ASTRONOMY & ASTROPHYSICS
SUPPLEMENT SERIES

Astron. Astrophys. Suppl. Ser. **143**, 491–493 (2000)

Oscillator strengths for As I-III

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Received November 10, 1999; accepted January 25, 2000

Abstract. Oscillator strengths for excitations of As I, As II, and As III from their ground states to various excited states are calculated using a semiempirical analytic independent-particle-model. The results are compared to experimental and theoretical data where possible. The results are of astrophysical interest.

Key words: oscillator strengths — As I, As II, As III — atomic data

1. Introduction

Accurate oscillator strengths are needed for the determination of chemical abundances in the atmospheres of astrophysical objects. Elemental abundance studies are used to address problems related to stellar evolution and chemically peculiar stars, to the interstellar medium, and to cosmology. The need for accurate oscillator strengths is particularly acute in ultraviolet astronomy, because of the dramatic increase in observational capabilities provided by orbiting observatories such as the Hubble Space Telescope. Most of the lines seen in spectra from the interstellar medium and stellar photospheres result from neutral and lowly ionized atoms. In the present work we study various transitions occurring in neutral arsenic, As I, and in singly- and doubly-ionized arsenic, As II and As III.

The first detection of arsenic in any star, including the sun, was made with the high-resolution Echelle spectrometer aboard the Hubble Space Telescope (Leckrone et al. 1991). The 1937.6 Å line of As I was detected for the first time in the ultraviolet spectrum of the bright, ultra-sharp-lined B-peculiar star, chi Lupi. This line results from the transition $4p^3(^4S^\circ_{3/2})\rightarrow 4p^2(^3P)5s(^4P_{3/2})$, which is discussed in Sect. 3 of the present work. Arsenic is known to be present in meteorites (Anders & Grevesse 1989). A knowledge of the oscillator strengths of As I is also important for an understanding of the mechanisms involved in arsenic lasers (Fowles et al. 1974).

The first detection of As II in the interstellar medium was made by the Goddard High Resolution Spectrograph aboard the Hubble Space Telescope (Cardelli et al. 1993). Oscillator strengths for various ultraviolet transitions in As II are discussed in Sect. 4 of this work. In Sect. 5 we present results for As III.

Table 1. Experimental and computed energy levels of As III. Units are in Rydbergs

Level	Experimental	Computed
4p	2.0813	2.0511
5s	1.1091	1.0920
6s	0.5970	0.5947
5p	0.8790	0.8807
4d	1.0087	1.0509
5d	0.5716	0.5762
4f	0.5859	0.5768
5g	0.3599	0.3605

2. Method of calculation

Each atom is a many-body system which may be described by an independent-particle-model. In this model, each electron moves independently in an effective potential determined by the nucleus and the other electrons. The potential for an electron in a neutral or ionized atom is assumed to have the form

$$V(r) = -(2/r)\{(Z-\eta)[H(e^{r/d}-1)+1]^{-1}+\eta\} \qquad (1)$$

where Z is the atomic number, and η is the ionicity: $\eta = 1, 2, 3$ for As I, As II, As III, respectively. The quantity r is the electron-nucleus distance, and d, H are adjustable parameters. The potential of equation (1) is inserted into the radial Schrödinger equation, which is then solved to obtain the energy eigenvalues and wave functions. The parameters d, H are adjusted so as to obtain agreement between the energy eigenvalues and the experimental single-particle energy levels. This procedure and all necessary formulas may be found in a previous article (Ganas 1995). The following values of the potential parameters were obtained: $d = 1.4196$, $H = 8.1745$ for As I; $d = 4.7814$, $H = 39.726$ for As II; $d = 0.6094$, $H = 3.0641$ for As III.

Table 2. Oscillator strengths, f, for the resonance transition $4p^3(^4S^\circ_{3/2}) \rightarrow 4p^2(^3P)5s(^4P_J)$ in As I, from the present calculations, other calculations, and experiment

J	λ(Å)	f (this calculation)	f (experiment)	f (other calculations)
1/2	1972.6	0.0532	0.059 ± 0.008^a	0.0584^d
			0.074^b, 0.0734^c	0.06^e, 0.03^f
3/2	1937.6	0.1064	0.123 ± 0.017^a	0.113^d
			0.14^b, 0.139^c	0.11^e, 0.06^f
5/2	1890.4	0.1596	0.21^b, 0.214^c	0.161^d, 0.16^e

[a] Bengtsson et al. (1992): uses time-resolved laser spectroscopy.
[b] Andersen et al. (1974): uses the beam-foil technique.
[c] Lotrian et al. (1980): uses emission spectroscopy.
[d] Verner et al. (1994): gives a critical review of f-values from previous compilations.
[e] Holmgren (1975): uses optimized Hartree-Fock-Slater local exchange approximation and relativistic wave functions.
[f] Lawrence (1967): uses an intermediate coupling theory.

Table 3. Oscillator strengths for As I for the transitions $4p^3(^4S^\circ_{3/2}) \rightarrow 4p^2(^3P)ns(^4P_J)$, $n > 5$, and $4p^3(^4S^\circ_{3/2}) \rightarrow 4p^2(^3P)nd(^4P_J)$, $n > 3$, from the present calculations

4p to	$J = 1/2$	$J = 3/2$	$J = 5/2$
6s	0.0075	0.0151	0.0226
7s	0.0027	0.0054	0.0081
8s	0.0013	0.0026	0.0039
9s	0.00072	0.0014	0.0022
4d	0.1981	0.3962	0.5943
5d	0.0551	0.1101	0.1652
6d	0.0234	0.0468	0.0702
7d	0.0123	0.0246	0.0369
8d	0.0072	0.0145	0.0217
9d	0.0050	0.0099	0.0149

Representative energy levels are given in Table 1 for As III. The computed levels and the experimental levels are in good agreement, the discrepancy being less than 2% in every case (except one).

3. Results for As I

The computed oscillator strengths for various transitions from the ground state of As I are presented in Tables 2 and 3. There is not a great deal of experimental and theoretical data available; in fact, there is data only for the resonance transition $4p^3(^4S^\circ_{3/2}) \rightarrow 4p^2(^3P)5s(^4P_J)$. For the $J = 1/2$ component of this transition, the presented calculated value, 0.0532, lies inside the range of experimental values, 0.059 ± 0.008 (Bengtsson et al. 1992), and is in reasonable agreement with the experimental values 0.074 (Andersen et al. 1974) and 0.0734 (Lotrian et al. 1980). Calculations have been performed using a variety of techniques. The present value, 0.0532, is in good agreement with the theoretical value 0.0584 (Verner et al. 1994) and lies between the theoretical values 0.03 (Lawrence 1967) and 0.06 (Holmgren 1975). For $J = 3/2$, the present value, 0.1064, lies just inside the experimental range 0.123 ± 0.017 (Bengtsson et al. 1992), and is in reasonable agreement with the experimental values 0.14 (Andersen et al. 1974) and 0.139 (Lotrian et al. 1980). The present value is in good agreement with the theoretical values 0.11 (Holmgren 1975) and 0.113 (Verner et al. 1994). For $J = 5/2$, the present value, 0.1596, is in reasonable agreement with the experimental values 0.21 (Andersen et al. 1974) and 0.214 (Lotrian et al. 1980), and is in excellent agreement with the theoretical values 0.16 (Holmgren 1975) and 0.161 (Verner et al. 1994).

In Table 3 we present our computed oscillator strengths for transitions to higher s-states and d-states. Due to the absence of any experimental or theoretical data on these transitions, no comparisons can be made.

Table 4. Oscillator strengths, f, for the transitions $4p^2(^3P_0) \rightarrow 4p(^2P^\circ)ns(^3P^\circ_1)$ and $4p^2(^3P_0) \rightarrow 4p(^2P^\circ)nd(^3P^\circ_1, {}^3D^\circ_1)$ from As II, from the present calculations, and other calculations

Upper State	λ (Å)	f (this calculation)	f (other calculations)
5s	1263.8	0.3547	0.32^a, 0.292^b, 0.26^c 0.23^d, 0.18^e
6s		0.0451	
7s		0.0150	
8s		0.00703	
9s		0.00392	
$4d(^3P^\circ_1)$	890.3	0.5166	0.20^d
$4d(^3D^\circ_1)$	1009.5	1.5497	1.4^d
$5d(^3P^\circ_1)$		0.0435	
$5d(^3D^\circ_1)$		0.1306	
$6d(^3P^\circ_1)$		0.0128	
$6d(^3D^\circ_1)$		0.0383	
$7d(^3P^\circ_1)$		0.00568	
$7d(^3D^\circ_1)$		0.0170	
$8d(^3P^\circ_1)$		0.00310	
$8d(^3D^\circ_1)$		0.00930	
$9d(^3P^\circ_1)$		0.00190	
$9d(^3D^\circ_1)$		0.00571	

[a] Cardelli et al. (1993): uses the Coulomb approximation with a Hartree-Slater core.
[b] Warner & Kirkpatrick (1969): uses scaled-Thomas-Fermi radial wave functions and intermediate coupling techniques.
[c] Bieron et al. (1991): uses a relativistic configuration interaction approach.
[d] Brage & Leckrone (1995): uses multiconfiguration Hartree-Fock and semiempirical configuration interaction techniques.
[e] Gruzdev (1968): uses the Coulomb approximation and an intermediate coupling scheme.

Table 5. Oscillator strengths, f, for the transitions $4s^2 4p(^2P^\circ_{1/2}) \rightarrow 4s^2 ns(^2S_{1/2})$ and $4s^2 4p(^2P^\circ_{1/2}) \rightarrow 4s^2 nd(^2D_{3/2})$ in As III, from the present calculations, other calculations, and experiment

Upper State	λ(Å)	f (this calculation)	f (experiment)	f (other calculations)
5s	937.3	0.1228	0.13 ± 0.02^a	0.125^b, 0.147^c 0.185^d
6s	613.9	0.0198		0.0192^b
7s		0.00738		
8s		0.00367		
9s		0.00212		
4d	850.0	0.9877	0.88 ± 0.15^a 1.30 ± 0.08^e	1.026^b, 1.437^f 1.531^d
5d	603.8	0.0797		0.0858^b, 0.153^d
6d		0.0223		
7d		0.00949		
8d		0.00500		
9d		0.00299		

[a] Andersen & Lindgard (1977): uses the beam-foil technique.
[b] Migdalek (1976): uses a relativistic semiempirical approach involving the Dirac equation.
[c] Migdalek (1983): uses a relativistic Hartree-Fock method.
[d] Marcinek & Migdalek (1993): uses a multiconfiguration Hartree-Fock method.
[e] Pinnington et al. (1981): uses the beam-foil technique.
[f] Aashamar et al. (1983): uses multiconfiguration optimized potential model.

4. Results for As II

The computed oscillator strengths for transitions from the ground state of As II are presented in Table 4. There is no experimental data available for any of the transitions considered, but there is some theoretical data available. For the $4p - 5s$ transition, the present value, 0.3547, is in good agreement with the theoretical value 0.32 (Cardelli et al. 1993), and is comparable to the theoretical values 0.292 (Warner & Kirkpatrick 1969), 0.26 (Bieron et al. 1991), and 0.23 (Brage & Leckrone 1995). For the $4p - 4d(^3D^\circ_1)$ transition, the present value, 1.5497, is in good agreement with the theoretical value 1.4 (Brage & Leckrone 1995). There appears to be no data available for the higher transitions.

5. Results for As III

The computed oscillator strengths for transitions from the ground state of As III are presented in Table 5. For the $4p - 5s$ transition, the present value, 0.1228, lies inside the range of experimental values 0.13 ± 0.02 (Andersen & Lindgard 1977). This value, 0.1228, is in good agreement with the theoretical value 0.125 (Migdalek 1976), and is comparable to the theoretical values 0.147 (Migdalek 1983) and 0.185 (Marcinek & Migdalek 1993). For the $4p - 6s$ transition, the present value, 0.0198, is in good agreement with the theoretical value 0.0192 (Migdalek 1976). For the $4p - 4d$ transition, the present value, 0.9877, lies inside the range of experimental values 0.88 ± 0.15 (Andersen & Lindgard 1977), but is outside the experimental range 1.30 ± 0.08 (Pinnington et al. 1981). The present value, 0.9877, is in good agreement with the theoretical value 1.026 (Migdalek 1976). For $4p - 5d$, the present value, 0.0797, is in good agreement with the theoretical value 0.0858 (Migdalek 1976). There is no experimental or theoretical data on the higher transitions $4p - ns$, $n > 6$, and $4p - nd$, $n > 5$.

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