly, the $2p^3$ configuration was dropped in the final odd parity state. This gives, for the initial state,

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Table 1
States of U^{86+} and U^{87+}

Label	J	Configuration	Mixing coefficient	Energy (10^4 a.u.)
		$1s^2 2s^2+$		
a	0	$2p_{1/2}^2$	1.000 + 00	−1.435 091
		$2p_{3/2}^2$	−7.126 − 03	
b	1	$2p_{1/2}2p_{3/2}$	1.000 + 00	−1.420 244
c	2	$2p_{1/2}2p_{3/2}$	1.000 + 00	−1.420 123
		$2p_{3/2}^2$	5.888 − 03	
d	2	$2p_{1/2}2p_{3/2}$	−5.888 − 03	−1.405 120
		$2p_{3/2}^2$	1.000 + 00	
e	0	$2p_{1/2}^2$	7.126 − 03	−1.404 861
		$2p_{3/2}^2$	1.000 + 00	
		$1s^2 2s^2+$		
f	1/2	$2p_{1/2}$	1.000 + 00	−1.320 589
g	3/2	$2p_{3/2}$	1.000 + 00	−1.305 368
		$1s^2 2s+$		
h	1/2	$2p_{1/2}^2$	9.997 − 01	−1.319 121
		$2p_{1/2}2p_{3/2}$	−2.292 − 02	
		$2p_{3/2}^2$	−7.263 − 02	
i	3/2	$2p_{1/2}2p_{3/2}$	−5.237 − 01	−1.304 343
		$2p_{1/2}2p_{3/2}$	8.518 − 01	
		$2p_{3/2}^2$	1.354 − 02	
j	5/2	$2p_{1/2}2p_{3/2}$	9.999 − 01	−1.304 098
		$2p_{3/2}^2$	1.537 − 02	
k	1/2	$2p_{1/2}^2$	2.303 − 02	−1.303 796
		$2p_{1/2}2p_{3/2}$	9.996 − 01	
		$2p_{3/2}^2$	1.589 − 02	
l	3/2	$2p_{1/2}2p_{3/2}$	8.517 − 01	−1.303 755
		$2p_{1/2}2p_{3/2}$	5.238 − 01	
		$2p_{3/2}^2$	−1.409 − 02	
m	5/2	$2p_{1/2}2p_{3/2}$	−1.537 − 02	−1.289 034
		$2p_{3/2}^2$	9.999 − 01	
n	1/2	$2p_{1/2}^2$	6.896 − 03	−1.288 560
		$2p_{1/2}2p_{3/2}$	−1.606 − 02	
		$2p_{3/2}^2$	9.999 − 01	
o	3/1	$2p_{1/2}2p_{3/2}$	1.909 − 02	−1.288 510
		$2p_{1/2}2p_{3/2}$	−4.156 − 03	
		$2p_{3/2}^2$	9.998 − 01	

three relativistic configurations $2p_{1/2}^2$, $2p_{1/2}2p_{3/2}$, and $2p_{3/2}^2$, and five total angular momentum states with $J = 0,2,2,1,0$, respectively, in order of their binding energy. The final $2s^2 2p$ state has two relativistic configurations $2s^2 2p_{1/2} J = 1/2$ and $2s^2 2p_{3/2} J = 3/2$. The $2s2p^2$ state has three; $2s2p_{1/2}^2$, $2s2p_{1/2}2p_{3/2}$, and $2s2p_{3/2}^2$. These give rise to eight J states, three for $J = 1/2$, three for $J = 3/2$ and two for $J = 5/2$. This information is shown in Table 1, where the states, configurations, mixing coefficients (the eigenvector components) and calculated binding energies in atomic units (1 a.u. = 27.2116 eV) are given.

3. Results and discussion

The calculated cross sections, including the Moeller interaction and exchange ionisation, are tabulated in Tables 2 and 3. Cross sections for combinations of initial and final states not appearing in Tables

Table 2
Cross sections for $2p$-electron ejection from C-like U ions by electron impact; X is the incident energy in units of the ionisation energy of the transition and Q the cross section in units of 10^{-23}cm^2

Transition	a–f		b–f		b–g		c–f		c–g		d–g		e–g	
J, J'	0,1/2		1,1/2		1,3/2		2,1/2		2,3/2		2,3/2		0,3/2	
I.P. (10^3 a.u.)	1.1450		0.9966		1.1488		0.9953		1.1475		0.9975		0.9949	
	X	Q	X	Q	X	Q	X	Q	X	Q	X	Q	X	Q
	1.25	2.51	1.25	1.73	1.25	1.25	1.25	1.74	1.25	1.25	1.25	3.48	1.25	3.52
	1.44	3.48	1.5	2.53	1.44	1.72	1.66	2.80	1.44	1.73	1.5	5.09	1.5	5.18
	1.60	3.97	1.66	2.78	1.60	1.97	1.85	3.00	1.60	1.97	1.66	5.57	1.66	5.60
	2.00	4.56	1.84	2.99	2.00	2.35	2.00	3.11	2.00	2.28	1.84	5.92	1.85	6.02
	2.41	4.78	2.25	3.18	2.40	2.38	2.25	3.21	2.40	2.38	2.50	6.43	2.30	6.45
	2.75	4.84	2.77	3.20	2.75	2.41	2.77	3.21	2.75	2.41	2.76	6.40	2.77	6.44
	3.00	4.81	3.00	3.17	3.00	2.40	3.00	3.18	3.00	2.40	3.00	6.34	3.00	6.37
	4.00	4.66	4.00	3.03	4.00	2.32	4.00	3.04	4.00	2.32	4.00	6.05	4.00	6.10
	5.00	4.43	5.00	2.84	5.00	2.21	5.00	2.85	5.00	2.21	5.00	5.68	5.00	5.71

2 and 3 involve either transitions forbidden by angular selection rules, or transitions only possible because of configuration mixing and for which the cross sections are small (of the order of 10^{-26} cm^2 or less) due to a weakly coupled initial or final configuration.

Calculations including only the Coulomb interaction, not given here, are about 15% lower than those obtained using the Moeller interaction. This result is similar to that obtained [5] for $2s$ ejection in Li-like U and Be-like U, illustrating the lesser importance of this relativistic effect in L-shell ejection compared with K-shell ejection, where it is much larger [5]. In all these calculations, strong destructive interference is found between the exchange and interference terms in the total cross section, both with and without the Moeller interaction.

An experimental verification of these results would be of great interest, but to date none have been reported. The previously published calculations for other ions were in very good agreement with data measured in the electron beam ion trap at Lawrence Livermore National Laboratory [9], and we look forward to similar measurements on C-like U ions in the near future.

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Table 3
Cross sections in units of 10^{-23} cm^2 for $2s$-electron ejection from C-like U ions by electron impact

	a–h	b–k	b–i	b–l	c–i	c–l	c–j	d–m	d–o	e–h
J, J''	0,1/2	1,1/2	1,3/2	1,3/2	2,3/2	2,3/2	2,5/2	2,5/2	2,3/2	0,1/2
I.P.	1.1597	1.1645	1.1590	1.1649	1.1578	1.1637	1.1603	1.1609	1.1661	1.1630
X	X	X	X	X	X	X	X	X	X	X
1.25	1.986	0.659	1.159	1.639	0.099	0.693	1.191	1.189	0.790	1.978
1.5	2.949	0.979	1.721	2.434	0.147	1.029	1.768	1.765	1.172	2.938
2.25	3.875	1.287	2.261	3.201	0.193	1.354	2.323	2.320	1.542	3.863
2.5	3.949	1.310	2.305	3.259	0.197	1.378	2.367	2.364	1.569	3.934
2.75	3.995	1.327	2.331	3.300	0.199	1.395	2.395	2.392	1.589	3.981
3.0	3.985	1.324	2.325	3.294	0.199	1.398	2.389	2.386	1.587	3.974
4.0	3.872	1.287	2.260	3.202	0.193	1.353	2.322	2.319	1.543	3.862
5.0	3.700	1.229	2.159	3.058	0.184	1.293	2.218	2.216	1.473	3.689

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