J. Astrophys. Astr. (2007) **28,** 157–166

Forbidden Transition Probabilities of Astrophysical Interest among Low-lying States of V III

Andrei Irimia
Department of Physics and Astronomy, Vanderbilt University, Nashville, Tennessee, 37235, USA.
e-mail: andrei.irimia@vanderbilt.edu

Received 2005 May 15; accepted 2007 August 7

Abstract. Electric and magnetic multipole transitions among low-lying states of doubly ionized vanadium were computed using the multi-configuration Hartree–Fock (MCHF) method with Breit–Pauli (BP) corrections to a non-relativistic Hamiltonian. Energy levels were determined up to and including $3d^2(^1G)4s$ b $^2G_{7/2}$ and computed energies were found to be in good agreement with experiment and other theories. In addition to Einstein A_{ki} coefficients for some E2 and M1 transitions, lifetime data and selected weighted oscillator strengths are also reported.

Key words. Atomic structure calculations—atomic data—oscillator strength—lifetimes.

1. Introduction

Vanadium transition data are useful in a wide range of scientific applications. Ionized vanadium, for example, has been used in plasma diagnosis (Wagatsuma & Danzaki 1999), where physical properties such as electron temperature and concentration can be determined by analyzing the intensity and width of spectral lines (Griem 1964). Lines of forbidden ionized vanadium were observed in the spectra of B[e] stars by Jaschek & Andrillat (1997) while Lodders (2002) studied the abundance of this element in low-mass dwarf stars. A chemical abundance study of brown dwarfs made use of vanadium spectroscopic data to determine its depletion in these astrophysical objects (Burrows *et al.* 2000; Gounelle *et al.* 2001) used spectral data of vanadium for a study of cosmic-ray irradiation in early solar-system rocks. Yields of this element in massive stars were modeled by Samland (1998), who made the observation that an accurate interpretation of the observational database for vanadium is restricted at the present time by the fact that abundance determinations for metal-poor and solar-metalicity stars are missing. Transition data in vanadium were also used by Whaling *et al.* (1985) and Biemont *et al.* (1989) to determine the solar abundance of this element.

Experimental studies of the Sc-like isoelectronic sequence are few in spite of dating as far back as the 1920s (Gibbs & White 1927; White 1929a, 1929b; Goly 1978;

Bromage 1978). Gibbs & White (1927) determined the wavelengths and relative positions of multiplets in the V III spectrum while White (1929a, 1929b) focused on investigating term separations for this ion. Ekberg (1976) observed the spectrum of V III in a vacuum sliding-spark discharge experiment and made contributions to our present understanding of this ion. Radiative lifetimes for excited states in V III were measured by Andersen *et al.* (1977) for a few $3d^2\ 4p$ levels using a beam-foil experiment, but their data do not include lifetimes for the metastable levels of the $3d^3$ and $3d^2\ 4s$ configurations. In recent years, Stark broadening parameters for spectral lines of V I, V II and V III were determined by Popovic & Dimitrijevic (2000).

Early theoretical investigations of V III include a spectrum calculation by Many (1946) and a study of d^3 and d^4 configurations of vanadium by Meshkov (1954). In 1963, Mendlowitz computed intermediate-coupling transition strengths for $d^2\ d \rightarrow d^2 p$ and $d^3 \rightarrow d^2 p$ allowed transitions.

A spin-dependent interaction calculation for this spectrum was performed by Pasternak & Godschmidt (1972) and some oscillator strengths were determined by Roberts (1973), who also computed the lifetimes of several $3d^2(a\ ^3F)4p$ levels. An atomic partition function calculation for some Ti and V ions – including V III – was done in 1988 by Halenka (1988), followed by Zilitis (2001), who employed the Dirac-Fock method to study the structure of the energy level system and to determine ionization potentials for 39 Sc-like ions.

In the scandium sequence, some forbidden transitions were computed by Luke (1997) for singly ionized vanadium and atomic data have also been published for V II (Roberts 1973; Halenka 1988) and V V (Berry 1976). Nevertheless, a similar study involving doubly ionized vanadium has not yet been performed. In a 2003 compilation of resonance absorption lines for wavelengths longward of the Lyman limit, Morton (2003) mentioned the lack of sufficient atomic data for V III and indicated the work of Kurucz (1998) as one of the very few recent sources of reliable tabulations for this ion.

Forbidden transitions play an important role in many astrophysical applications, particularly in the interpretation of spectra of diluted astrophysical plasmas, where energy is transfered to the plasma via excitation and ionization processes. Because astrophysical plasma densities are very low, the probability of collisions is small and many states decay by M1 or E2 transition radiation. This is why forbidden transitions are useful indicators of plasma densities, indicating a need for both experimental and theoretical data for such transitions (Hartman *et al.* 2003).

Forbidden lines of the Sc-like ions have recently come under much attention as a result of the FERRUM project (Hartman *et al.* 2003), in which the laser probing technique was extended at the CRYRING storage ring to measure extremely long lifetimes, such as that of the metastable $3d^2(^3P)4s$ b $^4P_{5/3}$ level in Ti II. With the recent lifetime measurement of a very long-lived (520^{+310}_{-140} s) metastable state in strontium (Yasuda & Katori 2004), the growing importance of atomic data for forbidden lines – including for the Sc-like sequence – cannot be overstated. In this paper, we present the results of a V III spectrum calculation for states up to and including $3d^2(^1G)4s$ b $^2G_{7/2}$ using the multi-configuration Hartree Fock (MCHF) method with Breit–Pauli corrections. In addition to energy levels and non-relativistic oscillator strengths, we report lifetimes for the excited states computed as well as A_{ki} coefficients for E2 and M1 transitions in this atom. This is the first theoretical investigation of forbidden lines and metastable state lifetimes for the lower portion of the V III spectrum.

2. Computational approach

In the non-relativistic MCHF approach (Froese Fischer 1991), the wave function Ψ of state γLS is written as

$$\Psi(\gamma LS) = \sum_j c_j \Phi\left(\gamma_j LS\right), \tag{1}$$

where γ denotes the dominant configuration as well as any other quantum numbers required to specify the state uniquely. The wave function Ψ is expanded in terms of configuration state functions (CSFs) that have an identical LS symmetry but different electronic configurations γ_j. A basis consisting of one-electron spin-orbital functions

$$\phi_{nlm_l m_s} = \frac{1}{r} P_{nl}(r) Y_{lm_l}(\theta, \phi)\, \chi_{m_s} \tag{2}$$

is used to build the CSFs. Radial functions are determined by the CSFs included in the expansion and they are subjected to the requirement of orthonormality within each l symmetry:

$$\int_0^\infty P_{n'l}(r) P_{nl}(r) dr = \delta_{n'n}. \tag{3}$$

Since the orbitals obtained using the MCHF procedure are eventually used in a Breit–Pauli configuration interaction (CI) calculation involving many LS terms, our method optimizes on a weighted linear combination of energy expressions thereby optimizing simultaneously for a group of terms. In the multiconfiguration self-consistent field (MC–SCF) approach, both radial functions and expansion coefficients are determined so that the energy functional

$$\langle \gamma LS | \mathcal{H} | \gamma LS \rangle \tag{4}$$

is left stationary. The iterative Davidson algorithm (Davidson 1975) is used to determine the desired eigenvalues and eigenvectors.

Because the Breit–Pauli interaction matrix must be computed from one orthonormal orbital basis, LS terms are grouped according to the term interaction. Simultaneous optimization of the radial functions is performed on all LS states that were grouped together. After obtaining the set of radial orbitals, relativistic corrections are taken into account within the BP approximation by diagonalizing the BP Hamiltonian (Froese Fischer 1997) to obtain the intermediate coupling functions

$$\Psi(\gamma J) = \sum_{LS} \sum_j c_j(LSJ) \Phi(\gamma_j LSJ). \tag{5}$$

The expansion coefficients $c_j(LSJ)$ and the corresponding energy $E(LSJ)$, are an eigenvector and eigenvalue, respectively, of the interaction matrix. All contributors to the Breit–Pauli Hamiltonian were included in the present calculation with the exception of the orbit–orbit interaction term, which does not contribute to interactions between CSFs from different LS terms. It is convenient to think of the Breit–Pauli interaction matrix as having a block structure, in that diagonal blocks are the interactions within an LS term, while off-diagonal blocks represent the interaction between the

terms. Two LS terms are referred to as interacting if, for some value of J, there are non-zero interactions in the off-diagonal block for the pair of LS terms.

Weighted oscillator strengths gf are computed here using the length and velocity gauges given by

$$g_i f_l(ik) = \frac{2}{3}\Delta E_{ik}\left|\left\langle \Psi_i \left|\left| \sum_j \mathbf{r}_j \right|\right| \Psi_k \right\rangle\right|^2 \tag{6}$$

and

$$g_i f_v(ik) = \frac{2}{3}\frac{1}{\Delta E_{ij}}\left|\left\langle \Psi_i \left|\left| \sum_j \nabla_j \right|\right| \Psi_k \right\rangle\right|^2, \tag{7}$$

respectively. In the equations above, g_i is the degeneracy factor, i.e., $g_i = (2L_i + 1)(2S_i + 1)$ for LS-coupled wave functions and $g_i = (2J_i + 1)$ for BP wave functions.

In the computational approach employed here, an active set (AS) of orbitals was used to determine wave function expansions. The latter were obtained for increasing sizes of the principal quantum number n and the convergence of the calculation was monitored by observing the agreement of the non-relativistic length and velocity gauges of the oscillator strength. Since the length gauge is correct to $\mathcal{O}(\alpha^2)$ while the velocity gauge requires a relativistic correction to the gradient operator (Drake 1972), both gauges are reported in this work. Throughout this paper, we refer to the $\{1s, 2s, 2p, \ldots, 3s, 3p, 3d\}$ set of orbitals as the $n = 3$ orbital set, $\{1s, 2s, 2p, \ldots, 4s, 4p, 4d, 4f\}$ as $n = 4$, etc. In the case of the present calculation, expansions were obtained for orbital sets with $n = 4, \ldots, 6$ and $s \leq l \leq g$ by means of generating single (S) and double (D) excitations from a multi-reference set, where $1s^2 2s^2 2p^6$ was considered to form a closed common core and the multi-reference set contained the configurations $3d^3$ and $3d^2 4s$. Configuration states from SD excitations which did not interact with at least one member of the multi-reference set were discarded.

The number of CSFs included in the calculation increases rapidly both with n and with the number of electrons outside the common core. Since large orbital sets can result in a considerable increase in computational time required for the problem, appropriate restrictions are necessary. For this reason, for each of $n = 7, 8, 9$, only expansions over even $3d\ nl\ n'l'$ configuration states (where nl and $n'l'$ are orbitals from the orbital set) were added to the existing set of CSFs.

Once radial functions were determined for each group, the Breit–Pauli CI calculations were performed and transition data determined for these wave functions. All E2, E3, M1, M2 and M3 transitions between the states targeted by the calculation were computed. To improve the reliability of the mixing of LS terms in the Breit–Pauli interaction matrix, fine-tuning (Hibbert 1993) was applied to its elements. In this process, adjustments were made to the matrix elements that shift all diagonal components of a given LS block by a fixed amount. This shift was the difference of an *ab initio* energy level and the observed level. If more than one eigenstate in a group had the same LS value as, for example, $3d^3$ a ^4F and $3d^2$b $4s^4F$, energy adjustments were made separately for each of the eigenstates with different shifts for ^4F.

Table 1. Breit–Pauli energies, energy differences (computed – observed (NIST), in cm^{-1}), splittings (in cm^{-1}), and lifetimes (in s) for excited states up to and including $3d^2(^1G)4s$ b $^2D_{3/2}$ after fine-tuning.

Config.	Term	J	Energy	Diff.	Splitting	Lifetime
$3d^3$	a ^4F	3/2	0.00			
		5/2	176.72	31.22	176.72	4.1984E+03
		7/2	400.29	58.79	400.29	2.0642E+03
		9/2	646.92	63.12	646.92	2.4716E+03
	a ^4P	1/2	11482.92	−30.88		2.3032E+01
		3/2	11618.03	26.23	135.12	2.3673E+01
		5/2	11774.37	4.67	291.46	2.5194E+01
	a ^2G	7/2	11948.37	−17.93		7.6451E+02
		9/2	12204.93	17.93	256.57	4.9393E+03
	a ^2P	3/2	15459.73	−90.57		9.8242E+02
		1/2	15670.38	90.58	210.65	1.1899E+04
	a ^2D	3/2	16205.37	−125.13		4.4811E+04
		5/2	16502.87	128.17	297.51	3.2689E+03
	a ^2H	9/2	16793.77	−17.13		1.4307E+04
		11/2	16994.74	17.14	200.97	5.9964E+03
	a ^2F	7/2	27724.56	−3.24		8.2104E+00
		5/2	27850.05	3.25	125.50	7.2835E+00
	b ^2D	5/2	42261.58	−5.82		1.6962E−01
		3/2	42371.21	0.01	109.64	1.6224E−01
$3d^2(^3F)4s$	b ^4F	3/2	43893.05	−49.44		1.1551E−02
		5/2	44095.10	−14.94	202.06	1.1435E−02
		7/2	44354.29	8.47	461.25	1.1297E−02
		9/2	44646.95	−0.01	753.90	1.1160E−02
	b ^2F	5/2	49314.12	−13.62		1.7603E−02
		7/2	49818.90	13.61	504.78	1.6899E−02
$3d^2(^1D)4s$	c ^2D	5/2	56204.84	44.42		1.1082E−02
		3/2	56212.33	−44.42	7.49	1.1234E−02
$3d^2(^3P)4s$	b ^4P	1/2	56567.40	38.10		4.5039E−03
		3/2	56703.31	34.26	135.91	4.4934E−03
		5/2	56850.12	−72.38	282.72	4.4967E−03
	b ^2P	1/2	61570.04	−8.70		1.2980E−02
		3/2	61785.86	8.71	215.82	1.2495E−02
$3d^2(^1G)4s$	b ^2G	9/2	63307.35	4.23		7.2629E−03
		7/2	63310.81	−4.24	3.45	7.1578E−03

Table 2. Convergence trends for some non-relativistic weighted oscillator strengths (gf values) in V III. Per cent differences were computed according to the formula $[gf(l) - gf(v)] \times 100/\max\{gf(l),\ gf(v)\}$.

$3d^3$ a $^4F - 3d^2(^1G)4s$ b ^4P				$3d^3$ a $^2H - 3d^2(^1G)4s$ b ^2G			
n	$gf(l)$	$gf(v)$	Diff. (%)	n	$gf(l)$	$gf(v)$	Diff. (%)
4	9.82E−7	7.74E−7	21.2	4	1.21E−6	8.99E−7	25.6
5	8.80E−7	7.32E−7	16.8	5	1.06E−6	8.78E−7	17.2
6	8.70E−7	7.55E−7	13.3	6	1.03E−6	9.00E−7	12.5
7	8.60E−7	7.90E−7	8.2	7	1.01E−6	9.46E−7	6.3
8	8.60E−7	7.91E−7	8.1	8	1.01E−6	9.49E−7	6.0
9	8.59E−7	7.92E−7	7.8	9	1.01E−6	9.50E−7	5.8

Table 3. Non-relativistic weighted oscillator strengths (gf values) in V III. Per cent differences were computed according to the formula $[gf(l) - gf(v)] \times 100/\max\{gf(l),\ gf(v)\}$.

Transition			$gf(l)$	$gf(v)$	Diff. (%)
$3d$ a ^2G	–	$3d$ a ^2D	1.518E−11	1.683E−11	9.8
$3d$ a ^2G	–	$3d$ a ^2G	5.290E−07	5.546E−07	4.6
$3d$ a ^2G	–	$3d^2(^3F)4s$ c ^2D	2.416E−07	2.545E−07	5.1
$3d$ a ^2G	–	$3d^2(^3P)4s$ b ^2P	9.975E−08	1.050E−07	5.0
$3d$ a ^2D	–	$3d^2(^1G)4s$ b ^2G	3.468E−08	3.548E−08	2.3
$3d^2(^3F)4s$ b ^2F	–	$3d^2(^3P)4s$ b ^2P	1.862E−09	1.775E−09	4.7

3. Results and discussion

In Table 1, we present our computed energies for the V III spectrum up to and including $3d^2(^1G)4s$ b $^2G_{7/2}$. In addition to LS term splittings, we also report energy differences (computed – observed (NIST Online Database)) and lifetimes for the excited states. The differences from observed are very good for these term energies. The separation between the levels of each term determines its spread and the computed separation would be the same as observed if term separations were exact.

One feature that makes the Sc-like isoelectronic sequence somewhat unusual is the fact that the ground state configuration changes along each of the first three members of the sequence. Thus, the ground state configuration changes from $3d\ 4s^2$ in Sc I to $3d^2\ 4s$ in Ti II to $3d^3$ in V III. The lowest odd-parity configuration in Sc I is $3d\ 4s\ 4p$, replaced by $3d^2\ 4p$ in both Ti II and V III. Although the separation between $3d^2\ 4s$ even-parity levels and the ground state increases from $Z = 21$ to $Z = 23$, this phenomenon occurs slower than it does for odd-parity $3d^2\ 4p$ levels. The net result of this is that $3d^2\ 4s$ remains the lowest excited configuration in V III, excluding the ground state configuration $3d^3$. Thus, the lowest portion of the V III spectrum is populated by 34 even-parity levels that belong to the $3d^3$ and $3d^2\ 4s$ configurations. As Table 1 shows, these levels are metastable because the excited electron can only decay via forbidden electric (E2, E4) and magnetic (M1, M3) multipole transitions. For

Table 4. Einstein A_{ki}-coefficients in s^{-1} for selected E2 transitions after fine-tuning[a]. Per cent differences were computed according to the formula $[A_{ki}(L) - A_{ki}(V)] \times 100/\max\{A_{ki}(L),\ A_{ki}(V)\}$.

Transition			$A_{ki}(L)$	$A_{ki}(V)$	Diff. (%)
$3d^3$ a $^2D_{5/2}$	–	$3d^2(^1D)4s$ c $^2D_{5/2}$	1.79E+01	1.86E+01	−3.85
	–	$3d^2(^1D)4s$ c $^2D_{3/2}$	6.69E+00	6.97E+00	−4.03
	–	$3d^2(^1D)4s$ b $^2P_{1/2}$	8.16E+00	8.74E+00	−6.55
$3d^3$ a $^2D_{3/2}$	–	$3d^2(^1D)4s$ c $^2D_{5/2}$	4.62E+00	4.77E+00	−3.21
	–	$3d^2(^1D)4s$ c $^2D_{3/2}$	1.61E+01	1.67E+01	−3.39
	–	$3d^2(^1D)4s$ b $^2P_{3/2}$	6.19E+00	6.58E+00	−5.94
	–	$3d^2(^1D)4s$ b $^2P_{1/2}$	1.21E+01	1.30E+01	−6.84
$3d^3$ a $^2D_{3/2}$	–	$3d^2(^1G)4s$ b $^2G_{7/2}$	2.27E+00	2.32E+00	−2.14
$3d^3$ a $^2D_{5/2}$	–	$3d^2(^1G)4s$ b $^2G_{9/2}$	2.61E+00	2.64E+00	−0.97
	–	$3d^2(^1G)4s$ b $^2G_{7/2}$	2.62E+00	2.65E+00	−1.31
	–	$3d^2(^1G)4s$ b $^2D_{5/2}$	1.79E+01	1.86E+01	−3.80
$3d^3$ a $^2D_{5/2}$	–	$3d^2(^1G)4s$ b $^2G_{9/2}$	2.61E+00	2.64E+00	−0.97
	–	$3d^2(^1D)4s$ b $^2G_{7/2}$	2.62E−01	2.65E−01	−1.31
$3d^3$ a $^2F_{7/2}$	–	$3d^2(^3F)4s$ b $^2F_{7/2}$	3.33E−01	3.19E−01	4.20
	–	$3d^2(^3F)4s$ b $^2F_{5/2}$	4.76E−02	4.77E−02	−0.21
$3d^3$ a $^2F_{5/2}$	–	$3d^2(^3F)4s$ b $^2F_{7/2}$	3.88E−02	3.74E−02	3.64
	–	$3d^2(^3F)4s$ b $^2F_{5/2}$	2.77E−01	2.79E−01	−0.83
$3d^3$ a $^2H_{11/2}$	–	$3d^2(^1G)4s$ b $^2G_{9/2}$	6.70E+01	6.70E+01	0.00
	–	$3d^2(^1G)4s$ b $^2G_{7/2}$	3.22E+00	3.22E+00	0.05
$3d^3$ a $^2H_{9/2}$	–	$3d^2(^1G)4s$ b $^2G_{9/2}$	3.93E+00	3.94E+00	−0.19
	–	$3d^2(^1G)4s$ b $^2G_{7/2}$	6.89E+01	6.90E+01	−0.15
$3d^2(^1D)4s$ c $^2D_{3/2}$	–	$3d^2(^1D)4s$ c $^2D_{5/2}$	7.98E−20	8.50E−20	−6.15
$3d^2(^3F)4s$ b $^2F_{7/2}$	–	$3d^2(^1D)4s$ c $^2D_{5/2}$	1.34E−05	1.29E−05	4.09
$3d^2(^3F)4s$ b $^2F_{5/2}$	–	$3d^2(^1D)4s$ c $^2D_{3/2}$	2.00E−05	1.95E−05	2.60

[a]The velocity form of the transition operator has neglected some relativistic corrections and hence, unlike the length form, is not correct in that, some terms of order α^2 have been omitted. The values of the length and velocity gauges have significance when term mixing is small and the transition is spin-allowed.

example, the lowest excited level $3d^3$ a $^4F_{5/2}$ has a very long lifetime of approximately 69 minutes. In the case of several other excited levels, the nature of the spectrum causes their primary decay channels to involve magnetic octupole (M3) transitions, which dramatically lengthens their associated lifetimes. As the table suggests, $3d^3$ levels are all very long-lived, while $3d^2$ $4s$ levels have shorter lifetimes, *albeit* still of the order of hundredths of a second.

Because the lifetimes of excited levels in V III involve highly forbidden transitions that have very small Einstein A_{ki} coefficients, the computation of transition proba-

Table 5. Einstein A_{ki}-coefficients in s^{-1} for selected M1 transitions after fine-tuning.

Transition			A_{ki}
$3d^3$ a $^4P_{3/2}$	–	$3d^3$ b $^4P_{5/2}$	6.18456E−05
$3d^3$ a $^2P_{1/2}$	–	$3d^3$ b $^2P_{3/2}$	8.40396E−05
$3d^3$ a $^2D_{3/2}$	–	$3d^3$ a $^2D_{5/2}$	2.84062E−04
$3d^3$ a $^2F_{7/2}$	–	$3d^3$ a $^2F_{5/2}$	3.04621E−05
$3d^3$ a $^2G_{7/2}$	–	$3d^3$ a $^2G_{9/2}$	2.02458E−04
$3d^3$ a $^2D_{5/2}$	–	$3d^3$ b $^2D_{5/2}$	8.46173E−11
$3d^3$ a $^2D_{5/2}$	–	$3d^3$ b $^2D_{3/2}$	4.33143E−02
$3d^3$ a $^2D_{3/2}$	–	$3d^3$ b $^2D_{5/2}$	2.95112E−02
$3d^3$ a $^2D_{3/2}$	–	$3d^3$ b $^2D_{3/2}$	1.40610E−11
$3d^3$ a $^2F_{7/2}$	–	$3d^2(^3F)4s$ b $^2F_{7/2}$	1.94999E−12
$3d^3$ a $^2F_{7/2}$	–	$3d^2(^3F)4s$ b $^2F_{5/2}$	3.96734E−04
$3d^3$ a $^2F_{5/2}$	–	$3d^2(^3F)4s$ b $^2F_{7/2}$	3.13588E−04
$3d^3$ a $^2F_{5/2}$	–	$3d^2(^3F)4s$ b $^2F_{5/2}$	2.37724E−13
$3d^3$ a $^4P_{5/2}$	–	$3d^2(^3F)4s$ b $^4P_{3/2}$	2.39644E−05
$3d^3$ a $^2D_{5/2}$	–	$3d^2(^1D)4s$ c $^2D_{5/2}$	3.32393E−13
$3d^3$ a $^2D_{5/2}$	–	$3d^2(^1D)4s$ c $^2D_{3/2}$	6.43609E−06
$3d^3$ a $^2D_{3/2}$	–	$3d^2(^1D)4s$ c $^2D_{5/2}$	6.21414E−06
$3d^3$ a $^2D_{3/2}$	–	$3d^2(^1D)4s$ c $^2D_{3/2}$	6.78299E−14
$3d^3(^3F)4s$ b $^2F_{5/2}$	–	$3d^2(^3F)4s$ b $^2F_{7/2}$	1.48676E−03
$3d^3(^3F)4s$ b $^4F_{7/2}$	–	$3d^2(^3F)4s$ b $^4F_{9/2}$	6.76096E−04
$3d^3(^3P)4s$ b $^4P_{3/2}$	–	$3d^2(^3P)4s$ b $^4P_{5/2}$	5.12022E−05

bilities in this ion requires a very high level of accuracy. To ensure the convergence of our calculation, the length and velocity gauges of the non-relativistic weighted oscillator strength (gf values) were monitored. If convergence is achieved as the active set of orbitals is expanded, the agreement between the two gauges should improve. In Table 2, we present convergence trends for two forbidden transitions between excited levels. In both cases, the label change is $3d \rightarrow 4s$, which makes such transitions suitable for testing how well correlation was captured by our calculation.

In Table 3, we present several other computed oscillator strengths for transitions between excited levels where the change $3d \rightarrow 4s$ occurs. We also include one case of a parent-changing ($^3F \rightarrow ^3P$) transition between two excited levels of the $3d^2\ 4s$ configuration. For all these transitions, the agreement of the two gauges is excellent in spite of their small magnitudes.

Some Einstein A_{ki} coefficients for electric quadrupole and magnetic dipole transitions in V III are made available in Tables 4 and 5, respectively. The selection of these A_{ki} values was made on the basis of their magnitudes and contributions to the associated decay channels. For many of the computed levels in V III, the accuracy of A_{ki}

values for E2 and M1 transitions is essential in determining the accuracy of lifetime data. This is because, for the most part, A_{ki} coefficients for E4 and M3 transitions were found to have much lower values than their E2 and M1 counterparts. This indicates that the corresponding E4 and M3 decay channels have negligible contributions to the reported lifetimes whenever E2 and/or M1 decay channels are also available for a certain level.

4. Conclusion

In summary, we have computed forbidden transitions of astrophysical interest among low-lying states of V III using the MCHF approach with BP corrections to a non-relativistic Hamiltonian. Excellent agreement was obtained between computed and observed energy levels and convergence trends for the weighted oscillator strengths were also satisfactory. Good agreement between the length and velocity gauges of these quantities was obtained, although typically this is notoriously difficult to achieve for forbidden transitions since the g_f values associated with them are usually small. Some Einstein A_{ki} coefficients were also presented.

References

Andersen, T., Petersen, P., Biemont, E. 1977, *J. Quant. Spectrosc. Radiat. Transfer*, **17**, 389.
Berry, H. G. 1976, *Phys. Scripta*, **13**, 36.
Biemont, E., Grevesse, N., Faires, L. M., Marsden, G., Lawler, J. E., Whaling, W. 1989, *Astron. Astrophys.*, **209**, 391.
Bromage, G. E. 1980, *Astron. Astrophys. Suppl.*, **41**, 79.
Burrows, A., Marley, M. S., Sharp, C. M. 2000, *Astrophys. J.*, **531**, 438.
Davidson, E. R. 1975, *J. Comput. Phys.*, **17**, 87.
Drake, G. W. R. 1972, *Phys. Rev. A*, **5**, 1979.
Ekberg, J. O. 1976, *Phys. Scripta*, **13**, 111.
Froese Fischer C. 1991, *Comput. Phys. Commun.*, **74**, 415.
Froese Fischer, C., Brage, T., Jönsson, P. 1997, *Computational Atomic Structure – An MCHF Approach* Bristol: IOP Publishing.
Gibbs, R. C., White, H. E. 1927, *Phys. Rev.*, **29**, 655.
Goly, A. 1978, *Astron. Astrophys.*, **68**, 79.
Griem, H. R. 1964, *Plasma Spectroscopy*, McGraw-Hill, NY.
Gounelle, M., Shu, F. H., Shang, H., Glassgold, A. E., Rehm, K. E., Lee, T. 2001, *Astrophys. J.*, **548**, 1051.
Halenka, J. 1988, *Astron. Astrophys. Suppl.*, **75**, 47.
Hartman, H. *et al.* 2003, *J. Phys. B: At. Mol. Opt. Phys.*, **36**, L197.
Hibbert, A. 1993, *Phys. Scripta*, **T65**, 104.
Jaschek, C., Andrillat, Y. 1997, *Astron. Astrophys. Suppl.*, **128**, 475.
Kurucz, R. L. 1998, http://kurucz.harvard.edu/atoms.html.
Lodders, K. 2002, *Astrophys. J.*, **577**, 974.
Luke, T. M. 1997, *J. Phys. B: At. Mol. Opt. Phys.*, **30**, 4223.
Many, A. 1946, *Phys. Rev.*, **70**, 511.
Mendlowitz, H. 1963, *Astrophys. J.*, **138**, 1277.
Meshkov, S. 1954, *Phys. Rev.*, **93**, 270.
Morton, D. C. 2003, *Astrophys. J. Suppl.*, **149**, 205.
NIST atomic spectra database (http://physics.nist.gov/cgi-bin/AtData/main_asd)
Pasternak, A., Goldschmidt, Z. B. 1972, *Phys. Rev. A*, **6**, 55.
Popovic, L. C., Dimitrijevic, M. S. 2000, *Phys. Scripta*, **61**, 192.
Roberts, J. R. 1973, *Astrophys. J.*, **181**, 578.
Samland, M. 1998, *Astrophys. J.*, **496**, 155.

Wagatsuma, K., Danzaki, Y. 1999, *J. Anal. At. Spect.*, **14**, 1727.
Whaling, W., Hannaford, P., Lowe, R. M., Biemont, E., Grevesse, N. 1985, *Astron. Astrophys.*, **153**, 109.
White, H. E. 1929a, *Phys. Rev.*, **33**, 672.
White, H. E. 1929b, *Phys. Rev.*, **33**, 914.
Yasuda, M., Katori, H. 2004, *Phys. Rev. Lett.*, **92**, 153004-1.
Zilitis, V. A. 2001, *Opt. Spectrosc.* **92**, 353.