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LIFETIMES AND OSCILLATOR STRENGTHS FOR THE $6p7s\,^3P_{0,1}$ LEVELS IN Bi II

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ABSTRACT

Lifetime measurements and empirical branching ratio estimates for the $6p7s\,^3P_0$ and $^3P_1$ levels in Bi II are reported, together with supporting theoretical calculations. These results are combined to yield absorption oscillator strengths between these levels and those of the $6p^2$ ground configuration. The results are discussed in the context of spectroscopic data obtained from orbiting telescopes.

Subject headings: atomic data — methods: laboratory

1. INTRODUCTION

Bismuth represents the last element in the chain of neutron capture nucleosynthesis that is radioactively stable. As such the quantitative analysis of its abundance in stellar atmospheres presents a constraint on the theories of nucleosynthesis for the very heavy elements. However, observations of its spectral lines in astronomical spectra have been limited to a scant few chemically peculiar stars. Jacobs & Dworetsky (1982) detected strong absorption lines of Bi II in the *International Ultraviolet Explorer* (*IUE*) satellite spectra of the HgMn-type star HR 7775 and determined that the abundance of bismuth in this star is approximately 6 orders of magnitude greater than in the solar system. Lines of Bi II have also been identified in the *IUE* spectra of the magnetic star HR 465 by Cowley (1987), using the wavelength coincidence statistic technique, and by Fuhrmann (1989). The latter study also finds strong evidence for lines of Bi II in the spectrum of the magnetic star α^2 CVn. Wahlgren et al. (1994) determined an upper limit abundance enhancement of 2.1 dex from the Bi II λ1902 Å line in the spectrum of the HgMn star χ Lupi using data from the *Hubble Space Telescope* Goddard High Resolution Spectrograph and a synthetic spectrum fitting technique.

Spectral searches among other chemically peculiar stars have not identified bismuth with any degree of certainty. The presence of Bi I lines in cooler stars, including the Sun, has not been detected. The meteoritic bismuth abundance (Anders & Grevesse 1989), along with theoretical nucleosynthesis calculations, imply that bismuth is a trace constituent, amounting to an abundance of $\log (N_{\rm Bi}/N_{\rm H}) = 0.7$, on a scale where $\log N_{\rm H} = 12.0$. Therefore, any search for bismuth spectral lines necessarily begins with its strongest transitions. For the warm chemically peculiar stars and certain components of the interstellar medium such lines would be the strongest lines of the singly ionized state, nearly all occurring at ultraviolet wavelengths. However, quantitative stellar abundance analyses are hindered by the limited number of lines for which oscillator strength data exist.

We report here oscillator strengths for $6s^26p^2$–$6s^26p7s$ transitions in Bi II, deduced from lifetime measurements of the $6p7s\,^3P^o_0$ and $6p7s\,^3P^o_1$ levels, and empirical estimates (based on measured energy level data) of the branching ratios of the $6p7s\,^3P^o_1$ to the $6p^2\,^3P_0$, $^3P_1$, $^3P_2$, $^1D_2$, and $^1S_0$ ground configuration levels. The work was supported by theoretical calculations that examine the validity of the single-configuration intermediate coupling (IC) approximation and determine the extent to which these levels are affected by configuration interaction (CI). The empirical approach was used to specify the IC in both the upper and lower levels through singlet-triplet mixing amplitudes determined from experimental energy level data (Kolyniak, Kornalewsky, & Roszkowska 1976; Crawford & McLay 1934). The results are compared with earlier theoretical (Beiroń, Marcinek, & Migdłek 1991; Gruzdev 1968) and experimental (Stanek, Musiol, & Labuz 1981) studies of the oscillator strengths as well as earlier investigations (Kwela, Zachara, & Hults 1981; Garstang 1964) of the degree of IC within the ground configuration.

2. EXPERIMENT

This experiment utilized the University of Toledo Heavy Ion Accelerator, and detailed descriptions of this facility are provided in the reports of earlier studies in this series (Irving et al. 1995; Henderson et al. 1996a, 1996b; Beideck et al. 1993a, 1993b), and in instrumentation reviews (Haar et al. 1993; Haar & Curtis 1993). Ions of Bi^+ and Bi^{2+} were produced in the ion source, accelerated through 20 kV, and magnetically analyzed. After momentum and mass-to-charge selection, the ions were postaccelerated to final energies (440 keV for Bi^{2+}). The ions then entered an electrostatic switchyard and were steered into the experimental station and collimated before passage through a thin carbon foil (ranging from 2.1 to 2.5 μg cm^{-2}). At the beam energy of 440 keV, the observed spectroscopic excitations were primarily in Bi II, Bi III, and Bi IV.

The Bi II emission lines were analyzed with an Acton 1 m normal incidence VUV monochromator, with three sets of concave gratings and detectors: a 1200 l mm^{-1} grating coupled with a solar blind detector for the 1437, 1777, and 1792 Å transitions, a 1200 l mm^{-1} grating coupled with a bi-alkali detector for the 1902 Å transition, and a 600 l mm^{-1} grating coupled with a bi-alkali detector for surveys of possible cascade transitions from higher lying states. Unfortunately, the most likely contributors to cascade repopulation have wavelengths long of 5100 Å, which are outside of our accessible detection window.

The postfoil velocity was determined from the machine calibration and foil energy loss to be 0.625 ± 0.016 mm ns^{-1}, with the tolerances including uncertainties in energy

calibration and foil thickness, as well as from possible beam divergence. The ions were produced from pure bismuth in the Danfysik Model 911A ion source. To minimize foil breakage, the current was limited to 100 particle nA.

Although the principal cascade repopulating transitions were not accessible to measurement, cascade distortions in the decay curves were found to be small and tractable. The fitting procedure was carried out using the nonlinear least-squares multiexponential fitting program DISCRETE (Provencher 1976). Since curve fitting of individual decay curves does not possess the internal consistency checks available when cascade-correlated decay curve analysis (ANDC) methods (Curtis, Berry, & Bromander 1971) are employed, nonstatistical errors were systematically investigated. The uncertainties in our multiexponential fits were computed by combining statistical uncertainties in the individual fits, scatter among the independent measurements, uncertainties in the beam velocity, and estimates of possible errors introduced by cascade corrections.

3. CALCULATIONS

3.1. *Theoretical Calculations*

Calculations of transition probabilities and intermediate coupling eigenvectors were performed using the program suite of Cowan (1981). The relativistic Hartree-Fock (HFR) mode was used, in which the leading single-particle relativistic corrections are included in the self-consistent–field procedure. Consistent results were obtained from four separate calculations: one single-configuration Hartree-Fock, and three CI calculations using 14 even-parity and 15 odd-parity configurations. The three CI calculations differed with regard to the empirical adjustment capability of the Cowan program RCG: in the first, no adjustments or scalings were done; in the second, the standard scaling was used, in which the electrostatic integrals are multiplied by 0.85 and the spin-orbit integrals by 0.95; in the third, we adjusted these scaling factors and the relevant individual energy integrals in order to reproduce the observed intervals within the $6p^2$ and $6p7s$ configurations. The transition probabilities and eigenvector percentages predicted by these four calculations agreed with each other quite well, generally to within 5%.

We chose to use the HFR method here rather than fully Dirac-relativistic ab initio multiconfiguration Dirac-Fock (MCDF) methods because we sought to assess the effects of CI on the branching fractions. As described above, the HFR method permits many configurations to be included with the option of optimizing through the use of observed energy level data. A comparative study of HFR and MCDF calculations of oscillator strengths has been carried out by Beiroń et al. (1991) which concludes that, for Bi II, the quasi-relativistic and fully relativistic approaches yield similar results.

3.2. *Empirical Calculations*

For a pure configuration, the intermediate coupling amplitudes are manifested both by the energy levels and by the transition probabilities of the levels. Thus, if the single configuration picture is valid, the measured energy level splittings within the upper and the lower configuration can be used to determine the mixing amplitudes, and these can then be used to specify (to within factors of the radial transition matrix) the relative transition probabilities. In the case of the sp and p^2 configurations, there are at most two normalized mixing amplitudes for a given value of J, which can be characterized by a singlet-triplet mixing angle θ_J. For sp the mixing between the $^3P_1$ and $^1P_1$ states can be characterized by θ_1, whereas for p^2 the mixing between the $^3P_0$ and $^1S_0$ states can be characterized by θ_0, and the mixing between the $^3P_2$ and $^1D_2$ can be characterized by θ_2. A formalism has been developed earlier (Curtis 1989) by which these mixing angles are first extracted from measured energy level data and then used to predict transition probabilities. For a p^2-sp manifold, the transitions from the upper level $sp\,^3P_1^o$ to the levels of the ground configuration p^2 can be deduced from this formalism (Curtis 1989) using the LS coupling angular transition matrices of Cowan (1981) to yield (using nominal LS notation)

$$\langle {}^3P_0 \,|\, \boldsymbol{r} \,|\, {}^3P_1^o \rangle = -\sqrt{20}\cos(\theta_1 + \theta_0)\langle p^2 \,|\, r \,|\, sp \rangle\,, \quad (1)$$

$$\langle {}^3P_1 \,|\, \boldsymbol{r} \,|\, {}^3P_1^o \rangle = \sqrt{15}\cos\theta_1\langle p^2 \,|\, r \,|\, sp \rangle\,, \quad (2)$$

$$\langle {}^3P_2 \,|\, \boldsymbol{r} \,|\, {}^3P_1^o \rangle = 5(2\sin\theta_1 \sin\theta_2 + \cos\theta_1 \cos\theta_2)\langle p^2 \,|\, r \,|\, sp \rangle\,, \quad (3)$$

$$\langle {}^1D_2 \,|\, \boldsymbol{r} \,|\, {}^3P_1^o \rangle = -5(2\sin\theta_1 \cos\theta_2 - \cos\theta_1 \sin\theta_2)\langle p^2 \,|\, r \,|\, sp \rangle\,, \quad (4)$$

$$\langle {}^1S_0 \,|\, \boldsymbol{r} \,|\, {}^3P_1^o \rangle = -\sqrt{20}\sin(\theta_1 + \theta_0)\langle p^2 \,|\, r \,|\, sp \rangle\,. \quad (5)$$

It should be noted that in a fully relativistic Dirac-Fock treatment the corresponding expressions would involve two separate jj-coupled radial transition matrices and will reduce to equations (1)–(5) only if these two radial matrices are equal. Theoretical studies of these quantities are currently in progress (Ellis, Brage, & Curtis 1996).

For pure sp and p^2 configurations the energy levels (and thereby the mixing angles) are specified (Curtis 1989) by three parameters which correspond to the energies associated with (1) the isotropic electrostatic interaction (F_0), (2) the angular dependent electrostatic electron-electron interaction, either direct (F_2) or exchange (G_1), and (3) the spin-orbit interaction (ζ_p). Since the sp and p^2 configurations contain four and five levels, respectively, the specification of these three parameters is overdetermined. We have handled this by first using the average energies ϵ_J of the $J = 0$, 1, and 2 levels to make a nonoverdetermined parametrization. We then computed the singlet-triplet splittings from this parametrization and tested the single configuration picture by comparing these results to the corresponding experimental splittings. Some authors (Trees 1951; Kwela et al. 1981) have instead removed the overdetermination by introducing additional empirical parameters to account for interactions with other configurations, but our results (both theoretical and empirical) indicate that CI effects for this system are small. Within this framework, the mixing angles θ_J can be determined from the relationships (Curtis 1989)

$$\cot(2\theta_J) = W_J\,, \quad (6)$$

where the sp mixing $J = 1$ level is given by

$$W_1 = \frac{\epsilon_2 - 3\epsilon_1 + 2\epsilon_0}{\sqrt{2}(\epsilon_2 - \epsilon_0)}\,, \quad (7)$$

and the p^2 mixing of the $J = 0$ and $J = 2$ levels is given by

$$W_0 = -\frac{10\epsilon_2 - 21\epsilon_1 + 11\epsilon_0}{4\sqrt{2}(5\epsilon_2 - 3\epsilon_1 - 2\epsilon_0)}\,, \quad (8)$$

$$W_2 = -\frac{5\epsilon_2 + 3\epsilon_1 - 8\epsilon_0}{2\sqrt{2}(5\epsilon_2 - 3\epsilon_1 - 2\epsilon_0)} . \quad (9)$$

In terms of the transition elements $\langle k|r|i\rangle$ given by equations (1)–(5), the oscillator strengths are given by

$$g_k f_{ki} = \left[\frac{303.75}{\lambda(\text{Å})}\right] |\langle k|r|i\rangle|^2 , \quad (10)$$

the transition probabilities are obtained from

$$A_{ik} = \frac{1}{3}\left[\frac{1265.38}{\lambda(\text{Å})}\right]^3 |\langle k|r|i\rangle|^2 , \quad (11)$$

and the branching fractions are defined as

$$BF_{ik} = A_{ik}/\sum_{k'} A_{ik'} . \quad (12)$$

4. RESULTS

The measured energy level data (Kolyniak et al. 1976; Crawford & McLay 1934) are given in Table 1, together with values obtained from the J-averaged IC parametrization and the subtracted differences. The values obtained for the energy parameters are listed in a footnote. Notice that, because of the overdetermination, the predicted singlet-triplet splittings are slightly narrower than the corresponding experimental values. This narrowing is 68 cm^{-1} (0.34%) for the $J = 1$ levels, 469 cm^{-1} (1.06%) for the $J = 0$ levels, and 540 cm^{-1} (3.2%) for the $J = 2$ levels, and indicates that the system is described quite well by the single configuration IC approximation. The theoretical calculations indicated that both the upper and lower configurations were relatively pure, with the relevant eigenvectors all showing less than 5% CI, further confirming that the system is accurately characterized by IC.

Our results for the measured lifetimes for the $6p7s\,^3P^o_0$ and $6p7s\,^3P^o_1$ levels are given in Table 2. The empirical reduction of the energy level data (Kolyniak et al 1976) yielded mixing angles $\theta_1 = 33.^\circ15$, $\theta_0 = -24.^\circ16$, and $\theta_2 = 42.^\circ83$. Earlier estimates for p^2 ground configuration mixing have been reported (Garstang 1964) as $\theta_0 = -24.^\circ4$ and $\theta_2 = 43.^\circ9$ and (Kwela et al. 1981) as $\theta_0 = -23.^\circ83$ and $\theta_2 = 45.^\circ24$. Assuming that the radial integrals are relatively insensitive over the supermultiplet, these mixing angles yield the branching ratios of the decay. The wavelengths (Reader & Corliss 1980; Wahlgren et al. 1994) for the various transitions from these two upper levels are given in Table 3, together with values for the branching ratios computed both theoretically (by adjusted HFR) and by the IC empirical method. The theoretical branching ratios were very close to the values obtained from the empirical methods, and we have chosen to use the empirical values because of their direct connection to experiment. Thus, the measurements for the lifetimes given in Table 2 were combined with the empirically computed branching fractions in Table 3 to yield the transition probabilities and absorption oscillator strengths, which are also listed in Table 3.

Calculations of these oscillator strengths have been reported using several alternative methods. Gruzdev (1968) applied the semiempirical Coulomb approximation to all of these transitions, and Wahlgren et al. (1994) made MCDF calculations for the 1902 Å transitions, and these results are listed in Table 3. Beiroń et al. (1991) explored various methods for including the effects of both relativity and CI,

TABLE 1

IC PARAMETRIZATION[a] OF ENERGY LEVELS

Level	E(obs)	E(IC)[b]	E(IC)–E(Obs)
$6p^2\,^3P_0$	0	235	+235
$6p^2\,^3P_1$	13325.57[c]	13326	0
$6p^2\,^3P_2$	17031.78[c]	17302	+270
$6p^2\,^1D_2$	33938.86[c]	33669	−270
$6p^2\,^1S_0$	44173.85[c]	43939	−235
$6p7s\,^3P^o_0$	69133[d]	69133	0
$6p7s\,^3P^o_1$	69598[d]	69632	+34
$6p7s\,^3P^o_2$	88769[d]	88769	0
$6p7s\,^1P^o_1$	89883[d]	89849	−34

[a] Curtis 1989; in cm^{-1}.

[b] $F_0 = 24{,}937$, $F_2 = 1168$, $\zeta_p = 11{,}540$ for $6p^2$; $F_0 = 83{,}013$, $G_1 = 790$, $\zeta_p = 13{,}091$ for $6p7s$.

[c] Kolyniak et al. 1976.

[d] Crawford & McLay 1934 (also reprinted by Moore 1957).

TABLE 2

MEASURED LIFETIMES

Level	$\tau(ns)$
$6p7s\,^3P_0$	1.56 ± 0.15
$6p7s\,^3P_1$	1.24 ± 0.08

TABLE 3

TRANSITION PROBABILITIES AND OSCILLATOR STRENGTHS

Transition	λ (Å)[a]	BF(Emp)[b]	BF(Theo)[c]	A (ns^{-1})[d]	gf[d]	gf_{other}
$6p^2\,^3P_1$–$6p7s\,^3P^o_0$	1791.93[e]	1.00	1.00	0.64	0.31	0.21[f], 0.28[g]
$6p^2\,^3P_0$–$6p7s\,^3P^o_1$	1436.83[e]	0.43	0.44	0.34	0.32	0.25[f], 0.31[g]
$6p^2\,^3P_1$–$6p7s\,^3P^o_1$	1777.11[e]	0.12	0.12	0.10	0.14	0.11[f], 0.18[g]
$6p^2\,^3P_2$–$6p7s\,^3P^o_1$	1902.31[h]	0.44	0.44	0.35	0.58	0.45[f], 0.57[g], 0.60[i]
$6p^2\,^1D_2$–$6p7s\,^3P^o_1$	2804.2[e]	0.004	0.006	0.003	0.01	0.01[f], 0.04[g]
$6p^2\,^1S_0$–$6p7s\,^3P^o_1$	3933.3[e]	0.0005	0.0009	0.0004	0.003	0.002[f], 0.01[g]

[a] Vacuum wavelengths.

[b] Empirical, using $\theta_1 = 33.^\circ15$, $\theta_0 = -24.^\circ16$, $\theta_2 = 42.^\circ84$.

[c] This work, adjusted HFR.

[d] This work, using measured τ and empirical BF.

[e] Reader & Corliss 1980.

[f] Gruzdev 1968, Coulomb approximation.

[g] Beiroń et al. 1991, MCDM-OL calculation.

[h] Wahlgren et al. 1994, strongest hfs component.

[i] Wahlgren et al. 1994, MCDF-EOL calculation.

obtaining a rather wide range of oscillator strengths. Our results reported in Table 3 are generally consistent with this range of values, but do not agree for all six transitions with any specific set of these calculations. Thus, we have selected for inclusion in Table 3 the geometric mean of the length and velocity gauges for the set of calculations denoted as MCDM-OL by Beiroń et al (1991). An emission measurement has been reported (Stanek et al. 1981) for the relative transition probability of the λ2804 line, which was normalized using a lifetime measurement (Osherovich & Tezikov 1978) for the $6p8p\,^3D_1$ level. This yielded a result $A(2804) = 0.07\ \mathrm{ns}^{-1}$ which is much larger than our value.

5. CONCLUSION

Lifetime measurements have been combined with branching ratios determined empirically from spectroscopic data to obtain oscillator strengths. The branching fractions are confirmed by nonrelativistic theoretical calculations, and the oscillator strengths are established (within the nonrelativistic framework) to a precision of 10%. The results presented here are consistent with the theoretical results used by Wahlgren et al. (1994) for the λ1902 transitions and thus do not alter the conclusions of that study. The revision of several oscillator strengths employed by Jacobs & Dworetsky (1982) is also small and thus does not alter their conclusions regarding the unusually high apparent surficial bismuth abundance in HR 7775.

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