

Magnetic quadrupole transition probabilities for the beryllium isoelectronic sequence

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The magnetic quadrupole transition probabilities for the $1s^2 2s 2p \ ^3P_2 - 1s^2 2s^2 \ ^1S_0$ and $1s^2 2s 2p \ ^3P_2 - 1s^2 2p^2 \ ^1S_0$ transitions of elements of the beryllium isoelectronic sequence are calculated using eigenfunctions obtained by the Z -expansion method. Matrix elements are presented for $Z = 6-30$ and transition probabilities are obtained for all elements with $Z \geq 6$ for which excitation energies are available. Good agreement is obtained with other calculations when common values for the transition energies are used.

I. INTRODUCTION

Reliable values for the allowed and forbidden transition rates between low-lying levels of elements of the beryllium isoelectronic sequence are of importance in the spectroscopic diagnostics of high-temperature plasmas. In the solar atmosphere, elements such as C, N, Ne, and Fe are abundant, and the study of the berylliumlike spectra of these atoms provides a valuable means for understanding the nature of the solar environment.¹

The determination of the electron density from the observed intensity ratio of the spin-forbidden electric dipole ($E1$) line, $2s^2 \ ^1S_0 - 2s 2p \ ^3P_1$, to the magnetic quadrupole ($M2$) line, $2s^2 \ ^1S_0 - 2s 2p \ ^3P_2$, requires knowledge of the transition probabilities between these levels. While a number of studies employing various theoretical methods have been made of the allowed and forbidden $E1$ transitions of the members of the beryllium sequence,^{2,3,4} the magnetic multipole transitions have received less attention. In this paper we calculate the $M2$ transition probabilities from the $1s^2 2s 2p \ ^3P_2$ state to the $1s^2 2s \ ^1S_0$ and $1s^2 2p^2 \ ^1S_0$ states using wave functions obtained by the Z -expansion method.

II. THEORY

The probability for the emission of magnetic J -pole radiation from an N -electron atom⁵ is, in atomic units,

$$A_{JM} = \frac{2(J+1)}{J(2J+1)[(2J-1)!!]^2 c^2} \left(\frac{\omega}{c}\right)^{2J+1} \times |\langle \Psi_i | Q_M^{(J)} | \Psi_f \rangle|^2, \quad (1)$$

where ω is the transition frequency, $c = 1/\alpha$, and the tensor operator of rank J is

$$Q_M^{(J)} = \sum_{i=1}^N q_M^{(J)}(i) \quad (2)$$

with the individual electron operator given by

$$q_M^{(J)}(i) = \left(\frac{4\pi}{2J+1}\right)^{1/2} [\vec{\nabla} r_i^J Y_{JM}(\hat{r}_i)] \cdot \left(\frac{\vec{1}_i}{J+1} + \vec{s}_i\right). \quad (3)$$

Using Eq. (1), we may express the probability for the $M2$ transition from the 3P_2 to the 1S_0 state, averaged over initial magnetic quantum numbers and summed over final magnetic quantum numbers, as

$$A = \frac{1}{15} (\omega^5/c^7) T, \quad (4)$$

where

$$T = \frac{1}{5} \sum_{M_J, M=-2}^2 |\langle 112M_J | Q_M^{(2)} | 0000 \rangle|^2 \quad (5)$$

and where the quantum numbers in the bras and kets are L, S, J , and M_J .

Using the Wigner-Eckart theorem, we write the squared matrix element as

$$T = \frac{1}{5} \sum_{M_J, M=-2}^2 \begin{pmatrix} 2 & 2 & 0 \\ -M_J & M & 0 \end{pmatrix}^2 |\langle 112 | Q_2^{(2)} | 000 \rangle|^2. \quad (6)$$

The reduced matrix element for the four-electron system can readily be expressed in terms of the matrix element of $Q_2^{(2)}$ between L, S, M_L, M_S states with the result that

$$|\langle 112 | Q_2^{(2)} | 000 \rangle|^2 = 5 |\langle 1111 | Q_2^{(2)} | 0000 \rangle|^2, \quad (7)$$

where in the reduced matrix element the quantum numbers are L, S , and J and in the matrix element on the right the numbers are L, S, M_L , and M_S . Performing the summation over M_J and M in Eq. (6) and inserting the result into Eq. (4) yields for the transition probability

$$A_{3P_2 \rightarrow 1S_0} = 3.03704 (\Delta E)^5 |\langle 1111 | Q_2^{(2)} | 0000 \rangle|^2 (\text{sec}^{-1}), \quad (8)$$

where ΔE is the excitation energy in atomic units.

A thorough discussion of the construction of the Z -expansion wave functions for atomic systems has

been given by Onello, Ford, and Dalgarno⁶ for states which are nondegenerate in a hydrogenic approximation. The case of a zero-order degeneracy removable in the first order of perturbation theory as occurs for the $1s^2 2s^2 \ ^1S_0$ and $1s^2 2p^2 \ ^1S_0$ states of the beryllium isoelectronic sequence has been treated by Watson and ONeil.²

Briefly, the Z -expansion method proceeds by choosing the unit of length to be Z^{-1} a.u. and the unit of energy to be Z^2 a.u. The Schrödinger equation for the four-electron system is, in these atomic units,

$$(H_0 + V/Z) |\Psi_n\rangle = E_n |\Psi_n\rangle \quad (9)$$

with

$$H_0 = \sum_{i=1}^4 \left(-\frac{1}{2} \nabla_i^2 - \frac{1}{r_i} \right),$$

$$V = \sum_{i < j=1}^4 \frac{1}{|\vec{r}_i - \vec{r}_j|},$$

where \vec{r}_i is the position of the i th electron with respect to the nucleus. The wave function $|\Psi_n\rangle$ and energy E_n are expanded in a power series in Z^{-1} :

$$|\Psi_n\rangle = \sum_{i=0}^{\infty} Z^{-i} |\Psi_n^{(i)}\rangle, \quad (10)$$

$$E_n = \sum_{i=0}^{\infty} Z^{-i} E_n^{(i)}. \quad (11)$$

Inserting these Z expansions into Eq. (9) and equating the coefficients of different powers of $1/Z$ equal to zero yields a set of equations for the expansion terms, with the lowest-order term in both Eqs. (10) and (11) being hydrogenic if there is no degeneracy.

The equations can be solved by finding the stationary values of the functionals⁷

$$J_n^{(s)} = \langle \Psi_n^{(s)} | H_0 - E_n^{(0)} | \Psi_n^{(s)} \rangle$$

$$+ 2 \langle \Psi_n^{(s)} | V - E_n^{(1)} | \Psi_n^{(s-1)} \rangle$$

$$- \sum_{\tau=2}^{2s-1} E_n^{(\tau)} \sum_{q=s-\tau}^{\tau} \langle \Psi_n^{(q)} | \Psi_n^{(2s-\tau-q)} \rangle \quad (12)$$

with respect to trial forms of $\Psi_n^{(s)}$. Following Dalgarno and Drake,⁸ the trial form $\Psi_n^{(s)}$ is chosen to be a linear combination of N orthonormal functions ϕ_k , one of which is $\Psi_n^{(0)}$, with the set $\{\phi_k\}$ satisfying

$$\langle \phi_i | H_0 | \phi_j \rangle = \epsilon_i \delta_{ij}, \quad i, j = 1, 2, \dots, N.$$

This procedure leads to iterative solutions for $|\Psi_n^{(s)}\rangle$ and $E_n^{(s)}$. Because of the hydrogenic degeneracy of the $1s^2 2s^2 \ ^1S_0$ and $1s^2 2p^2 \ ^1S_0$ states, appropriate linear combinations of the zero-order wave functions must be chosen so as to diagonalize the perturbing potential V in the usual manner of

degenerate Rayleigh-Schrödinger perturbation theory.

III. CALCULATIONS

The basis set $\{\phi_k\}$ and the matrix elements of the interelectron potential V between these states, required for the evaluation of $|\Psi_n^{(s)}\rangle$ and $E_n^{(s)}$, were obtained using a modified version² of a configuration-interaction program written by Schaefer.⁹ This program uses L - S configurations of the form

$$\Phi = \sum_i b_i D_i,$$

where b_i is a symmetry-adapted coefficient and D_i is a determinant constructed from atomic orbitals Θ_j . Each spin orbital is a product of a radial factor, a spherical harmonic, and an α or β spin function. The radial factor is expanded as a sum of Slater-type orbitals so that the individual spin orbitals assume the form

$$\Theta_j = \left(\sum_k a_{jk} \frac{(2\xi)^{n+1/2}}{[(2n)!]^{1/2}} r^{n-1} e^{-\xi r} \right) Y_{l, m_j}(\theta, \phi) \begin{cases} \alpha \\ \beta \end{cases},$$

where ξ is the orbital exponent. The orbital exponents for the $1s$, $2s$, and $2p$ orbitals were chosen so that these wave functions correspond to hydrogenic orbitals in order to produce the correct high- Z limit behavior. These and the remaining exponents are the same as those chosen by Watson and ONeil in their study of electric dipole transitions in the beryllium isoelectronic sequence. Sixty configurations were used in calculating the wave function for each state. The orbitals, orbital exponents, and configurations used for the 1S and 3P states are given in Tables I and II of Ref. 2.

The calculation of the matrix element of Eq. (8)

$$\langle 1111 | Q_2^{(2)} | 0000 \rangle$$

is reduced to the evaluation of the matrix element of the tensor operator between single particle l, s, m_l, m_s spin orbitals which are then expressed in terms of l, s, j, m_j states using vector addition coefficients. The matrix element

$$\langle l's'j'm'_j | Q_2^{(2)} | l s j m_j \rangle$$

is simplified by using the Wigner-Eckart theorem and the resulting reduced matrix element is evaluated by standard tensor algebra methods.¹⁰

Since the excitation energy ΔE is raised to the fifth power in the expression for the transition probability, Eq. (8), it is essential to employ accurate energies if the transition probabilities are to be reliable. The energy differences used have been obtained from the compilation by Fawcett¹¹ of $2s^2$, $2s2p$, and $2p^2$ energy levels for elements of the beryllium isoelectronic sequence.

TABLE I. Z -expansion coefficients for the square of the transition matrix element for the $2s2p\ ^3P_2-2s^2\ ^1S_0$ and $2s2p\ ^3P_2-2p^2\ ^1S_0$ transitions. A (B) denotes $A \times 10^B$.

i	$T_i(2s^2\ ^1S_0)$	$T_i(2p^2\ ^1S_0)$
0	3.2927(1)	3.0729
1	1.4156(2)	1.4721(1)
2	4.1253(2)	5.7212(1)
3	1.0421(3)	1.6709(2)
4	3.6995(3)	-1.1182(2)
5	1.3895(4)	-3.5067(3)
6	1.8638(4)	-1.1381(4)
7	-1.5040(5)	1.8497(4)
8	-1.0964(6)	2.8213(5)
9	-3.8810(6)	1.0165(6)
10	-9.0851(6)	7.7224(5)

IV. RESULTS AND DISCUSSION

Use of the Z -expansion wave functions leads to an expansion series for the square of the transition matrix element of Eq. (4):

$$T = \frac{1}{Z^2} \sum_{i=0}^{\infty} Z^{-i} T_i. \quad (13)$$

Table I presents the first 11 expansion coefficients, T_i , for the $1s^22s2p\ ^3P_2-1s^22s^2\ ^1S_0$ and $1s^22s2p\ ^3P_2-1s^22p^2\ ^1S_0$ transitions. With the understanding that the initial level for both transitions is the $1s^22s2p\ ^3P_2$ state, we label the transitions by the configuration of the 1S_0 state.

The squared matrix elements, T , obtained by retaining 50 terms in the expansion of Eq. (13), are given in Table II for $Z = 6 - 30$. For the $2s^2\ ^1S_0$ transition, the 11 terms of Table I yield a value for T within 0.1% of the full 50-term sum for $Z \geq 7$, while for the $2p^2\ ^1S_0$ transition the first 11 terms converged to within 0.2% of the full sum for $Z \geq 7$. The eigenfunction of the $2p^2\ ^1S_0$ state is not as accurate as the eigenfunctions of the $2s^2\ ^1S_0$ or $2s2p\ ^3P_2$ states which are the lowest states of their respective symmetries and some loss of accuracy will occur when calculating the squared matrix element $T(2p^2\ ^1S_0)$ using the $2p^2\ ^1S_0$ Z -expansion wave function.

TABLE II. Squared matrix elements T , excitation energies ΔE in a.u. and transition probabilities A in sec^{-1} , for the $1s^22s2p\ ^3P_2-1s^22s^2\ ^1S_0$ and $1s^22s2p\ ^3P_2-1s^22p^2\ ^1S_0$ transitions. $A(B)$ denotes $A \times 10^B$.

Z	Ion	Squared matrix element		Excitation energy ^a		Transition probability	
		$T(2s^2\ ^1S_0)$	$T(2p^2\ ^1S_0)$	$\Delta E(2s^2\ ^1S_0)$	$\Delta E(2p^2\ ^1S_0)$	$A(2s^2\ ^1S_0)$	$A(2p^2\ ^1S_0)$
6	C III	2.1191	2.0564(-1)	0.2390	0.5927	5.02(-3)	4.57(-2)
7	N IV	1.3603	1.3407(-1)	0.3072	0.7652	1.13(-2)	1.07(-1)
8	O V	9.4266(-1)	9.3561(-2)	0.3754	0.9365	2.13(-2)	2.05(-1)
9	F VI	6.9066(-1)	6.8631(-2)	0.4440	1.1070	3.62(-2)	3.47(-1)
10	Ne VII	5.2747(-1)	5.2322(-2)	0.5135	1.2778	5.72(-2)	5.41(-1)
11	Na VIII	4.1589(-1)	4.1127(-2)	0.5843	1.4485	8.60(-2)	7.96(-1)
12	Mg IX	3.3628(-1)	3.3137(-2)	0.6564	1.6201	1.24(-1)	1.12
13	Al X	2.7750(-1)	2.7248(-2)	0.7314	1.7917	1.76(-1)	1.53
14	Si XI	2.3288(-1)	2.2789(-2)	0.8080	1.9658	2.44(-1)	2.03
15	P XII	1.9821(-1)	1.9336(-2)	0.8881	2.1406	3.33(-1)	2.64
16	S XIII	1.7074(-1)	1.6608(-2)	0.9718	2.3167	4.49(-1)	3.37
17	Cl XIV	1.4861(-1)	1.4417(-2)	1.0596	2.4958	6.03(-1)	4.24
18	Ar XV	1.3051(-1)	1.2632(-2)	1.1518	2.6780	8.04(-1)	5.28
19	K XVI	1.1553(-1)	1.1158(-2)	1.2495	2.8634	1.07	6.52
20	Ca XVII	1.0299(-1)	9.9273(-3)	1.3534	3.0531	1.42	8.00
21	Sc XVIII	9.2377(-2)	8.8892(-3)	1.4642	3.2487	1.89	9.77
22	Ti XIX	8.3327(-2)	8.0056(-3)	1.5827	3.4495	2.51	1.19(1)
23	V XX	7.5544(-2)	7.2473(-3)	1.7099		3.35	
24	Cr XXI	6.8802(-2)	6.5918(-3)	1.8464		4.48	
25	Mn XXII	6.2923(-2)	6.0213(-3)	1.9934		6.01	
26	Fe XXIII	5.7767(-2)	5.5217(-3)	2.1516		8.09	
27	Co XXIV	5.3219(-2)	5.0818(-3)				
28	Ni XXV	4.9188(-2)	4.6924(-3)				
29	Cu XXVI	4.5597(-2)	4.3461(-3)				
30	Zn XXVII	4.2386(-2)	4.0367(-3)				

^aFawcett, Ref. 11.

TABLE III. Comparison of the $1s^2 2s 2p \ ^3P_2 - 1s^2 2s^2 \ ^1S_0$ Z-expansion transition probabilities in sec^{-1} , with other works. Quantities in brackets have been obtained by adjusting for the different values of the excitation energy used in the various calculations. A (B) denotes $A \times 10^B$.

	Present work	Ref. 12	Ref. 13	Ref. 14
C III	5.02(-3)	5.23(-3)	5.15(-3) ^{13a}	5.08(-3)
Ne VII	5.72(-2)	5.76(-2)	5.74(-2)	5.70(-2)
Si XI	2.44(-1)	2.38(-1)	4.8(-1) ^{13b}	
		[2.42(-1)]	[2.45(-1)]	
Ca XVII	1.42	1.41	2.12	
		[1.39]	[1.40]	
Fe XXIII	8.09	7.69	1.02(1)	
		[7.81]	[7.86]	

The values for the excitation energies are also listed in Table II. The squared matrix element $T(2p^2 \ ^1S_0)$ is an order of magnitude smaller than $T(2s^2 \ ^1S_0)$, but $\Delta E(2p^2 \ ^1S_0)$ is more than twice $\Delta E(2s^2 \ ^1S_0)$. Because ΔE enters to the fifth power in Eq. (8), the $1s^2 2s 2p \ ^3P_2 - 1s^2 2p^2 \ ^1S_0$ transition probability is five to ten times greater than the $1s^2 2s 2p \ ^3P_2 - 1s^2 2s^2 \ ^1S_0$ value.

The transition probabilities for the magnetic quadrupole decay of the $1s^2 2s 2p \ ^3P_2$ states for C III through Fe XXIII are presented in Table II.

Also given are the probabilities for the $1s^2 2s 2p \ P_2 - 1s^2 2p^2 \ ^1S_0$ transition for C III through Ti XIX. Relativistic effects need to be taken into account for the more highly charged elements. They affect the excitation energy more strongly than the transition matrix,^{13(b)} and we have used the nonrelativistic matrix elements to calculate transition probabilities for all ions for which the excitation energies are available.

A comparison with other values for the $2s 2p \ ^3P_2 - 2s^2 \ ^1S_0$ transition probability is given in Table III. The C III and Ne VIII results are in close agreement. For Si XI, Ca XVII, and Fe XXIII the discrepancies can be attributed largely to the different values employed for the excitation energies. Use of the excitation energies given in Table II yields the modified values given in brackets in Table III which agree well with our transition probabilities.

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