



Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

New atomic data for Ge XX

Waleed Othman Younis^{a,*}, Alan Hibbert^b^a Physics Department, Faculty of Science, Beni-Suef University, Beni-Suef City, Egypt^b School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, UK

ARTICLE INFO

Article history:

Received 20 March 2015

Received in revised form

29 July 2015

Accepted 29 July 2015

Available online 28 August 2015

Keywords:

Oscillator strengths

Transition rates

Lifetimes

Configuration interaction

ABSTRACT

We have performed large-scale configuration interaction (CI) calculations using CIV3 for the lowest (in energy) 155 fine-structure levels of aluminum-like germanium ion. We have calculated the energies and lifetimes of these levels, together with oscillator strengths, and transition probabilities for the electric-dipole (optically allowed and intercombination) transitions among the levels of ground state $3s^23p$ (2P) and higher energy levels of states $3s3p^2$, $3s^23d$, $3p^3$, $3s3p3d$, $3p^23d$, $3s3d^2$, $3p3d^2$, $3d^3$, $3s^2$ ($4s$, $4p$, $4d$, $4f$) of Ge XX in the LSJ coupling scheme. The present results include relativistic effects through the Breit–Pauli operator. Improvements to the *ab initio* calculations are made by applying a “fine-tuning” technique in which small adjustments are made to some diagonal elements of the Hamiltonian matrix so as to bring the calculated energy separations into as close agreement as possible with experimental values. Comparisons are made with other available experimental and theoretical results and the accuracy of the present results is assessed.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

The spectra of Al-like ions with $Z > 30$ have received a great deal of attention both experimentally and theoretically. In previous experimental works, which mainly make use of high-energy lasers or tokamak discharges, the spectra of some Al-like ions in plasmas have been measured, though for the heavier ions such as germanium, selenium, molybdenum and silver only the spectra from the transitions between $3s3p^2$ and $3s^23d$ configurations have been identified by Hinnov et al. [1] and by Sugar et al. [2] for copper through molybdenum. Transitions in Ge XX between the $3s^23p$, $3s3p^2$, $3s^23d$, $3p^3$ and $3s3p3d$ configurations were identified in the extreme-ultraviolet spectra emitted from linear plasmas, produced using line-focused laser beams [3].

Large-scale theoretical studies of Al-like ions have been performed using different methods: systematic studies of oscillator strengths for fine-structure transitions in the aluminum isoelectronic sequence [4]; relativistic many-body calculations of electric-dipole lifetimes, transitions rates and oscillator strengths for $n=3$ states in Al-like ions [5].

Critical data compilations based on available theoretical and experimental sources are given in National Institute of Standards and Technology (NIST), Atomic Spectra Database (ASD) [6].

In this work, we have chosen to use the CIV3 program [7,8] to calculate energy levels and oscillator strengths. In a wide range of previous calculations this code has demonstrated its ability to obtain accurate results, especially when strong mixing occurs. The present study involves extensive calculations and gives results for optically allowed and intercombination electric-dipole transitions amongst the lowest 155 energy levels of the Ge XX ion by including configuration interaction (CI) to represent valence shell correlation effects.

* Corresponding author.

E-mail addresses: waleedegy2005@yahoo.com, waledosman@science.bsu.edu.eg (W.O. Younis).

2. Theoretical method

The wavefunctions describing the atomic states included in these calculations were obtained using configuration interaction code CIV3 of Hibbert [7,8]. The CI

wavefunctions are represented as

$$\psi(J) = \sum_{j=1}^M a_{ij} \phi_j(\propto_j L_j S_j J), \quad (1)$$

where (ϕ_j) denotes a set of single-configuration wavefunctions (configuration state functions: CSFs); (α_j) defines the coupling of the angular momenta of the electrons; and the orbital L_j and spin S_j angular momenta are coupled to give the total angular momentum J . The mixing coefficients (a_{ij}) are obtained by diagonalizing the Breit–Pauli Hamiltonian with respect to the basis (ϕ_j) .

The Hamiltonian used in this work consists of the non-relativistic electrostatic terms plus the one-body mass correction, the Darwin term, and the spin–orbit, spin–other-orbit, and spin–spin operators of the Breit–Pauli Hamiltonian. The inclusion of the mass correction and Darwin terms shifts the energy of a configuration as a whole, while the spin–orbit, spin–other-orbit and spin–spin terms give rise to the fine-structure splitting. The general configuration-interaction code CIV3 uses orthonormal orbitals. Their radial functions $P_{nl}(r)$ are expressed as superpositions of normalized Slater-type Orbitals (STOs) of the form

$$P_{nl}(r) = \sum_{j=1}^k C_{jnl} \chi_{jnl}(r), \quad (2)$$

where C_{jnl} are the Clementi-type [9] coefficients and

$$\chi_{jnl}(r) = \frac{(2\xi_{jnl})^{I_{jnl} + \frac{1}{2}}}{[(2I_{jnl}!)^{\frac{1}{2}}]} r^{I_{jnl}} \exp(-\xi_{jnl} r) \quad (3)$$

with the integer

$$I_{jnl} \geq l + 1$$

The parameters C_{jnl} and ξ_{jnl} are determined variationally while the parameters I_{jnl} are normally kept fixed in any optimization process. The radial functions are chosen to satisfy the orthonormality condition

$$\int_0^\infty P_{nl}(r) P_{n'l}(r) dr = \delta_{nn'}; \quad l + 1 < n' \leq n \quad (4)$$

Table 1
Radial function parameters for optimized orbitals of Al-like Ge XX.

Orbitals (nl)	Expansion coefficients (C_{jnl})	Power of r (I_{jnl})	Exponents (ξ_{jnl})
3d	0.0768888	3	13.6044828
	0.9416767	3	7.2784949
	0.0033590	3	3.3769297
4s	−1.7810545	4	5.2772495
	0.0071013	4	3.2983472
	2.2740362	3	7.3552125
	0.0112894	3	2.7572943
	−1.1918070	2	8.2033091
4p	0.1380578	1	23.9226036
	3.4588210	4	5.4838356
	0.1294863	4	13.6449050
	−3.2431628	3	5.2874429
	0.1214499	3	3.9884308
4d	0.3424522	2	13.9180855
	−1.3406807	4	4.6181499
	0.1747193	4	3.1520884
	−0.0311369	3	1.7274663
	0.7434741	3	7.8346912
4f	0.9417413	4	5.2748413
	0.0677806	4	3.6034363
	5.7226171	1	2.7557600
5s	−17.0442927	2	5.0267621
	8.2829726	3	3.4616527
	8.3735165	4	11.4040566
	−5.0226538	5	4.2541872
	16.0477928	2	4.2665146
5p	−18.4549978	3	7.1073204
	8.9776521	4	7.1349628
	−8.4608734	5	6.0800546
	1.3594932	3	9.6533726
5d	3.2152389	4	6.0685123
	−4.3486283	5	8.7436015
	2.9310063	4	6.5130178
5f	−2.7708161	5	6.3994632

Table 2
Method of determining the radial functions.

Orbital	Process of optimization	
1s, 2s, 2p, 3s, 3p	Hartree–Fock orbitals of $3s^2 3p^2 P^0$ of Ge XX (Clementi and Roetti [9])	
	Eigenvalue minimized	
	Configurations	
	Real spectroscopic	
3d	$3s^2 3d^2 D$	$3s^2 3d^2 D$
4s	$3s^2 4s^2 S$	$3s^2 4s^2 S$
4p	$3s^2 4p^2 P$	$3s^2 4p^2 P, 3s^2 3p^2 P^0$
4d	$3s^2 4d^2 D$	$3s^2 4d^2 D, 3s^2 3d^2 D$
4f	$3s^2 4f^2 F$	$3s^2 4f^2 F$
	Valence correlation	
5s	$3s^2 5s^2 S$	$3s3pnd (3 \leq n \leq 5), 3s3dnp (n = 4, 5), 3s3dnf (n = 4, 5), 3s4pnd (n = 4, 5), 3s4dnf (n = 4, 5), 3s4d5p, 3s4f5d, 3s5p5d,$
5p	$3s^2 5p^2 P$	$3s5d5f, 3p3dns (n = 4, 5), 3p4snp (n = 4, 5), 3p4snd (n = 4, 5), 3p4d5s, 3p5s5d, 3d4p5s, 3d5s5p, 4s4pnd (n = 4, 5),$
5d	$3s^2 5d^2 D$	$4s4d5p, 4s5p5d, 4p4d5s, 4p5s5d, 4d5s5p, 5s5p5d$
5f	$3s^2 5f^2 F$	

Download English Version:

<https://daneshyari.com/en/article/5427853>

Download Persian Version:

<https://daneshyari.com/article/5427853>

[Daneshyari.com](https://daneshyari.com)