

Seminar

Institute for Plasma Research

Title: Atomic Structure studies of ionized mercury atoms: Hg III - Hg VI
Speaker: Dr. Aadil Rashid
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Date: 05th December 2024 (Thursday)
Time: 04:00 PM
Venue: Join the talk online
<http://meet.google.com/ttf-chdh-cjo>

Abstract

The postdoctoral presentation entitled, “**Atomic Structure studies of ionized mercury atoms: Hg III – Hg VI**” comprises of an introduction, theoretical aspect of atomic spectra, experimental details followed by the detailed structure studies of four different ions of mercury (Hg III – Hg VI). For all the experiments described, the source of radiation was a triggered spark. The majority of experimental data used were recorded at the Antigonish laboratory, Canada, and at the National Institute of Standards and Technology (NIST), USA. The experiments performed to record the spectral data cover the vacuum ultraviolet wavelength region of the electromagnetic spectrum. Atomic data in the vacuum ultraviolet region are an intrinsic part of data retrieved over all regions of the electromagnetic spectrum, these data are required to ascertain correlation between the normal state of the atom and its excited states.

The theoretical method of atomic structure calculations based on Hartree-Fock formalism with relativistic corrections, and superposition of configurations incorporated in Cowan’s code. Multifarious central problems which need to be solved in quantum mechanics are all about atoms or molecules. These problems involve a number of electrons around several atomic nuclei. The method was proposed by Hartree in 1928, assuming each electron moving under the influence of the averaged potential. The wavefunction of the anticipated quantum number in that potential is chosen and presumed that this wavefunction is to be engaged for finding the charge density of all the other electrons.

The specifics of experiments performed to record mercury spectra in vacuum ultraviolet wavelength region. The spectrum of mercury was recorded on a 3-m normal incidence vacuum spectrograph (NIVS) in Canada, and on a 10.7 m grazing incidence spectrograph, USA. A 3-m normal incidence vacuum spectrograph (NIVS) set up at the Antigonish laboratory (Canada) used to record the data for the present analysis is a sort of cylindrical cavity of about 30 inches in diameter. The spectrum of mercury was predominantly recorded in the wavelength range 300 Å – 2000 Å using a triggered spark source- a modified spark source with improved control over spark in the voltage range of 2 kV - 10 kV. It consists of a low inductance fast-charging capacitor (14.5µF) chargeable up to 20 kV. Another set of spectra were recorded in grazing incidence on a 10.7m grazing incidence spectrograph installed at the National Institute of Standards and Technology (NIST), USA, having 1200 lines/mm grating, which gives the first order inverse dispersion of about 0.225 – 0.258 Å/mm at 200 Å. The recording of the spectrum was done in the wavelength region of 250 Å – 565 Å.

The structure of doubly ionized mercury (Hg III) having the closed subshell 5d10(1S0) as its ground energy state, and the first excited configurations are of the type 5d9nℓ (n ≥ 5). The spectrum (mercury) was recorded on a 3-m normal incidence vacuum spectrograph (NIVS) at the Antigonish laboratory in Canada. A triggered spark source was used to record the spectrum in the wavelength region of 300 – 2000 Å. The theoretical calculations were executed by Cowan’s *pseudo*-relativistic Hartree-Fock code using superposition of interacting configurations for the proper interpretation of energy eigenvalues. Least-squares fitted (LSF) parametric calculation was applied to illustrate the observed energy level structure. The spectroscopic interpretation of triply ionized mercury (Hg IV). It is the fourth member of Ir isoelectronic sequence with ground state electronic configuration [Xe]4f145d9. The regular excitations are of the type 5d8nℓ (n ≥ 5; ℓ ≥ 0), while the doubly excited

configurations lead to the 5d76s2, 5d76p2, 5d76d2, 5d75f2, 5d76s6p etc. The primal work on Hg IV spectrum was reported by Subbaraya [16] establishing 5d86s 4F9/2 as its lowest energy level, with 5d9 2D5/2 at 2192 cm-1 and 5d9 2D3/2 at 10376 cm-1 with an energy separation of 8184 cm-1. However, Joshi *et al.* completely revised the work reported by Subbaraya, and found the ground state configuration of Hg IV to be 5d9 instead of 5d86s configuration as reported earlier with a 2D doublet separation of 15684.7 cm-1.

The spectrum of quadruply ionized mercury (Hg V) which is isoelectronic with neutral osmium (Os I) having [Xe]4f145d8 as its ground configuration. The regular excitation leads to 5d7n ℓ ($n \geq 5$; $\ell \geq 0$). The spectrum of Hg V was first reported by Raassen *et al.* They studied the 5d8 and 5d76p configurations, classifying 188 spectral lines in the wavelength range 400 – 592 Å. They had established 8 of 9 energy levels belonging to the 5d8 configuration, and 62 out of 110 energy levels of the 5d76p configuration. We present a unified and extended atomic data of Hg V, comprising **142** energy levels and **569** classified lines with their corresponding uncertainty measures and other extensive factors.

Lastly the sixth spectrum of mercury (Hg VI) having [Xe]4f145d7 as the ground-state configuration. We report comprehensive atomic data related to this ion that could be used for the interpretation of stellar spectra. *Ab-initio* calculations were performed for Ir III-like Pt IV, Au V, and Hg VI using a *pseudo*-relativistic Hartree-Fock method (HFR). These calculations yielded theoretical energy levels and transition data for the electric-dipole (E1) transitions. The obtained results are in rational arbitration with the available experimental data. More precisely, the agreements of our theoretical calculations with the experimental values for Pt IV and Au V allowed us to perform precise calculations for Hg VI by scaling the Slater parameters analogous to Au V, which is proximate to Hg VI in Re isoelectronic sequence. Most of our theoretical energy levels and transition rates for Re-like Hg VI were not reported earlier. To our knowledge, the available calculations of energy levels and transition parameters among these three ions are limited to Pt IV and Au V, while for Hg VI spectrum no inclusive calculations have been reported so far, except a calculated transition rate for a single transition, [4f14]5d7 4F9/2 – 5d66p 6D7/2 [25]. Our results for Hg VI and some additional transition parameters for Au V are the first to be reported in the literature.
