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Interpretation of the satellite spectrum that follows ionization in the 5s and 5p shells of Xe at low photon energy

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An interpretation of the photoelectron satellite spectrum of Xe at 33-eV photon energy is proposed. On the basis of an extended analysis of the Xe II spectrum it is shown that an interpretation in terms of $\underline{5p}$ satellites can explain the strength of the spectrum relative to the main $\underline{5s}$ line as well as the occurrence of new satellites at low photon energy.

The satellite spectrum of Xe following photoionization in the 5s and 5p shells has been the subject of many recent investigations. In particular, with the development of synchrotron radiation sources it has become possible to study the spectrum as a function of the energy of the incoming photon. At high photon energy (1487 eV) good agreement exists between measurements by Gelius[1] and an interpretation[2,3] based on the assumptions that the satellite spectrum is (a) due to ionization of a 5s electron and (b) caused by final ionic-state configuration interaction.

The situation is different at low photon energies. Final ionic-state configuration interaction has recently been invoked[4] to explain the disagreement between the observed β factor for the main $\underline{5s}$ line[5] and calculations[6] using the relativistic random-phase approximation (RRPA) which does not include this type of interaction but has been very successful in reproducing the experimental data at higher energies. However, later calculations[7] using the relativistic time-dependent local-density approximation (RTDLDA) give good agreement with the observed values of β although final ionic-state configuration interaction is not taken into account.

At first sight the situation for the satellite intensities is similar. At high photon energy, the total strength of the satellites is approximately equal to that of the main line. At 75.5 eV, the total satellite strength has *decreased*[8] whereas at 40.8 eV Süzer and Hush[9] report an *increase* in satellite intensity. Recently, Fahlman, Krause, and Carlson,[10] in a remarkable experiment, were able to record the satellite spectrum at 33 eV. At this photon energy the probability for 5s ionization has a (Cooper) minimum and Fahlman *et al.* established that the satellite spectrum is 7.6 times stronger than the main $\underline{5s}$ line. An interpretation of the spectrum in terms of 5s ionization combined with final ionic-state configuration interaction was attempted by Fahlman *et al.*,[10] but a mechanism for the apparent increase in the satellite intensities has not been established. Fahlman *et al.* note, in particular, the appearance of new satellites at low photon energy which have not been observed at higher energies.

In this Rapid Communication we argue that the major part of the satellite spectrum at 33-eV photon energy is due to ionization in the 5p shell and associated with excitation to $5s^2 5p^4 6p, 7p$ and possibly $4f$ states. These satellites overlap the $\underline{5s}$ satellites but, due to an analysis[2,3] of the Xe II spectrum which is in progress, it is possible to disentangle the $\underline{5s}$ and $\underline{5p}$ contributions in some detail.

The proposed interpretation explains a number of puzzling features in the experimental observations.

(a) It explains the strength of the satellite spectrum which, as mentioned, is 7.6 times stronger than the main $\underline{5s}$ line but only 10% of the intensity of the main $\underline{5p}$ lines. This seems a reasonable figure for the intensity of satellites in the outermost p shell of the rare gases.[11]

(b) It explains the occurrence of new satellites at low photon energy.

(c) It explains why the asymmetry parameters measured by Fahlman *et al.*[10] have values in disagreement with that observed for the main $\underline{5s}$ peak.[5] This result is also peculiar to the low-energy region.

Table I shows the details of our interpretation of the photoelectron spectra recorded by Fahlman *et al.*[10] at 33.0 eV and by Süzer and Hush[9] at 40.8-eV photon energy. The numbering of the peaks in Table I, column 1, is taken from Fahlman *et al.* Column 3 shows the observed intensities measured at the magic angle relative to the main $\underline{5s}$ peak. Reference 10 reports also the strength of the satellites relative to the total intensity of the main $\underline{5s}$ and $\underline{5p}$ peaks. Using this information the strengths relative to the main $\underline{5p}$ lines of the *new* features appearing at 33.0 eV can be estimated by assuming the strength of the $\underline{5s}$ satellite spectrum to be the same at 33.0 and 1487 eV (column 4). Column 6 shows the intensities measured by Süzer and Hush[9] at 90° relative to the main $\underline{5s}$ peak. In this experiment only satellites with energies less than 28.3 eV were accessible. However, the resolution obtained is somewhat better, as shown by a comparison of columns 2 and 5 of Table I.

The last three columns of Table I contain the data relevant to our interpretation, i.e., the energies and labels established in the Xe II analysis[2,3] (in some cases the energy values are predicted values) and, in the last column, our most recent[3] prediction of the $\underline{5s}$ satellite intensities. The calculation for this prediction is similar to that described briefly in Ref. 2 but the new calculation is in better agreement with the satellite intensities observed[1] at 1487 eV. At low photon energy the $\underline{5s}$ intensities might be somewhat different.[12]

A realistic calculation of the $\underline{5p}$ satellite intensities is more difficult. We have estimated that shakeup is insufficient to explain the strength of the satellite spectrum and we expect

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TABLE I. Interpretation of the $\underline{5s}$ and $\underline{5p}$ photoelectron satellite spectrum of Xe at 33.0- and 40.8-eV photon energies.

	Observed spectrum					Present interpretation		
	33.0 eV, Ref. 10			40.8 eV, Ref. 9				
Label[a]	Energy (eV)	Intensity[b]	Intensity[c]	Energy (eV)	Intensity[b]	Energy (eV)	Label[d]	Intensity[b]
(1)	22.63 (5)[e]							
$\underline{5s}$	23.397[f]	100		23.394[f]	100	23.397	$5s5p^6\,^2S_{1/2}$	100
(2)	23.9 (1)	5 (2)		23.93 (2)	2 (1)			
						24.139	$(^3P)5d\,^4D_{1/2}$	0
(3)	24.64 (5)[g]	< 5		obscured		24.672	$(^3P)6s\,^4P_{1/2}$	10
						25.055	$(^3P)5d\,^2P_{1/2}$	1
(4)	25.4 (1)	36 (8)	0.44	25.28 (2)	5 (2)	25.266	$(^3P)5d\,^4P_{1/2}$	5
						25.385	$(^3P)6s\,^2P_{1/2}$	1
						25.991	$(^3P)6p\,^4P_{3/2}$	
(5)	26.38 (5)			26.37 (2)	12 (4)	26.224	$(^3P)6p\,^2P_{1/2}$	
		117 (16)	1.72	26.63 (4)	4 (2)	26.609	$(^3P)6p\,^2P_{3/2}$	
(6)	26.8 (1)			26.88 (2)	5 (2)	27.060	$(^3P)6p\,^4D_{1/2}$	
						27.154	$(^3P)6p\,^4P_{1/2}$	
						27.210	$(^3P)6p\,^4D_{3/2}$	
						27.412	$(^3P)6p\,^2P_{3/2}$	
						27.540	$(^3P)6p\,^2D_{3/2}$	
(7)	27.6 (1)			27.54 (2)	32 (5)	27.575	$(^3P)6p\,^2S_{1/2}$	
				27.93 (2)	14 (4)	27.877	$(^1D)5d\,^2P_{1/2}$	10
		207 (23)	2.72					
						28.155	$(^1S)6s\,^2S_{1/2}$	12
(8)	28.1 (1)			28.24 (4)	6 (2)	28.207	$(^1D)6p\,^2P_{3/2}$	
						28.487	$(^1D)6p\,^2D_{3/2}$	
						28.588	$(^1D)6p\,^2P_{1/2}$	
(9)	28.9 (1)	41 (7)				28.875	$(^1D)5d\,^2S_{1/2}$	26
						29.061	$(^3P)6d\,^2P_{1/2}$	6
						29.330	$(^3P)6d\,^4P_{1/2}$	18
(10)	29.33 (5)	84 (13)	0.97			29.388	$(^3P_2)7p\,[1]_{3/2}$	
						29.426	$(^3P_2)4f\,[2]_{3/2}$	
						29.489	$(^3P_2)7p\,[1]_{1/2}$	
						29.511	$(^3P_2)4f\,[1]_{1/2}$	
						29.530	$(^3P_2)4f\,[1]_{3/2}$	
						29.597	$(^3P)7s\,^4P_{1/2}$	1
						29.851	$(^3P)7s\,^2P_{1/2}$	0
						30.135	$(^3P)6d\,^4D_{1/2}$	0
						30.45[h]	$(^3P_0)7p$	
						30.508	$(^1S)6p\,^2P_{1/2}$	
(11)	30.7 (1)	268 (43)	3.67			30.527	$(^3P_1)4f\,[2]_{3/2}$	
						30.628	$(^1S)6p\,^2P_{3/2}$	
						30.65[h]	$(^3P_1)7p$	
						30.66[h]	$(^3P)7d\,^4P_{1/2}$	0
						30.71[h]	$(^3P)7d\,^2P_{1/2}$	0
						31.271	$(^1D)6d\,^2P_{1/2}$	3
						31.40[h]	$(^3P)8s\,^4P_{1/2}$	5
						31.406	$(^1D_2)4f\,[1]_{3/2}$	
						31.5[h]	$(^3P)8d\,^4P_{1/2}$	. . .
(12)	31.4 (1)					31.47[h]	$(^1D)6d\,^2S_{1/2}$	10
						31.510	$(^1D_2)4f\,[2]_{3/2}$	
						31.56[h]	$(^1D_2)7p$	

[a]Numbering taken from Fig. 1, Ref. 10.
[b]Normalized to the intensity of the $\underline{5s}$ peak.
[c]Normalized to the intensity of $\underline{5p}$ peaks, the intensity of the $\underline{5s}$ satellites is not included, see text.
[d]Except for $5s5p^6\,^2S_{1/2}$ all states belong to configurations $5s^25p^4(\overline{SL})nlSLJ$, written $(\overline{SL})nlSLJ$. Except for the $7p$ and $4f$ levels, LS coupling is used but jK coupling would in most cases provide better designations.
[e]Auger line, Ref. 10.
[f]Used to calibrate the experimental energies.
[g]Possibly Auger line component, Ref. 10.
[h]Predicted level. For $7p$, the predictions are for the center of gravity of all levels built on a particular parent.

that correlation in the Xe ground state is the primary reason for the strength of the satellites. Dyall and Larkins[13] have made calculations of the $\underline{5p}$ satellites at high photon energy including correlation in the initial state. The calculated total satellite intensity is between 2 and 2.5% as compared to the experimental value of 9.5%. However, also for Ar, the calculation of Dyall and Larkins seems to give $\underline{3p}$ satellites weaker than observed and compared to the results obtained by Carlson, Krause and Moddeman[11] for Ne and Ar the observed $5p$ satellite spectrum in Xe is rather weak.

The coupling conditions in $6p$, $7p$, and $4f$ are closer to jK than to LS coupling.[3] This means that we cannot use the results of the calculation by Dyall and Larkins since it neglects the spin-orbit interaction. We expect that most levels with $J=\frac{1}{2}$ or $\frac{3}{2}$ can give rise to observable satellites and in Table I we have included all presently known odd levels in the relevant energy range in addition to a few predicted levels.

A comparison of the measurements by Süzer and Hush[9] with our interpretation indicates that the $\underline{5s}$ satellite intensities are the same at 40.8 and 1487 eV. The intensities of the 25.28- and 27.93-eV satellites (column 6) agree with the calculated values (column 9). The $(^1S)6s\,^2S_{1/2}$ satellite at 28.24 eV is apparently somewhat weak. However, it is situated very close to the cutoff in this experiment. The good agreement for the $\underline{5s}$ satellites provides further support for identifying the remaining lines at 40.8 and by implication at 33 eV as $\underline{5p}$ satellites. A detailed comparison between observed and predicted satellite structure at 33 eV is given below with reference to Table I.

According to Fahlman *et al.*[10] peak (1) is an Auger line. Peak (2) is very weak and cannot be explained as a $\underline{5s}$ or $\underline{5p}$ satellite while the weak peak (3), which was obscured in the experiment of Süzer and Hush,[9] probably is a $\underline{5s}$ satellite. The most serious flaw in our interpretation concerns peak (4) which is very strong at 33-eV photon energy. A weak $\underline{5s}$ but no $\underline{5p}$ satellites are predicted at this position. Peaks (5) and (6), which are strong and not observed at high photon energy, can be explained as due to $6p$ states although the agreement in energy for peak (5) is worse than expected from the experimental accuracy. Süzer and Hush[9] have resolved three lines in this energy range which agrees with our prediction but the agreement in energy is not perfect. The strongest satellites, peaks (7) and (8), agree well in energy with $6p$ states. Peak (9) is interpreted as the strongest $\underline{5s}$ satellite. The observed intensity is in agreement with this assignment which is also supported by the observed β value as explained later. Peak (10) has an energy close to the lowest $7p$ level while peak (11) lies close to the $(^1S)6p\,^2P$ levels. Finally, peak (12) is close to the observed position of $(^1D)4f\,^2P$ which, according to Dyall and Larkins,[13] should give an observable satellite but also close to the predicted position of $(^1D)7p$.

The observed β value for peak (9), 1.6, is similar to that for the main $\underline{5s}$ peak[5] while β for all other peaks has values[10] between -0.1 and 0.8. These values do not correspond to the β values for the main $\underline{5p}$ peaks[14] but, unlike the $\underline{5s}$ satellites, the $\underline{5p}$ satellites are believed to be due to a different component of the initial wave function than the main line and can, therefore, be expected to have a different value of β. At higher energy, the β values for all the satellites are similar to that for the main $\underline{5s}$ line[15] and this is further support for the interpretation that the bulk of the satellites at low photon energy has a different origin.

In conclusion, we note that the disagreement in energy for some satellites is the only discouraging feature of our interpretation. However, the experimental-energy determination is very difficult at these low energies and is made even more difficult by the large number of unresolved lines. In addition, post-collision effects might influence the observed energies at this energy. However, our interpretation explains so many features of the observed spectrum which are difficult to understand in terms of $\underline{5s}$ satellites that it must be essentially correct. Nevertheless, a calculation of satellite intensities and β values, in which correlation, relativity, and the dependence of the dipole matrix element on the photon energy is included, is needed to confirm the details of the interpretation.

After this work was completed we received a report of work prior to publication[16] of an experimental study of the satellite structure at a number of photon energies between 28.5 and 74.8 eV. In this work it is suggested that $5p$ ionization might contribute to some of the observed satellites although no detailed analysis is attempted.

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