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Spectral analysis of the 4d⁹6s configuration in eight times ionized xenon, Xe IX

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Abstract

A capillary light source was used to observe the spectrum of eight times ionized xenon, Xe IX, in the vacuum ultraviolet range, 270–2000 Å. Sixteen transitions have been identified as combinations between energy levels of the $4d^96s$ with $4d^95p$ configuration, and all $4d^96s$ levels have been determined. The present analysis is based on an accurate extrapolation of energy parameters and experimental energy level values in the Pd I isoelectronic sequence. The energy parameters were obtained with Hartree–Fock relativistic calculations. Least-squares parametric calculation has been carried out to study the fit between experimental and theoretical values.

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1. Introduction

Palladium-like xenon, Xe IX, has a closed $4d^{10}$ shell in its ground state. Data for higher members of the Pd I sequence are important for achieving the laser action at shorter wavelengths, and laser effect was demonstrated for Xe IX at the wavelength of 418, 1 Å [1]. Resonant transitions against the $4d^9(np+n'f)$ configurations were studied in the Pd I isoelectronic sequence from Cd III to Cs X by Churilov et al. [2], and also in [3].

The spectra of Cd III, In IV, and Sn V, were studied by Joshi and van Kleef [4,5], and the previous studies on Sb VI and Te VII [6] were revised and extended, including I VIII, by Churilov et al. [7], and Xe IX [8,9]. Recent analysis of the Cs X–Ce XIII, and Pr XIV–Nd XV [10,11] has been published.

Spectroscopic data from rare gases can be used in studies related with collision physics, photoelectron spectroscopy, fusion diagnostic, and as mentioned, in laser physics. For a better understanding of the eight times ionized xenon atomic structure, the present investigation was undertaken to study the $4d^96s$ configuration of the Xe IX ion, and all energy levels belonging to this configuration were determined by $4d^95p-4d^96s$ transitions.

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The spectral analysis was supported by theoretical calculation using the Cowan codes [12] and by means of least squares fits along the Pd I sequence for the 4d⁹6s configuration [7]. For this configuration we also extrapolated accurate energy level values along the isoelectronic sequence, using the multiconfiguration Dirac Fock (MCDF) method [13], and Hartree–Fock relativistic calculations [12].

2. Experimental

To excite the xenon spectra we used a capillary pulsed discharge that is a Pyrex tube, 100 cm long, and with an inner diameter of 0.3 cm. The electrodes, placed 80 cm apart, were made of tungsten covered with indium, this one, used to avoid the impurities coming from the electrodes. At one side of the tube there is an inlet connected via a pressure reduction system to the bottle of xenon. In this way a continuous flow of gas was achieved during the exposures.

Gas excitation is produced by discharging a bank of low-inductance capacitors of 240 nF and charged up to 19 kV through the tube. The gas pressure was measured by a thermocouple vacuum gauge before and after the exposures. The pressure range was varied between 5 and 150 mTorr. Light emitted axially was analysed using a 3 m normal incidence vacuum spectrograph with a concave diffraction grating with 1200 lines/mm, blazed for 1200 Å, with plate factor 2.77 Å/mm in the first diffraction order. Ilford Q-2 and Kodak SWR plates were used to record the spectra. Known lines of Xe and C, N, O, were used as internal wavelength standards.

The wavelength values of the measured lines are estimated to be correct to ± 0.02 Å. The intensities figures are visual estimates of photographic density, and are on a uniform scale only within limited wavelength ranges. To distinguish among different states of ionization, we studied the behaviour of the spectral lines intensity as a function of pressure.

3. Results and discussion

Theoretical predictions were used in the analysis of the spectra. To obtain these predicted energy level values and the transition probabilities from de Cowan computer codes [12], we included into calculation the even $4d^{10}$, $4d^9$ ns (n = 5, 6), $4d^9$ nd (n = 5, 6), $4d^8$ 5s², $4d^8$ 5s⁵d, $4d^8$ 5d², $4p^5$ 5d¹⁰ 5p and $4p^5$ 5d¹⁰ nf (n = 4, 5) configurations and the odd 4d⁹ np (n = 5, 6), $4d^9$ nf (n = 4 - 6), $4d^8$ 5s⁵p, $4d^8$ 5p⁵d, $4d^8$ 5s nf (n = 4, 5), $4p^5$ 4d¹⁰ 5s and $4p^5$ 4d¹⁰ 5d configurations. The radial parameters were scaled to 0.85 of their ab initio Hartree–Fock values.

The transitions observed in the present investigation are listed in Table 1. They are shown as combinations between energy levels of the $4d^96s$ configuration, against levels of the $4d^95p$ configuration, taken from the work of Churilov et al. [9]. The intensities of the observed lines, marked by Int. in the table, are based on visual estimates and the wavenumber values given in the calculated column are deduced from the optimized level values. The level values were determined in a procedure where the wavenumbers of the observed lines are weighted according to their estimated uncertainties. We also presented in this table the calculated transition probabilities (gA, where g is the statistical weight of the upper level and A, the Einstein coefficient for spontaneous emission).

Theoretical calculations along the isoelectronic sequence were also made using the MCDF code of Grant [13]. We also use the predicted MCDF and HFR [12,13] energy levels together the reported experimental 4d⁹6s energy levels in the sequence, to help us in the search of the energy levels. Studying the behaviour of the difference between the observed and calculated energies along the isoelectronic sequence and using the energy of ³D₃ as reference value, we established all the extrapolated energy level values of the configuration. Fig. 1 shows the ³D₁–³D₃ and ³D₂–³D₃ energy level differences using $E_{obs}-E_{cal}$ (HFR) values, along the isoelectronic sequence.

Table 2 shows the experimental energy level values of the 4d⁹ 6s configuration and the percentage composition of the 4d⁹6s energy levels in L–S coupling. The designation of the levels ${}^{1}D_{2}$ and ${}^{3}D_{2}$ is a little ambiguous. The contribution to the ${}^{3}D_{2}$ level is 54% ${}^{3}D$ and 46% ${}^{1}D$. The same fact can be seen with these levels in other ions belonging to the isoelectronic sequence.

To give the best possible fit between the calculated eigenvalues and the observed energy levels, the radial integrals E_{av} , F^k , G^k , ζ and R^k were considered as adjustable parameters, whose values were determined considering their behaviour through the isoelectronic sequence. The accuracy of the fit is measured by means of the standard deviation in a least-squares calculation [12].

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