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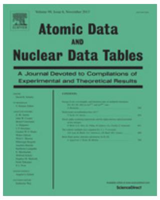

Electric quadrupole transition probabilities for atomic lithium

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ABSTRACT

Electric quadrupole transition probabilities for atomic lithium have been calculated using the weakest bound electron potential model theory (WBEPMT). We have employed numerical non-relativistic Hartree–Fock wavefunctions for expectation values of radii and the necessary energy values have been taken from the compilation at NIST. The results obtained with the present method agree very well with the Coulomb approximation results given by Caves (1975). Moreover, electric quadrupole transition probability values not existing in the literature for some highly excited levels have been obtained using the WBEPMT.

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Contents

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1. Introduction

The alkali atoms such as lithium have long served as a test system for various theoretical developments aimed at the accurate determination of spectroscopic data such as transition probabilities, oscillator strengths, and lifetimes. Electric quadrupole (E2) transitions are very difficult to detect in ordinary experimental conditions, because the transition intensity is extremely weak compared to electric dipole allowed transitions. Therefore, the importance of the theoretical study still exists. Up to the present, several calculations of spectroscopic data belonging to E2 transitions for atomic lithium have been reported. The calculation of some matrix elements has been made by Boggard and Orr [1] using a Coulomb approximation and by Boyle and Murray [2] using Weiss's Hartree–Fock functions for atomic lithium. Weighted oscillator strengths for different E2 transitions have been calculated using analytic Hartree–Fock wavefunction for Li I, Be II, and B III by Sengupta [3]. Caves has calculated the transition probabilities and oscillator strengths for a large number of E2 lines using a generalized Coulomb approximation [4]. Beck has studied many-electron effects on E2 transition probabilities for Li I and some alkali-like systems using both analytic and numerical restricted Hartree–Fock wavefunctions [5]. Recently a critical evaluation of available literature sources has been reported by Wiese and Fuhr [6].

In the present article, we present the results of calculation of the E2 transition probabilities for multiplet lines belonging to excited levels of atomic lithium by using the weakest bound electron potential model theory (WBEPMT). In the calculations, many of transition arrays are considered.

2. Theory

The WBEPMT has been widely employed to calculate many spectroscopic data such as energy levels, transition probabilities, oscillator strengths, and lifetimes. According to the WBEPMT, the radial wavefunction of the weakest bound electron can be obtained as [7–10]

$$R_{nl}(r) = \left(\frac{2Z^*}{n^*}\right)^{l^*+3/2}\left[\frac{2n^*}{(n-l-1)!}\,\Gamma\,(n^*+l^*+1)\right]^{-1/2} \times \exp\left(-\frac{Z^*r}{n^*}\right) r^{l^*} L^{2l^*+1}_{n-l-1}\left(\frac{2Z^*r}{n^*}\right). \quad (1)$$

Here, the parameters n^* and l^* are

$$n^* = n + d, \qquad l^* = l + d. \quad (2)$$

In addition, the quantities Z^*, n^*, and l^* are defined to be the effective nuclear charge, effective principal quantum number, and effective orbital quantum number, respectively, and d is an adjustable parameter. These parameters can be obtained by solving energy and expectation value expressions given in Eqs. (3) and (4) together [7–10], namely,

$$I = -\varepsilon = \frac{Z^{*2}}{2n^{*2}}, \quad (3)$$

$$\langle r\rangle = \frac{3n^{*2} - l^*(l^*+1)}{2Z^*}. \quad (4)$$

Here I is the ionization energy and $\langle r\rangle$ is the expectation value for radius of the weakest bound electron. The ionization energies and expectation values for radii of all states must be known for the parameters Z^*, n^*, and l^* to be determined. In the WBEPMT, the ionization energies for the weakest bound electron are taken from experimental energy values in the literature and the expectation value of radius of the weakest bound electron is obtained from different theoretical methods.

In this work, the radial transition integral is obtained using the WBEPMT radial wavefunctions given in Eq. (1). According to this theory, the radial transition integral for E2 transitions can be obtained as [11]

$$\begin{aligned}
\langle R_{nl}|Q(r)^{(2)}|R_{n'l'}\rangle &= \int_0^\infty r^4\, R_{n_il_i}(r)\; R_{n_fl_f}(r)\; dr \\
&= (-1)^{n_f+n_i+l_f+l_i}\left(\frac{2Z_f^*}{n_f^*}\right)^{l_f^*}\left(\frac{2Z_i^*}{n_i^*}\right)^{l_i^*} \times \left(\frac{Z_f^*}{n_f^*} - \frac{Z_i^*}{n_i^*}\right)^{-l_f^*-l_i^*-5} \\
&\times \left[\frac{n_f^{*4}\,\Gamma\,(n_f^*+l_f^*+1)}{4Z_f^{*3}\,(n_f-l_f-1)!}\right]^{-1/2} \times \left[\frac{n_i^{*4}\,\Gamma\,(n_i^*+l_i^*+1)}{4Z_i^{*3}\,(n_i-l_i-1)!}\right]^{-1/2} \\
&\times \sum_{m_1=0}^{n_f-l_f-1}\sum_{m_2=0}^{n_i-l_i-1}\frac{(-1)^{m_2}}{m_1!m_2!}\left(\frac{Z_f^*}{n_f^*} - \frac{Z_i^*}{n_i^*}\right)^{m_1+m_2} \\
&\times \left(\frac{Z_f^*}{n_f^*} + \frac{Z_i^*}{n_i^*}\right)^{-m_1-m_2} \times \Gamma\,(l_f^*+l_i^*+m_1+m_2+5) \\
&\times \sum_{m_3=0}^{S}\binom{l_i^*-l_f^*+m_2+3}{n_f^*-l_f^*-1-m_1-m_3} \\
&\times \binom{l_f^*-l_i^*+m_1+3}{n_i^*-l_i^*-1-m_2-m_3} \\
&\times \binom{l_i^*+l_f^*+m_1+m_2+m_3+4}{m_3}, \quad (5)
\end{aligned}$$

where Γ is the gamma function and $S = \min\{n_f - l_f - 1 - m_1,\ n_i - l_i - 1 - m_2\}, 2 > -l_f^* - l_i^* - 3$.

The E2 transition probability A_{E2} (in s^{-1}) for a transition between two states within the *LS* coupling is given by [11,12]

$$A_{E2} = \frac{32\pi^5\alpha\, c\, a_0^4}{15\,\lambda^5 g'}S_{E2} = \frac{1.11995\times 10^{18}}{\lambda^5 g'}S_{E2}. \quad (6)$$

Here, α is the fine structure constant, λ is the wavelength in angstroms, c is the speed of light (cm/s), a_0 is the Bohr radius (cm), g' is the degeneracy of the initial level, and S_{E2} is the E2 line strength in atomic units. Line strength is determined according to the coupling schemes in atomic or ionic systems. *LS* coupling is the dominant coupling scheme in many light atoms and the E2 line strength in atomic units ($e^2a_0^4$) for transitions between two