Journal of Basic and Applied Engineering Research
Print ISSN: 2350-0077; Online ISSN: 2350-0255; Volume 2, Number 12; April-June, 2015 pp. 1028-1030
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http://www.krishisanskriti.org/jbaer.html

Energy level Prediction of $4s^24p5d$ Configuration in RbVI

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Abstract—*Five times ionized rubidium ions have germanium like structure with $4s^24p^2$ ground state configuration. Only two exited configurations $4s4p^3$ and 4p5s of Rb VI have been studied so far and all others are still unknown. The energy levels belonging to $4s^24p5d$ configuration has been predicted empirically by means of Ge I isoelectronic sequence study. Calculations are carried out using Cowan code with relativistic Hartree-Fock method by inclusion of large number of interacting configurations [$4s^24p$ (4f+5p+5g), 4s4p (4d+5s), $4p^3$ (4d+5s)].*

1. INTRODUCTION

Highly ionized ions are subject to various investigations in science & technology. Scientists in astrophysics, plasma physics, physical chemistry, atomic physics and nuclear physics as well as many related fields rely heavily on the proper identification of atomic energy levels. Germanium like ions has been widely applied in the laboratory and in astronomical plasmas [1]. The Rb VI is one of the elements of Ge-I isoelectronic sequence.

Five-time ionized rubidium (Rb VI) has neutral germanium-like (Ge I) spectrum with $3d^{10}4s^24p^2$ ground configuration with the exited configurations $4s4p^3$, $4s^24pnd$ (n<4) and $4s^24pns$ (n<5); and further excitations can lead to $3d^{10}4s^24p$ (5p, 6p, 4f, 5f), $3d^{10}4s(4p^24d, 4p^25s)$, $3d^{10}4p^4$.

Theoretical calculations for Rb VI ground state configurations were published first in 1986 by Biemont and Hansen [2]. Litzen and Reader in 1989 studied the Rb VI transitions experimentally. They reported the $4s^24p^2$ ground configuration and exited $4s4p^3$ configuration with the exception of $4s4p^3\ {}^5S_2$ energy level, which is predicted from fitted parameters [3]. In the studied of O'Sullivan for laser produced plasma spectrum of Rb, They found transitions of $4s^24p5s$ configurations in the 320-390 Å range of Rb VI [4]. The resolution of Reader et al. is greater than O'Sullivan.

In this paper we have report the extension of these analysis to include the $4s^24p^2$, $4s4p^3$, 4p5s and 4p4d of Rb VI.

2. THE LEVEL STRUCTURE

The level structure of the predicted $4s^24p5d$ configurations has been analyzed by means of least-squares fits of energy parameters consisting of ${}^3P_1$, ${}^3D_1$, ${}^1P_2$, ${}^3P_2$, ${}^1D_2$, ${}^3F_2$, ${}^3P_2$, ${}^3D_2$, ${}^3D_3$, ${}^3F_3$ and ${}^1F_3$ levels (Fig. 1).

A calculation consisting of the even configuration 4^24p^2 and the odd configurations 4s4p3, $4s^24p$ (4f+5p+5g), 4s4p (4d+5s), $4p^3$ (4d+5s) was thus carried out using the Cowan code. Energy parameters were used in the calculation, with the empirical scaling factors 0.85 for electrostatic integrals (F_k) integrals, 0.75 for G_k integrals and 1.0 for spin-orbital integral.

The 4p4d transitions of Y VIII, Zr IX , Nb X and MO XI earlier studied by Rahimullah et al. in 1978 [5]. The interaction parameters of $4s^24p4d$ were fixed at scaled HXR values, 0.866 for the electrostatic and 0.81 for the G_k integrals keeping spin-orbital integral 1.0, according to the trend of 4p4d slater parameters based on reported values of Ge-like elements [5,6].

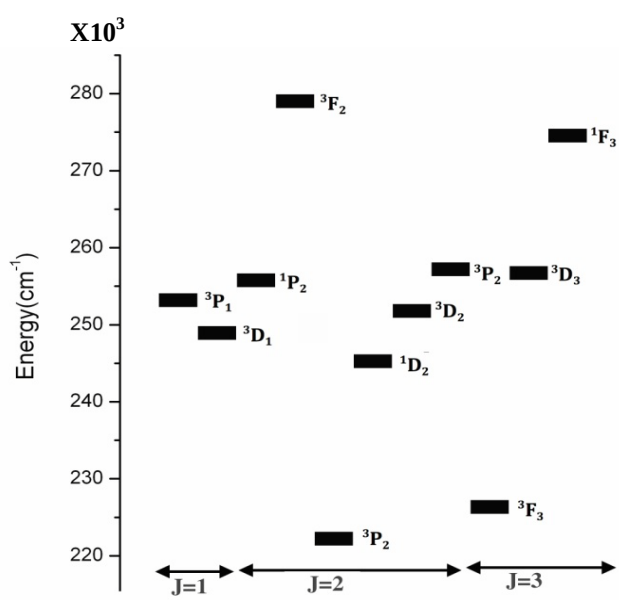

Fig. 1

Table 1: Hartree-Fock and Least squares fit values of Rb VI along with 4p4d.

J E(obs) E(LSF) diff. LS-composition.

Even Configurations

0 0.0 49.0 -49.0 96% <2>3P + 4% <0>1S

45201.0 45151.0 50.0 96% <0>1S + 4% <2>3P

1 5140.0 5085.0 55.0 100% <2>3P

2 9899.0 9815.0 84.0 89% <2>3P + 11% <2>1D

23746.0 23887.0 -141.0 89% <2>1D + 11% <2>3P

Odd Configurations

0 168930.0 168987.0 -57.0 92% 4s 4p3 (<1>2P)3P + 7% 4s2 4p 4d 3P

253168.0 253618.0 -450.0 90% 4s2 4p 4d 3P + 7% 4s 4p3 (<1>2P)3P

303480.0 303464.0 16.0 98% 4s2 4p 5s 3P

1 148531.0 148815.0 -284.0 87% 4s 4p3 (<3>2D)3D + 8% 4s2 4p 4d 3D

169477.0 169364.0 113.0 88% 4s 4p3 (<1>2P)3P + 7% 4s2 4p 4d 3P

208835.0 208635.0 200.0 79% 4s 4p3 (<3>4S) 3S + 16% 4s 4p3 (<1>2P) 1P

220609.0 220698.0 -89.0 72% 4s 4p3 (<1>2P)1P + 17% 4s 4p3 (<3>4S)3S

+ 9% 4s2 4p 4d 1P

248898.3 249644.0 -745.7 47% 4s2 4p 4d 3P + 40% 4s2 4p 4d 3D

255749.7 255453.0 296.7 47% 4s2 4p 4d 3D + 42% 4s2 4p 4d 3P

+ 4% 4s 4p3 (<3>2D) 3D

278982.0 278980.0 2.0 84% 4s2 4p 4d 1P + 9% 4s 4p3 (<1>2P)1P

304640.0 304656.0 -16.0 80% 4s2 4p 5s 3P + 17% 4s2 4p 5s 1P

317070.0 317067.0 3.0 80% 4s2 4p 5s 1P + 17% 4s2 4p 5s 3P

2 148667.0 148829.0 -162.0 85% 4s 4p3 (<3>2D)3D + 8% 4s2 4p 4d 3D

+ 5% 4s 4p3 (<1>2P) 3P

170125.0 169787.0 338.0 81% 4s 4p3 (<1>2P)3P + 7% 4s2 4p 4d 3P

+ 5% 4s 4p3 (<3>2D) 3D

188065.0 188309.0 -244.0 62% 4s 4p3 (<3>2D)1D + 32% 4s2 4p 4d 1D

222196.3 222436.0 -239.7 96% 4s2 4p 4d 3F

245249.0 245484.0 235.0 40% 4s2 4p 4d 3P + 29% 4s2 4p 4d 1D

+ 15% 4s 4p3 (<3>2D) 1D + 9% 4s2 4p 4d 3D

251768.0 251715.0 -53.0 35% 4s2 4p 4d 1D + 27% 4s2 4p 4d 3P

+ 16% 4s 4p3 (<3>2D) 1D + 15% 4s2 4p 4d 3D

257162.3 256691.0 471.3 65% 4s2 4p 4d 3D + 23% 4s2 4p 4d 3P

+ 6% 4s 4p3 (<3>2D) 3D

313630.0 313633.0 -3.0 98% 4s2 4p 5s 3P

3 150434.0 150263.0 171.0 91% 4s 4p3 (<3>2D) 3D + 8% 4s2 4p 4d 3D

226314.7 225776.0 538.7 96% 4s2 4p 4d 3F

256694.4 256397.0 297.4 87% 4s2 4p 4d 3D + 7% 4s 4p3 (<3>2D)3D

274542.0 274522.0 20.0 95% 4s2 4p 4d

3. THEORETICAL APPROXIMATIONS

The Hamiltonian of an atomic system having N electrons is of the form

$$H = H_{kin} + H_{e-nuc} + H_{e-e}$$

$$= \sum_i \frac{\hbar}{2m_e} \nabla_i^2 - \sum_i \frac{Ze^2}{r_i} + \sum_{i \neq j} \frac{e^2}{r_{ij}}$$

Where, H_{kin}, $H_{e\text{-}nuc}$ and $H_{e\text{-}e}$ belongs to the kinetic energy of electrons, the Coulomb potential and the energy of electrostatic interaction of electrons respectively and r_i is the distance between the ith electron and nucleus, and $r_{ij} = |r_i - r_j|$.

On solving the Schrödinger equation in the case of multiple electrons, multiple wave functions obtain. But because of the appearance of the term of interaction of electrons, an exact solution could not be obtained. And the other thing is that the interaction term is comparable with the Coulomb potential term, so it cannot be ignored. An approximate solution is to adopt the method of central force field. It assumed that every electron moves in the central force field of the nucleus and also in the mean force field produced by other electrons, then we have the following effective Hamiltonian:

$$H^{eff} = \sum_{i=1}^{N} H_i^{eff} = -\sum_{i=1}^{N} \left[\frac{1}{2}\frac{p_i^2}{m_e} + \frac{Ze^2}{r_i} - V_i^{eff}(r_i)\right].$$

The Hartree-Fock (HF) approximations assumes that the atomic wave function of n-electron atom be written as the product of n one-electron wave functions, which can be written as Slater Determinant [7-10].

$$\Psi(r_1, \ldots, r_N) = \frac{1}{\sqrt{N!}} \begin{pmatrix} \phi_1(r_1) & \phi_1(r_2) \ldots & \phi_1(r_N) \\ \vdots & \vdots \ddots & \vdots \\ \phi_N(r_1) & \phi_N(r_2) \ldots & \phi_N(r_N) \end{pmatrix}$$

4. RESULTS & DISCUSSIONS

The theoretical calculations have been performed using the Hartree-Fock method with relativistic corrections included in the Cowan code. All energy levels of the calculations along with predicted one are shown in Table 1. The *ab initio*

calculations have been performed for $4s4p^3$, $4s^24p5s$ and 4s4p4d configurations for Rb VI by Hartree-Fock method with relativistic corrections. The Hartree-Fock-Slater method is the most typical method. Cowan revised this method and developed the RCN/RCG program which was used in our study [8]. The program is very effective. The energy levels for allowed transitions were yielded. A large number of interacting configurations [$4s4p^2(4f+5p+5g)$, $4s4p(4d^2+5s^2)$, 4p3(4d+5s)] are taken for input. The calculations are semi empirical because they made use of experimental data to derive scaling factors for the theoretical parameters.

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