

PHYSICAL REVIEW LETTERS

VOLUME 20

4 MARCH 1968

NUMBER 10

PHOTOIONIZATION OF THE M SHELL OF XENON*

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(Received 26 January 1968)

New measurements of the continuum photoionization cross sections of xenon in the region 670–800 eV are reported which reveal, in the region of the M_{IV} and M_V edges, extreme nonhydrogenic behavior previously observed only at longer wavelengths.

Within the past few years, large-scale nonhydrogenic behavior of the photoionization cross section has been observed at progressively higher photon energies. This particular behavior is characterized by a small absorption jump at threshold followed by a delayed slow rise in absorption to several times its extrapolated value over a region two or more Rydbergs in extent. This was found for Xe $4d$ electrons by Ederer¹ and by Lukirskii, Brytov, and Zimkina.² Similar effects have been found in a number of other elements among which tin³ and the rare earths⁴ are typical.

The phenomenon has been found to be generally explicable in simple physical terms⁵ and is semiquantitatively accounted for in a recent extension by Cooper and Manson⁶ of the Hartree-model calculation of Cooper.⁷ This note shows the effect strikingly in the case of Xe $3d$ electrons. The region near 700 eV is one in which the normal, large threshold jump followed by a monotonic decrease in cross section might already be expected to be in force. Indeed, in a remarkable set of measurements, Lukirskii, Brytov, and Gribovskii⁸ (working with discrete line sources) show data all of which save one at 705 eV (Fe $L\alpha$) fall nicely on the usual linear plot of $\ln\mu$ vs $\ln\lambda$.

The data reported here were obtained using

continuum radiation as a source permitting photon energy to be incremented in small steps (~ 0.5 eV). In addition, measures were taken to establish an accurate energy scale. Absolute cross-section values were obtained by pressure measurements with an oil manometer on the contents of a cell of length 5.10 ± 0.05 cm.

The measurements were carried out on a vacuum double-crystal Bragg spectrometer⁹ using potassium acid phthalate (KAP) crystals.¹⁰ The instrument was operated as a single-crystal instrument with the second crystal replaced by a Soller collimator having an angular divergence of 0.15° . The detector was a gas-flow counter using illuminating gas from a laboratory tap. Illuminating gas was used in place of an argon-methane mixture in order to avoid a background pulse arising from the escape of an argon $K\alpha$ photon following absorption of fluorescent potassium K radiation from the crystal.

Figure 1 shows the experimental results of this investigation (at intervals of 0.05° in Bragg angle) along with the previous values obtained by Lukirskii, Brytov, and Zimkina.⁸ Theoretical values obtained according to Cooper and Manson⁶ are indicated by the dashed curve.¹¹

The energy scale indicated in Fig. 1 depends on two experimental parameters. Firstly, it is

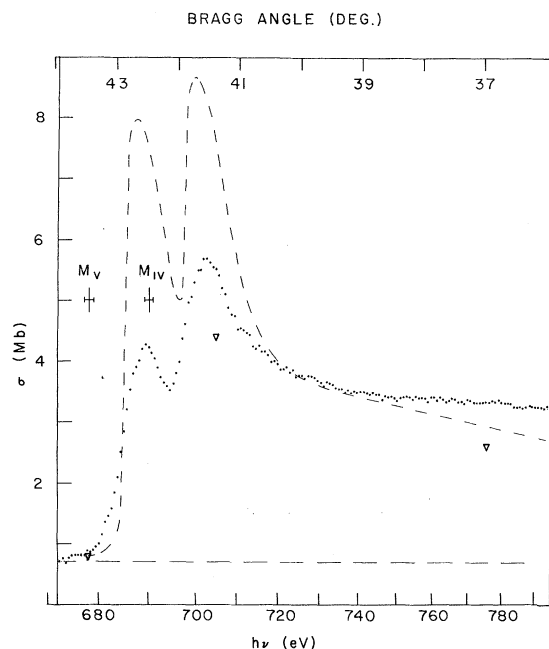


FIG. 1. Total photoattenuation cross section in xenon near the photoionization thresholds for $3d$ electrons. Spectral-window width at half-maximum is about equal to the interpoint spacing. Thresholds as measured by M. Krause using a photoelectron spectroscopic method are indicated by the vertical bars. Previous measurements (Ref. 7) using characteristic line radiation are indicated by the inverted triangles. Theoretical calculations due to Cooper and Manson (Refs. 5 and 10) are indicated by the dashed curve; the calculations have been plotted using the experimental thresholds. Cross-section values indicated in the figure have an estimated uncertainty of 0 ± 0.1 Mb near 4 Mb. Lower and higher values are somewhat less good owing to systematic problems.

assumed that the grating spacing of the analyzing crystal is $d_{\text{eff}} = 13.2942 \text{ \AA}^*$; this value is obtained from a d_{∞} value¹² of $13.3159 \pm 0.0002 \text{ \AA}^*$ and an index-of-refraction correction, neglecting anomalous dispersion, amounting to -0.0216 \AA^* . Secondly, the entire discrepancy between this scale and the proper one is assigned to an error in phase of the Bragg-angle measurement procedure which arose from the mechanical placement of the Soller collimator. This error was evaluated in the M_{IV}, V region by noting the location of $\text{Co } L\alpha_1$ whose wavelength¹³ of $15.972 \pm 0.006 \text{ \AA}^*$ gives a Bragg-angle reference of 36.921° . The observed location is $36.850 \pm 0.005^\circ$ and the implied additive correction of $0.07 \pm 0.01 \text{ deg}$ has been applied to the data of Fig. 1. The indicated limits represent estimates of overall uncer-

tainty. The energy scale was obtained from the wavelength scale through the conversion value¹⁴ of $12398.1 \text{ \AA}^* \text{ eV}$, whose uncertainty is not significant on the scale of Fig. 1. These errors would combine to yield an uncertainty of approximately 0.2 eV for the energy scale. Consideration of systematic errors suggests that 0.4 eV is a more appropriate estimate of the uncertainty.

Also shown in Fig. 1 are two bars marking the location of the binding energies for M_V and M_{IV} electrons as obtained by Krause¹⁵ by photoelectron spectroscopy. The presence of structure below the lower energy threshold is suggested by the data. These resonances would lead to the $3d - \epsilon p$ continuum because the f continuum is expected to be relatively small at threshold. The second or M_{IV} threshold is not evident in the x-ray data, but the splitting between the delayed maxima of the $3d - \epsilon f$ continuum are in agreement with the level splitting of Krause.

I am most grateful to Dr. Manfred Krause, Oak Ridge National Laboratory, for permission to quote his M_V - and M_{IV} -term measurements and to Dr. S. T. Manson for the theoretical values. I have also enjoyed many useful discussions with U. Fano and J. W. Cooper regarding these problems.

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¹D. L. Ederer, Phys. Rev. Letters **13**, 760 (1964).

²A. P. Lukirskii, I. A. Brytov, and T. M. Zimkina, Opt. Spektrosk. **17**, 438 (1964) [translation: Opt. Spectrosc. **17**, 234 (1964)].

³K. Codling, R. P. Madden, W. R. Hunter, and D. W. Angel, J. Opt. Soc. Am. **56**, 189 (1966).

⁴T. M. Zimkina, B. A. Fomichev, S. A. Gribovskii, and I. I. Zhukova, Fiz. Tverd. Tela **9**, 1447 (1967) [translation: Soviet Phys.—Solid State **9**, 1128 (1967)].

⁵J. W. Cooper, Phys. Rev. Letters **13**, 762 (1964).

⁶J. W. Cooper and S. T. Manson, Phys. Rev. **165**, 126 (1968).

⁷J. W. Cooper, Phys. Rev. **128**, 681 (1962).

⁸A. P. Lukirskii, I. A. Brytov, and S. A. Gribovskii, Opt. Spektrosk. **19**, 368 (1965) [translation: Opt. Spectrosc. **20**, 203 (1966)].

⁹R. D. Deslattes, Rev. Sci. Instr. **38**, 616 (1967).

¹⁰A. J. Bearden and F. Huffman, Rev. Sci. Instr. **34**, 1233 (1963).

¹¹I am indebted to S. T. Manson for performing these calculations according to the model of Ref. 5.

¹²This value was obtained from a measurement of the tenth-order diffraction angle for $\text{Cu } K\alpha_1$ on a double-crystal spectrometer. It is in reasonable agreement

with Ref. 8.

¹³J. A. Bearden, Rev. Mod. Phys. **39**, 78 (1967).

¹⁴J. A. Bearden and A. F. Burr, Rev. Mod. Phys. **39**,

125 (1967).

¹⁵M. Krause, private communications and to be published.

EXCITATION OF $n=2$ STATES IN HYDROGEN BY ELECTRON IMPACT

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(Received 15 January 1968)

A possible source of incompleteness is pointed out in the most recent close-coupling calculations for the excitation cross sections of the $n=2$ levels in hydrogen, some of the results of which disagree with experiment. We present a method which removes this difficulty by the implicit inclusion of all important effective polarization potential terms of order α/r^4 .

A serious discrepancy presently exists between rather refined theoretical and experimental determinations of the total $1s-2s$ excitation cross section.¹ The purpose of this note is to suggest a possible source of incompleteness in the most recent calculations² which lies in their failure to include the full effective polarizabilities that arise. Methods for incorporating the full ground-state polarizability into low-energy calculations for the elastic-scattering cross section have been given,³ and in the following we present the extension to the excitation of the $n=2$ states.

Starting with the complete set of radial coupled equations, we specialize at once to the case where the only open channels are those containing the $1s$, $2s$, and $2p$ atomic states. The asymptotic forms of the closed-channel radial functions may be expressed in terms of the open-channel functions, since they provide an oscillatory asymptotic coupling.⁴ When they are substituted into the right-hand side of the open-channel equations, one obtains the following set of asymptotic relations between the four open-channel radial functions:

$$\left(\mathcal{E}_L + \frac{\alpha(1s-p-1s)}{r^4} + k_1^2\right)F_0 = -\frac{\alpha(1s-p-2s)}{r^4}F_1 + \frac{2}{r^2} \frac{\langle u_{10} r u_{21} \rangle}{[3(2L+1)]^{1/2}} [L^{1/2}F_2 - (L+1)^{1/2}F_3], \quad (1)$$

$$\left(\mathcal{E}_L + \frac{\alpha(2s-p-2s)}{r^4} + k_2^2\right)F_1 = -\frac{\alpha(2s-p-1s)}{r^4}F_0 + \frac{2}{r^2} \frac{\langle u_{20} r u_{21} \rangle}{[3(2L+1)]^{1/2}} [L^{1/2}F_2 - (L+1)^{1/2}F_3], \quad (2)$$

$$\begin{aligned} \left(\mathcal{E}_{L-1} - \frac{2(L-1)}{5(2L+1)} \frac{\langle u_{21} r^2 u_{21} \rangle}{r^3} + \frac{1}{(2L+1)r^4}\right) \left\{ L\alpha(2p-s-2p) + \frac{7L+3}{5} \alpha(2p-d-2p) \right\} + k_2^2 F_2 \\ = \frac{2}{r^2} \left[\frac{L}{3(2L+1)} \right]^{1/2} [\langle u_{21} r u_{10} \rangle F_0 + \langle u_{21} r u_{20} \rangle F_1] - \frac{6[L(L+1)]^{1/2}}{5(2L+1)} \frac{\langle u_{21} r^2 u_{21} \rangle}{r^3} F_3, \end{aligned} \quad (3)$$

$$\begin{aligned} \left(\mathcal{E}_{L+1} - \frac{2(L+2)}{5(2L+1)} \frac{\langle u_{21} r^2 u_{21} \rangle}{r^3} + \frac{1}{(2L+1)r^4}\right) \left\{ (L+1)\alpha(2p-s-2p) + \frac{7L+4}{5} \alpha(2p-d-2p) \right\} + k_2^2 F_3 \\ = -\frac{2}{r^2} \left[\frac{L+1}{3(2L+1)} \right]^{1/2} [\langle u_{21} r u_{10} \rangle F_0 + \langle u_{21} r u_{20} \rangle F_1] - \frac{6[L(L+1)]^{1/2}}{5(2L+1)} \frac{\langle u_{21} r^2 u_{21} \rangle}{r^3} F_2, \end{aligned} \quad (4)$$

where

$$\mathcal{E}_L = \frac{d^2}{dr^2} - \frac{L(L+1)}{r^2}.$$

The notation is as follows: The channel indices 0, 1, 2, and 3 refer to the combinations of quantum numbers $nl'l'L=10LL$, $20LL$, $21L-1L$, and $21L+1L$, respectively, where nl are the atomic principal and orbital quantum numbers (radial function u_{nl}), l' is the free-electron orbital angular momentum, and L is the total coupled orbital angular momentum. The above asymptotic equations apply to both singlet and triplet scattering since the exchange terms in the close-coupling equations fall off more rapidly than the ones included. Only the leading asymptotic term in each of the coupling