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Oscillator strengths and interstate transition energies involving ^2S and ^2P states of the Li atom

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ABSTRACT

We report high accuracy calculations of the ground and excited doublet S and P states of lithium atom. Overall, 24 states corresponding to dominant electronic configurations $1s^2\,ns$ and $1s^2\,np$ ($n = 2, \ldots, 13$) are considered in the framework of the Ritz variational method. The nonrelativistic wave function of each of these states is generated in an independent calculation by expanding it in terms of a large number ($K = 11,000 - 17,000$) of all-electron explicitly correlated Gaussian functions (ECG) whose nonlinear parameters are extensively optimized with a procedure that employs analytic energy gradient determined with respect to these parameters. The Hamiltonian used in the calculations explicitly depends on the mass of the nucleus. The leading relativistic and quantum electrodynamics (QED) corrections to the energy levels are subsequently computed using the perturbation-theory approach and the variational nonrelativistic wave functions as the zeroth-order functions. As these functions are generated in the finite-nuclear-mass (FNM) calculations, the energy corrections include the nuclear recoil effects. The obtained energy levels allow us to determine highly accurate interstate transition frequencies for both the naturally occurring stable lithium isotopes, ^{6}Li and ^{7}Li, and the lithium atom with an infinitely heavy nucleus, $^\infty$Li. The nonrelativistic wave functions are used to compute the transition dipole moments and the corresponding oscillator strengths. These quantities are reported for 144 S–P transitions of each isotope. The data set generated in this work is considerably more accurate and comprehensive than the data available from the previous theoretical calculations. It can be useful in guiding future spectroscopic measurements of the lithium atom.

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Contents

1. Introduction

Designing and building synthetic quantum systems have been one of the most interesting research frontiers in recent years [1]. An example of the quantum systems that have attracted particular attention are systems of individually controlled neutral atoms either in the ground states or in Rydberg excited states. These types of systems can potentially be used as elements of quantum computers. Manipulation of individual atoms with optical tweezers into arrays of weakly interacting Rydberg species may provide a promising platform for well controlled quantum systems for various applications. To master this new technology, the quantum phenomena observed experimentally in these systems have to be explained using theoretical models that are amenable to computational simulations and interpretations. The relatively large scales of these models, as they have to include larger number of atoms (in some cases 50 or more), may require making several approximations that may affect accuracy of the calculations and the validity of the results. An attractive feature of studying the models is the ability to vary the parameters of the studied system in ranges inaccessible in experiments, thus providing a way to better understand the relevant properties of these systems [2,3] and the possibility of controlling their properties [3].

Some tools that allow to control individual atoms and tune their interactions have been developed by physicists. Subsequently, quantum systems represented by Hamiltonian with tunable parameters that allow to prepare an atom in specific quantum states for use in specific applications including quantum computers have been designed and, in some cases, practical implementation has been followed [4]. Individual atoms can be placed in arrays where large entangled states can be generated. Correlations between these types of states can be useful to overcome the standard quantum limits, thus leading to enhanced precision of such devices as clocks, sensors, etc. [4]. In quantum computers, each atom in the array would carry a single quantum bit [5–7]. Such an architecture would significantly increase the density of the stored information.

Development of fully controlled, coherent, many-body quantum systems is an outstanding problem for science and engineering. Such systems, in particular, systems with strong quantum correlation and involving strong quantum entanglement [8], are promising candidates for components of quantum information processors [9]. Another type of strongly correlated quantum systems involves assembles of coherently coupled neutral atoms excited to Rydberg states [10,11]. The realization of such assembles requires a detail knowledge of the Rydberg spectra of the individual atoms forming the assembles. The energies of individual levels and the interstate transition probabilities have to be known to fabricate effective assembles. These quantities can be predicted using quantum mechanical computations.

The present work involves performing these types of calculations for two stable isotopes of lithium, ^{6}Li and ^{7}Li. The considered states are the twelve lowest ^2S states and the twelve lowest ^2P states. The calculations employ large basis set of all-electron explicitly correlated Gaussian functions (ECGs). The nonlinear parameters of the Gaussians are variationally optimized using a procedure that employs analytically determined energy gradient calculated with respect to these parameters. The Hamiltonian used in the calculations has a finite nuclear mass (FNM). The nonrelativistic wave functions are used to calculated the leading relativistic and quantum electrodynamics (QED) energy corrections. The relativistic corrections include the spin–orbit interaction which results in splitting of energy levels into sub-levels. Thus, for example, each ^2P level of the lithium atom splits into two sub-levels corresponding to two possible values of the quantum number J: 3/2 and 1/2.

In order to put the present calculations in perspective of the previous theoretical studies, in Table 1 we show a survey of the progress achieved over the years in calculating the nonrelativistic energies of S and P states of the lithium atom with an infinite nuclear mass (INM). Results obtained with different methods are included in the table; though most of the methods are variational. More detailed discussion of the energies calculated in the current work and their comparison with the energies obtained in the prior works are presented in Section 3.

1.1. Basis functions

In the present calculations we used all-electron explicitly correlated Gaussian functions to construct the spatial parts of the wave functions for the P and S states considered in this work. The S-type Gaussians have the following form:

$$\phi_k = \exp\left[-\mathbf{r}'\mathbf{A}_k\mathbf{r}\right], \tag{1}$$

where the prime symbol stands for vector transpose and $\mathbf{A}_k$ is a $3n \times 3n$ real symmetric matrix of exponential parameters. $\mathbf{A}_k$ is constructed as $\mathbf{A}_k = A_k \otimes I_3$, where A_k is a $n \times n$ dense

Table 1
Comparison of nonrelativistic energies of $^{\infty}$Li obtained with various theoretical methods, i.e., Hartree–Fock (HF), configuration interaction (CI), many-body perturbation theory (MBPT), variational method employing the Hylleraas-type functions (Hy), Hylleraas-CI (Hy-CI), multiconfiguration Hartree–Fock (MCHF), variational method employing explicitly correlated Gaussian functions (ECG) and exponentially correlated Slater functions (ECS), and diffusion Monte Carlo (DMC). Some of the quoted values represent an extrapolation to the infinite basis set limit. All energies are given in atomic units.

$2\,^2S$

Work	Year	Method	Basis size	Energy
Wilson [12]	1933	HF		−7.419 2
James and Coolidge [13]	1936	Hy		−7.476 075
Walsh and Borowitz [14]	1959	Hy		−7.395
Roothaan *et al.* [15]	1960	HF		−7.432 73
Burke [16]	1963	Hy	13	−7.477 95
Ohrn and Nordling [17]	1966	Hy	5	−7.474 1
Seung and Wilson [18]	1967	MBPT		−7.472 62
Larsson [19]	1968	Hy	100	−7.478 025
Ishida and Nakatsuji [20]	1973	MCSCF		−7.447 54
Sims and Hagstrom [21]	1975	Hy-CI	150	−7.478 023
Perkins [22]	1976	Hy	30	−7.477 93
Muszynska *et al.* [23]	1980	Hy-CI	139	−7.478 044
Ho [24]	1981	Hy	92	−7.478 031
Pipin and Woznicki [25]	1983	Hy-CI	170	−7.478 044
Weiss [26]	1961	CI	45	−7.477 10
King and Shoup [27]	1986	Hy	352	−7.478 058
Hijikata *et al.* [28]	1987	Hy	100	−7.478 032
King [29]	1989	Hy	602	−7.478 059
Kleindienst and Beutner [30]	1989	Hy	310	−7.478 058 24
King and Bergsbaken [31]	1990	Hy	296	−7.478 059 53
Chung [32]	1991	CI	1 017	−7.477 925 06
		CI	∞	−7.478 059 7(9)
McKenzie and Drake [33]	1991	Hy	1 134	−7.478 060 326(10)
Jitrik and Bunge [34]	1991	CI	$l <= 8$	−7.477 906 662
		CI	∞	−7.478 062 4(7)
Pipin and Bishop [35]	1992	Hy-CI	1 618	−7.478 060 1
Luchow and Kleindienst [36]	1992	Hy-CI	976	−7.478 060 252
Tong *et al.* [37]	1993	MCSCF	$l = 10$	−7.477 968 61
		MCSCF	∞	−7.478 060 9
Kleindienst and Lüchow [38]	1993	Hy-CI	854	−7.478 060 21
Lüchow and Kleindienst [39]	1994	Hy-CI	1 420	−7.478 060 320 8
King [40]	1995	Hy	760	−7.478 060
Yan and Drake [41]	1995	Hy	1 589	−7.478 060 321 56
		Hy	∞	−7.478 060 323 10(31)
Pestka and Woźnicki [42]	1996	Hy-CI	386	−7.478 060 1
Langfelder *et al.* [43]	1997	DMC		−7.477 92
Jitrik and Bunge [44]	1997	CI	$l <= 13$	−7.478 025 4(7)
King [45]	1997	Hy		−7.478 060 19
Fische *et al.* [46]	1998	MCSCF		−7.478 567 258
Yan *et al.* [47]	1998	Hy	3 502	−7.478 060 323 618 9
		Hy	∞	−7.478 060 323 650 3(71)
Komasa [48]	2001	ECG	1 536	−7.478 060 314 3
Pachucki and Komasa [49]	2003	ECG	2 000	−7.478 060 315(10)
Pachucki and Komasa [50]	2006	ECG	5 200	−7.478 060 320(4)
Puchalski and Pachucki [51]	2006	Hy	9 576	−7.478 060 323 889 7
		Hy	∞	−7.478 060 323 904 1(+10,−50)
Brown *et al.* [52]	2007	DMC		−7.478 060(2)
Stanke *et al.* [53]	2007	ECG	7 000	−7.478 060 323 2
Yan and Drake [54]	2008	Hy	9 577	−7.478 060 323 892 4
Stanke *et al.* [55]	2008	ECG	10 000	−7.478 060 323 81
Puchalski and Pachucki [56]	2008	Hy	10 000	−7.478 060 323 889 7
		Hy	∞	−7.478 060 323 906(8)
Bubin *et al.* [57]	2009	ECG	10 000	−7.478 060 323 8
Puchalski *et al.* [58]	2009	Hy	13 944	−7.478 060 323 909 560
		Hy	∞	−7.478 060 323 910 10(32)
Sims and Hagstrom [59]	2009	Hy-CI	16 764	−7.478 060 323 451 9
Puchalski *et al.* [60]	2010	Hy	30 632	−7.478 060 323 910 097
		Hy	∞	−7.478 060 323 910 2(2)
Puchalski *et al.* [61]	2010	ECS	512	−7.478 060 323 448
Wang *et al.* [62]	2011	Hy	26 520	−7.478 060 323 910 134 843
		Hy	∞	−7.478 060 323 910 143 7(45)
Seth *et al.* [63]	2011	DMC		−7.478 067(5)
Wang *et al.* [64]	2012	Hy	12 168	−7.478 060 323 910 044 374
		Hy	34 020	−7.478 060 323 910 146 894
		Hy	∞	−7.478 060 323 910 147(1)
Ruiz *et al.* [65]	2013	Hy-CI	693	−7.478 058 969
		Hy-CI	∞	−7.478 060(2)

(*continued on next page*)

Table 1 (*continued*).

		CI	991	−7.477 192
		CI	∞	−7.477 20(1)
Bubin and Adamowicz [66]	2013	ECG	6 500	−7.478 060 323 89
Wang *et al.* [67]	2017	Hy	∞	−7.478 060 323 910 150(5)
Bralin *et al.* [68]	2019	ECG	10 500	−7.478 060 323 906
Nasiri and Zahedi [69]	2020	DMC		−7.478 06(5)
This work	2022	ECG	11 000	−7.478 060 323 906 57
		ECG	12 000	−7.478 060 323 907 70
		ECG	∞	−7.478 060 323 909 95(3)
$2\,^2P$				
Ahlenius and Larsson [70]	1973	Hy	78	−7.409 99
Sims and Hagstrom [21]	1975	Hy-CI	120	−7.410 053
Ahlenius and Larsson [71]	1978	Hy	97	−7.410 078
Muszynska *et al.* [23]	1980	Hy-CI	120	−7.410 097
Pipin and Woznicki [25]	1983	Hy-CI	170	−7.410 106
Chung [32]	1991	CI		−7.410 157 8(9)
Tong *et al.* [37]	1993	MCSCF	$l = 8$	−7.409 965 46
			∞	−7.410 153 1
Yan and Drake [41]	1995	Hy	1 715	−7.410 156 518 4
		Hy	∞	−7.410 156 521 8(13)
Pestka and Woźnicki [42]	1996	Hy-CI		−7.410 155 91
Yan *et al.* [47]	1998	Hy	3 463	−7.410 156 531 721
		Hy	∞	−7.410 156 531 763(42)
Puchalski and Pachucki [56]	2008	Hy	9 576	−7.410 156 532 628 6
		Hy	∞	−7.410 156 532 665(14)
Wang *et al.* [62]	2011	Hy	30 224	−7.410 156 532 650 66
Wang *et al.* [62]		Hy	∞	−7.410 156 532 651 6(5)
Bressanini [72]	2012	DMC		−7.410 14(1)
Bubin and Adamowicz [73]	2012	ECG	7 000	−7.410 156 532 44
Wang *et al.* [64]	2012	Hy	20 000	−7.410 156 532 652 104
	2012	Hy	32 200	−7.410 156 532 652 370
		Hy	∞	−7.410 156 532 652 41(4)
Ruiz *et al.* [65]	2013	Hy-CI	616	−7.410 149 407
		Hy-CI	∞	−7.410 150(6)
		CI	1 430	−7.408 619
		CI	∞	−7.408 70(9)
Strasburger [74]	2014	ECG	1 065	−7.410 156 511
		ECG	∞	−7.410 156 550(39)
Wang *et al.* [67]	2017	Hy	∞	−7.410 156 532 652 41(3)
Nasiri *et al.* [75]	2021	ECG	13 500	−7.410 156 532 647 90
This work	2022	ECG	12 000	−7.410 156 532 645 74
		ECG	17 500	−7.410 156 532 650 37
		ECG	∞	−7.410 156 532 652(2)

symmetric matrix and I_3 is a 3×3 identity matrix. Symbol $\otimes$ denotes the Kronecker product. To be used as a basis function in expanding the wave function of a bound state of the atom, function $\phi_k(\mathbf{r})$ needs to be square-integrable. This happens when the matrix A_k is positive definite. To fulfill this requirement, A_k is represented in the Cholesky-factored form as $A_k = L_k L_k'$, where L_k is a lower triangular matrix. The A_k matrix given in the Cholesky-factored form is always positive definite regardless of the values of the L_k matrix elements. Thus, if these matrix elements are used as the variational parameters of the Gaussians and adjusted to minimize the total energy of the state of the system under the consideration, they can be varied without any constrains from $-\infty$ to ∞. This is convenient, because any constraint imposed on the variational parameters would make the optimization more cumbersome.

For expanding the wave functions of states of the atom with one or more p electrons, one needs to include pre-exponential angular factors [76,77]. In our previous works, we implemented ECG basis functions with pre-exponential factors being Cartesian spherical harmonics. For P states of atoms whose dominant configuration includes just one electron in a single-particle p state, while all others are in single-particle s states, such as the ^2P Rydberg states of the lithium atom considered in this work, the following Gaussians have been used:

$$\phi_k(\mathbf{r}) = z_{i_k} \exp\left[-\mathbf{r}'\mathbf{A}_k\mathbf{r}\right], \tag{2}$$

Here z_{i_k} is the z-coordinate of the i_k-th electron. Subscript i_k (the label of the electron in a p state) can vary in the range $(1, \ldots, n)$ and can be considered to be an adjustable integer variational parameter. The parameter is specific for each basis function, ϕ_k, and its optimal value is determined variationally when the ECG is first added to the basis set. For more information on the basis sets see [76–80].

2. Formalism

2.1. Nonrelativistic nuclear-mass-dependent Hamiltonian

Let us consider quantum bound states of an atom. In general, these states represent the motion of the particles forming the atom, i.e., the nucleus and the electrons, around the center of mass of the atom. To study such states, one needs to first derive a Hamiltonian operator that describes the intrinsic motion of the particles forming the atom. In our approach, such a Hamiltonian is derived by starting with the standard nonrelativistic lab-frame Hamiltonian representing the kinetic and potential energies of the nucleus and the electrons. The laboratory frame nonrelativistic all-particle Hamiltonian of an atom consisting on a nucleus and $N-1$ electrons is (in atomic units):

$$H_{\mathrm{nr}}^{\mathrm{lab}} = \sum_{i=1}^{N} \frac{\mathbf{P}_i^2}{2M_i} + \sum_{i=1}^{N}\sum_{j\neq i}^{N} \frac{Q_i Q_j}{|\,\mathbf{R}_i - \mathbf{R}_j\,|}, \tag{3}$$

where M_i, Q_i, $\mathbf{R}_i$, $\mathbf{P}_i$ are the mass, charge, the Cartesian coordinates and the corresponding linear momenta of the ith particle, respectively. The above Hamiltonian can be rigorously separated

into two independent Hamiltonians describing the motion of the system as a whole and the Hamiltonian corresponding to the intrinsic motion. This can be done by means of a coordinate transformation from the lab frame coordinates $\mathbf{R}_i$ to a new set of coordinates. In our approach this new set is chosen to consist of three Cartesian coordinates of the center of mass and $(3N-3)$ "internal" coordinates. We chose the internal coordinates, denoted as $\mathbf{r}_i$ $(i = 1, \ldots, N-1)$, to be the position vectors of particles 2 to N with respect to particle 1. Particle 1 is called the reference particle. While any particle in the atom can be chosen to be the reference particle, it is natural to assign this role to the heaviest one, the nucleus. Thus, the new coordinate system consists of the lab frame coordinates of the center of mass, $\mathbf{r}_{\rm CM}$ and the internal coordinates, $\mathbf{r}_i$. The internal nonrelativistic Hamiltonian depends only on coordinates $\mathbf{r}_i$ and has the following form:

$$H_{\rm nr}^{\rm int} = -\frac{1}{2}\left(\sum_{i=1}^{n}\frac{1}{\mu_i}\nabla_{\mathbf{r}_i}^2 + \sum_{i=1}^{n}\sum_{j\neq i}^{n}\frac{1}{m_0}\nabla_{\mathbf{r}_i}'\nabla_{\mathbf{r}_j}\right) + \sum_{i=1}^{n}\frac{q_0 q_i}{r_i} + \sum_{i=1}^{n}\sum_{j<i}^{n}\frac{q_i q_j}{r_{ij}}. \tag{4}$$

Here we define $n \equiv N-1$. For the lithium atom $q_0 = Q_1 = 3$ (the charge of the nucleus), $q_i = -1$, $i = 1, 2$, and 3, (the electron charges), $m_0 = M_1$ is the nuclear mass, $\mu_i = m_0 m_i/(m_0 + m_i)$ is the reduced mass of the ith electron, $m_1 = m_2 = m_3 = 1$, and $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$. In this work, we adopted the following values for the nuclear masses in ^{7}Li and ^{6}Li, respectively: $m_0 = 12\,786.392\,282(9)m_e$ and $m_0 = 10\,961.898\,653(3)m_e$ [81], where m_e is the mass of the electron. The calculations involving the nonrelativistic Hamiltonian $H_{\rm nr}^{\rm int}$ can be carried out for both a finite and an infinite mass of the Li nucleus. By setting m_0 to infinity in $H_{\rm nr}^{\rm int}$, one gets the INM Hamiltonian that is used in the standard calculations based on the Born–Oppenheimer approximation. Both the finite nuclear mass (FNM) and INM Hamiltonians are used in the present calculations. When the FNM Hamiltonian is used, both the energy and the wave function explicitly depend on the mass of the nucleus. In the tables reported in this work, we report the results for both finite and infinite nuclear mass. The latter are useful for comparison with literature data.

2.2. Relativistic and QED corrections

Calculations performed at the nonrelativistic level of the theory, even if they are very accurate, are insufficient to determine the total energies and the interstate transition energies with an accuracy comparable to that of high resolution spectroscopic results. To achieve the spectroscopic accuracy, the leading relativistic and QED corrections to the energy must be included in the calculations. The most practical way for calculating these effects for few-electron systems is to use the perturbation theory and to expand the total energy in powers of the fine-structure constant, α [82,83]. The first term in this expansion is the nonrelativistic energy, $E_{\rm nr}$, of the considered state:

$$E_{\rm total} = E_{\rm nr} + \alpha^2 E_{\rm rel}^{(2)} + \alpha^3 E_{\rm QED}^{(3)} + \alpha^4 E_{\rm HQED}^{(4)} + \ldots. \tag{5}$$

The second term, $\alpha^2 E_{\rm rel}^{(2)}$, represents the leading relativistic corrections, the third term, $\alpha^3 E_{\rm QED}^{(3)}$, represents the leading QED corrections, the fourth term, $\alpha^4 E_{\rm HQED}^{(4)}$, represents higher-order QED corrections, and so on. It should be noted that this expansion also includes logarithmic terms of α, but in (5) we label terms according to the integer power of α. The energy corrections are evaluated as expectation values of some effective operators representing the respective physical effects using the nonrelativistic wave function. This wave function can be obtained either in an INM or FNM calculation. The use of an FNM wave function automatically includes the so called nuclear recoil effects in the case of $E_{\rm rel}^{(2)}$. In the calculations of higher order corrections we only use the INM wave function.

In the present work, the $\alpha^2 E_{\rm rel}^{(2)}$ term is calculated as the expectation value of the Dirac–Breit Hamiltonian in the Pauli approximation, $H_{\rm rel}$ [84,85]. This Hamiltonian contains the following terms:

$$H_{\rm rel} = H_{\rm MV} + H_{\rm D} + H_{\rm OO} + H_{\rm SS} + H_{\rm SO}, \tag{6}$$

where operators labeled as $H_{\rm MV}$, $H_{\rm D}$, $H_{\rm OO}$, and $H_{\rm SS}$ represent the mass–velocity, Darwin, orbit–orbit, spin–spin and spin–orbit corrections, respectively. Their explicit forms in the internal coordinates are [76]:

$$H_{\rm MV} = -\frac{1}{8}\left[\frac{1}{m_0^3}\left(\sum_{i=1}^{3}\nabla_{\mathbf{r}_i}\right)^4 + \sum_{i=1}^{3}\frac{1}{m_i^3}\nabla_{\mathbf{r}_i}^4\right], \tag{7}$$

$$H_{\rm D} = -\frac{\pi}{2}\left(\sum_{i=1}^{3}\frac{q_0 q_i}{m_i^2}\delta(\mathbf{r}_i) + \sum_{\substack{i,j=1\\ j\neq i}}^{3}\frac{q_i q_j}{m_i^2}\delta(\mathbf{r}_{ij})\right), \tag{8}$$

$$\begin{aligned} H_{\rm OO} = & -\frac{1}{2}\sum_{i=1}^{3}\frac{q_0 q_i}{m_0 m_i}\left(\frac{1}{r_i}\nabla_{\mathbf{r}_i}'\nabla_{\mathbf{r}_i} + \frac{1}{r_i^3}\mathbf{r}_i'\left(\mathbf{r}_i'\nabla_{\mathbf{r}_i}\right)\nabla_{\mathbf{r}_i}\right) \\ & -\frac{1}{2}\sum_{\substack{i,j=1\\ j\neq i}}^{3}\frac{q_0 q_i}{m_0 m_i}\left(\frac{1}{r_i}\nabla_{\mathbf{r}_i}'\nabla_{\mathbf{r}_j} + \frac{1}{r_i^3}\mathbf{r}_i'\left(\mathbf{r}_i'\nabla_{\mathbf{r}_i}\right)\nabla_{\mathbf{r}_j}\right) \\ & +\frac{1}{2}\sum_{\substack{i,j=1\\ j>i}}^{3}\frac{q_i q_j}{m_i m_j}\left(\frac{1}{r_{ij}}\nabla_{\mathbf{r}_i}'\nabla_{\mathbf{r}_j} + \frac{1}{r_{ij}^3}\mathbf{r}_{ij}'\left(\mathbf{r}_{ij}'\nabla_{\mathbf{r}_i}\right)\nabla_{\mathbf{r}_j}\right), \end{aligned} \tag{9}$$

$$H_{\rm SS} = -\frac{8\pi}{3}\sum_{\substack{i,j=1\\ j>i}}^{3}\frac{q_i q_j}{m_i m_j}\left(\mathbf{s}_i'\mathbf{s}_j\right)\delta(\mathbf{r}_{ij}), \tag{10}$$

and

$$\begin{aligned} H_{\rm SO} = & -\sum_{i=1}^{n}\frac{q_0 q_i}{2m_i}\left(\frac{1}{m_i} + \frac{2}{m_0}\right)\frac{1}{r_i^3}\mathbf{s}_i'(\mathbf{r}_i \times \mathbf{p}_i) \\ & -\sum_{\substack{i,j=1\\ j\neq i}}^{n}\left\{\frac{q_0 q_i}{m_0 m_i}\frac{1}{r_i^3}\mathbf{s}_i'(\mathbf{r}_i \times \mathbf{p}_j) \right. \\ & \left. + \frac{q_i q_j}{2m_i}\frac{1}{r_{ij}^3}\mathbf{s}_i'\left[\mathbf{r}_{ij} \times \left(\frac{1}{m_i}\mathbf{p}_i - \frac{2}{m_j}\mathbf{p}_j\right)\right]\right\} \\ = & H_{\rm SO_1} + H_{\rm SO_2}. \end{aligned} \tag{11}$$

In the above expressions $\delta(\mathbf{r}_i) = \delta(x_i)\delta(y_i)\delta(z_i)$ is the three-dimensional Dirac delta function, $\mathbf{p}_i = -i\nabla_{\mathbf{r}_i}$ is the linear momentum operator for the ith pseudo-particle, $\mathbf{s}_i$ are spin operators for the ith pseudo-particle ($\mathbf{s}_i \equiv \mathbf{S}_{i+1}$), and $H_{\rm SO_1}$ and $H_{\rm SO_2}$ are the one- and two-electron parts of the $H_{\rm SO}$ operator, respectively. For all states considered in this work, the scalar product $\mathbf{s}_i'\mathbf{s}_j$ yields a factor $-3/4$ in the expectation value of $H_{\rm SS}$ defined in Eq. (10). As noted previously, $E_{\rm rel}^{(2)}$ effectively contains both non-recoil and recoil contributions, if the nonrelativistic variational wave function used in the calculation of the expectation values of the relativistic and QED operators is generated using a finite mass of the nucleus in the nonrelativistic Hamiltonian.

In the present calculations, the total spin–orbit correction is a sum of the expectation value of Hamiltonian H_{SO} multiplied by α^2 and the expectation value of the following Hamiltonian representing the correction due to anomalous magnetic moment (AMM) of the electron. This latter expectation value is multiplied by $2\kappa\alpha^2(\approx \frac{\alpha^3}{\pi})$:

$$H_{\mathrm{AMM}} = -\sum_{i=1}^{n} \frac{q_0 q_i}{2m_i^2} \frac{1}{r_i^3} \mathbf{s}_i'(\mathbf{r}_i \times \mathbf{p}_i) - \sum_{\substack{i,j=1\\ j\neq i}}^{n} \frac{q_i q_j}{2m_i} \frac{1}{r_{ij}^3} \mathbf{s}_i' \left[\mathbf{r}_{ij} \times \left(\frac{1}{m_i}\mathbf{p}_i - \frac{1}{m_j}\mathbf{p}_j \right) \right] = H_{\mathrm{AMM}_1} + H_{\mathrm{AMM}_2}, \tag{12}$$

where H_{AMM_1} and H_{AMM_2} are the one- and two-electron parts of the H_{AMM} operator, respectively. The above formula is derived within the INM approach and, in particular, the first term, H_{AMM_1}, corresponds to the INM limit of the one-electron part of the spin–orbit interaction represented by operator H_{SO_1}. In general, the $2\kappa\alpha^2$ correction to the fine-structure splitting also contains the two-electron spin–spin term . This spin–spin term vanishes for ^2P states of the Li atom. The value of electron magnetic moment anomaly $\kappa = 1.15965218128(18) \times 10^{-3}$ is taken from CODATA 2018 [86].

Quantity $E^{(3)}_{\mathrm{QED}}$ in Eq. (5) represents the leading QED correction. For an atomic system, it accounts for the two-photon exchange, the vacuum polarization, and the electron self-energy effects. The explicit form of the corresponding operator is:

$$H_{\mathrm{QED}} = \sum_{\substack{i,j=1\\ j>i}}^{3} \left[\left(\frac{164}{15} + \frac{14}{3}\ln\alpha \right) \delta\left(\mathbf{r}_{ij}\right) - \frac{7}{6\pi}\mathcal{P}\left(\frac{1}{r_{ij}^3}\right) \right] + \sum_{i=1}^{3} \left(\frac{19}{30} - 2\ln\alpha - \ln k_0 \right) \frac{4q_0}{3} \delta\left(\mathbf{r}_i\right), \tag{13}$$

where the first sum represents the Araki–Sucher term [87–91], while the expectation value of $\mathcal{P}\left(1/r_{ij}^3\right)$ is defined as

$$\left\langle \mathcal{P}\left(\frac{1}{r_{ij}^3}\right) \right\rangle = \lim_{a\to 0} \left\langle \frac{1}{r_{ij}^3} \Theta\left(r_{ij} - a\right) + 4\pi\left(\gamma + \ln a\right) \delta\left(\mathbf{r}_{ij}\right) \right\rangle. \tag{14}$$

In the above equation, Θ is the Heaviside step function and $\gamma = 0.577215\ldots$ is the Euler–Mascheroni constant. The last term in Eq. (13) represents the electron self-energy. It contains a contribution involving the so-called Bethe logarithm, $\ln k_0$. The main difficulty in accurately computing the QED correction for a multi-electron atomic system comes from $\ln k_0$. However, it has been known that this quantity mostly depends on the wave function of the core electrons. Therefore, $\ln k_0$ can be approximated with sufficient accuracy (for the purpose of this work) based on its values for the lowest states of Li atom and Li^+ ion. A description of this procedure is described in the next section.

The last term in Eq. (5) is the $E^{(4)}_{\mathrm{HQED}}$ term. It can be approximately calculated as the expectation value of the following operator (for more information, see Ref. [92]):

$$H_{\mathrm{HQED}} = \pi q_0^2 \left(\frac{427}{96} - 2\ln 2 \right) \sum_{i=1}^{n} \delta\left(\mathbf{r}_i\right). \tag{15}$$

E_{HQED} includes the dominant electron–nucleus one-loop radiative correction, but neglects the two-loop and higher order corrections. The expectation value of operator (15) provides only a rough approximation to $E^{(4)}_{\mathrm{HQED}}$ for light atoms

The expectation values of the H_{QED} and H_{HQED} Hamiltonians are calculated in this work with the infinite-nuclear-mass wave functions. This is because the formulae used in the calculations were derived for the clamped nucleus [93,94]. Thus, the $E^{(3)}_{\mathrm{QED}}$ and $E^{(4)}_{\mathrm{HQED}}$ corrections computed in this work do not include the recoil effects.

Some of the operators used in the calculations of the relativistic and QED effects include singular terms. Examples of such terms are the $\nabla^4_{\mathbf{r}_i}$ operator and the one- and two-electron Dirac delta functions, $\delta(\mathbf{r}_i)$ and $\delta(\mathbf{r}_{ij})$. The convergence of the expectation values of Hamiltonians involving such singular terms with the number of basis functions used to expand the wave function of the atom is usually much slower than for non-singular operators. The number of the converged significant figures in the expectation value of a singular operator evaluated directly is typically about twice smaller. However, the convergence can be improved significantly by means of adopting various regularization techniques [95–100]. One way to improve the convergence of the expectation value of a particular singular operator is to employ an expectation-value identity, which involves a certain global operator whose expectation value coincides with the expectation values of the singular operators in the case when the exact wave function is used in the expectation-value calculation. The original idea was laid out by Drachman [100] based on the work of Trivedi [98]. In this work, we also adopt Drachman's approach to compute the expectation values of $\nabla^4_{\mathbf{r}_i}$, $\delta(\mathbf{r}_i)$, and $\delta(\mathbf{r}_{ij})$. More details on this can be found in Refs. [75,101,102].

2.3. Bethe logarithm fitting

Eq. (13) contains a term that includes the Bethe logarithm, $\ln k_0$, which represents the dominant part of the electron self-energy. As mentioned, an accurate calculation of this quantity for multi-electron systems represents a major difficulty. In recent years, some procedures have been developed to calculate this quantity with an increasing accuracy. However, all of the reported calculations have been limited to a few lowest states; mostly the ground state. For instance, the Bethe logarithm for the $2\,^2S$ and $2\,^2P$ states of lithium atom were studied by Puchalski et al. [104], Stanke et al. [105] and Yan et al. [54,67,106], while the $3\,^2S$ state was only considered by Yan et al. [54,67,106]. To our knowledge, no $\ln k_0$ values have been reported in the literature for higher states of lithium.

Drake and Goldman [103] showed that the value of the Bethe logarithm for atomic Rydberg states has the following asymptotic behavior: $A + B/n^3$, where n is the principal quantum number of the state and A and B are constants. In this work, we employ a fitting procedure that employs the above expression to estimate the values of the Bethe logarithm for all considered S and P states using the available $\ln k_0$ values for the S ($2\,^2S$, $3\,^2S$) and P ($2\,^2P$) states of the Li atom. In the fitting procedure, the Bethe logarithm value for the ground $2\,^1S$ state of Li^+ ion [54] is used as the limit when $n \to \infty$. The values of $\ln k_0$ adopted for the S and P states of Li considered in this work are shown in Table 2. To show how these values differ from the ground state value of the hydrogen-like atom, in Table 2 we also list the values of $\ln k_0/q_0^2$, where $q_0 = 3$ is the nuclear charge.

2.4. Oscillator strength

In this work, both the length and velocity formalisms are employed to calculate the absorption oscillator strength, f_{if}. The oscillator strength for a transition between initial state i and final state f is expressed as [107–109]:

$$\text{Length form} \qquad f^{\,L}_{if} = \frac{2}{3g_i}\left(\frac{Z_r}{Z_p}\right) \Delta E_{if} \left|\langle\psi_i|\boldsymbol{\mu}|\psi_f\rangle\right|^2 \tag{16}$$

Table 2
Approximate values of the Bethe logarithm adopted in the present calculations of the QED corrections for all considered ^2S and ^2P states of the lithium atom.

State	Ref.	$\ln k_0$	$\ln(k_0/q_0^2)$
$2\,^2S$	[67]	5.17817	2.98094
$3\,^2S$	[67]	5.17943	2.98221
$4\,^2S$		5.17964	2.98241
$5\,^2S$		5.17974	2.98252
$6\,^2S$		5.17979	2.98256
$7\,^2S$		5.17981	2.98259
$8\,^2S$		5.17982	2.98260
$9\,^2S$		5.17983	2.98261
$10\,^2S$		5.17984	2.98261
$11\,^2S$		5.17984	2.98261
$12\,^2S$		5.17984	2.98262
$13\,^2S$		5.17984	2.98262
$2\,^2P$	[67]	5.179793	2.982568
$3\,^2P$		5.179832	2.982607
$4\,^2P$		5.179842	2.982617
$5\,^2P$		5.179845	2.982621
$6\,^2P$		5.179847	2.982622
$7\,^2P$		5.179848	2.982623
$8\,^2P$		5.179848	2.982624
$9\,^2P$		5.179849	2.982624
$10\,^2P$		5.179849	2.982624
$11\,^2P$		5.179849	2.982624
$12\,^2P$		5.179849	2.982624
$13\,^2P$		5.179849	2.982624
$1\,^1S$ Li^+	[54]	5.1798492	2.982625
$2\,^1S$ H	[103]	2.984128	2.984128

Velocity form
$$f_{if}^{V} = \frac{2}{3\,g_i\,\Delta E_{if}}\left(\frac{Z_p}{Z_r}\right)\left|\langle\psi_i|\mathbf{p}|\psi_f\rangle\right|^2 \tag{17}$$

where $g_i = 2J_i + 1$ is the statistical weight of the lower level, $\Delta E_{if} = |E_i - E_f|$ is the nonrelativistic transition energy, $Z_r = \frac{q_0 m_e + m_0}{n m_e + m_0}$ and $Z_p = \frac{q_0 m_e + m_0}{m_0}$ are the effective radiative charges (q_0 is the charge of the nucleus, m_0 is the nuclear mass, m_e is the mass of the electron, and n is the number of electrons), $\boldsymbol{\mu}$ and $\mathbf{p}$ are the electric dipole moment and linear momentum operators, respectively. For an n-electron atom,

$$\boldsymbol{\mu} = \sum_{i=1}^{n} q_i \mathbf{r}_i\,, \quad \mathbf{p} = -i\sum_{i=1}^{n}\nabla_{\mathbf{r}_i}\,, \tag{18}$$

where q_i and $\mathbf{r}_i$ are the charge of the ith electron and its position in the internal coordinate system, respectively, and $\nabla_{\mathbf{r}_i}$ is the gradient with respect to $\mathbf{r}_i$. It is worth mentioning that for a charge-neutral system, $\boldsymbol{\mu}$ has the same value regardless of the choice of the origin of the coordinate system. ψ_i and ψ_f are non-relativistic wave functions obtained in the variational calculations with Hamiltonian (4). Due to the dependence of the Hamiltonian on the nuclear mass, the resulting wave functions, ψ_i and ψ_f, also explicitly depend on the nuclear mass. Thus, the wave functions for ^{6}Li, ^{7}Li, and $^\infty$Li are slightly different. The matrix elements associated with the $i \to f$ transition can be written in the following form:

$$\begin{aligned}|\boldsymbol{\mu}_{if}|^2 &= \left|\langle\psi_i|\boldsymbol{\mu}|\psi_f\rangle\right|^2\\ &= \left|\langle\psi_i|\mu_x|\psi_f\rangle\right|^2 + \left|\langle\psi_i|\mu_y|\psi_f\rangle\right|^2 + \left|\langle\psi_i|\mu_z|\psi_f\rangle\right|^2.\end{aligned} \tag{19}$$

$$\begin{aligned}|\mathbf{p}_{if}|^2 &= \left|\langle\psi_i|\mathbf{p}|\psi_f\rangle\right|^2\\ &= \left|\langle\psi_i|p_x|\psi_f\rangle\right|^2 + \left|\langle\psi_i|p_y|\psi_f\rangle\right|^2 + \left|\langle\psi_i|p_z|\psi_f\rangle\right|^2.\end{aligned} \tag{20}$$

For oscillator strengths, only the matrix elements between the S ($L = 0, M_L = 0$) and P ($L = 1, M_L = 0$) states need to be evaluated. Moreover, for P states with $M_L = 0$ only the last term in Eqs. (19) and (20) are non-zero. The transition matrix elements in the length and velocity forms with ECG basis functions (1) and (2) can be evaluated in a similar way as overlap matrix elements [80,110,111] Ref. [80] contains a derivation of these elements in the length forms. Here, we only present the expression for the transition matrix elements in the velocity form. For the sake of consistency, we adopt the same notation scheme as used in Refs. [80,110,111]. The z-component of the transition matrix element between S ($L = 0, M_L = 0$) and P ($L = 1, M_L = 0$) ECGs can be expressed as:

$$\begin{aligned}&\left\langle\hat{P}_k\phi_k^{(0)}\right|(p_i)_z\left|\hat{P}_l\phi_l^{(1)}\right\rangle = \left\langle(p_i)_z\,\tilde{\phi}_k^{(0)}\middle|\tilde{\phi}_l^{(1)}\right\rangle\\ &= \int\left(i\frac{\partial}{\partial z_i}\,\exp[-\mathbf{r}'(\tilde{A}_k\otimes I_3)\mathbf{r}]\right)z_{\tilde{m}_l}\exp[-\mathbf{r}'(\tilde{A}_l\otimes I_3)\mathbf{r}]\,d\mathbf{r}\\ &= 2\,i\int(\mathbf{v}^{i\prime}\tilde{\mathbf{A}}_k\mathbf{r})\exp[-\mathbf{r}'\tilde{\mathbf{A}}_k\mathbf{r}]\,(\tilde{\mathbf{v}}^{l\prime}\mathbf{r})\exp[-\mathbf{r}'\tilde{\mathbf{A}}_l\mathbf{r}]\,d\mathbf{r}\end{aligned} \tag{21}$$

Here $\hat{P}_k$ and $\hat{P}_l$ are the electron permutation operators for the *bra* and *ket* wave functions, respectively, $\mathbf{A}_k \equiv A_k \otimes I_3$, $\mathbf{A}_l \equiv A_l \otimes I_3$, and $\mathbf{v}^l \equiv v^l \otimes \boldsymbol{\epsilon}^z$, where $\boldsymbol{\epsilon}^{z\prime} \equiv (0, 0, 1)$. v^l is a sparse n-component vector with all components equal to zero, except the m_l-th component. The scalar product of a $3n$-component vector $\mathbf{v}^l$ with another $3n$-component vector $\mathbf{r}$ yields a single coordinate, $z_{m_l} = \mathbf{v}^{l\prime}\mathbf{r}$. The tilde symbol denotes the action of the permutation matrices $\mathbf{P}_k \equiv P_k \otimes I_3$ and $\mathbf{P}_l \equiv P_l \otimes I_3$ corresponding to operators $\hat{P}_k$ and $\hat{P}_l$ on matrices $\mathbf{A}_k$, $\mathbf{A}_l$, and vector $\mathbf{v}^l$:

$$\tilde{\mathbf{A}}_k = \mathbf{P}_k'\mathbf{A}_k\mathbf{P}_k,\ \tilde{\mathbf{A}}_l = \mathbf{P}_l'\mathbf{A}_l\mathbf{P}_l,\ \tilde{\mathbf{v}}^l = \mathbf{P}_l'\mathbf{v}^l,\ z_{\tilde{m}_k} = \tilde{\mathbf{v}}^{l\prime}\mathbf{r},\ \frac{\partial}{\partial z_i} = \mathbf{v}^{i\prime}\nabla.$$

The integral in Eq. (21) is given by formula (28) in Ref. [111]. In that formula, it is necessary to replace $v^k \to v^i$. With that expression (21) becomes:

$$\left\langle\tilde{\phi}_k^{(0)}\right|(p_i)_z\left|\tilde{\phi}_l^{(1)}\right\rangle = i\,\pi^{\frac{3n}{2}}\,\frac{v^{i\prime}\tilde{A}_k\tilde{A}_{kl}^{-1}\tilde{v}^l}{\left|\tilde{A}_{kl}\right|^{3/2}}, \tag{22}$$

where $\tilde{A}_{kl} = \tilde{A}_k + \tilde{A}_l$.

3. Results

The lowest twelve Rydberg ^2S states and the lowest twelve Rydberg ^2P states of the lithium are studied in the present work.

In the first step of the calculations, the nonrelativistic wave functions and the corresponding energies are obtained using the standard Rayleigh–Ritz variational method. In generating the ECG basis set for each state, the internal Hamiltonian explicitly dependent on the mass of the nucleus of the ^{7}Li isotope, i.e., FNM Hamiltonian (4), is used. The basis sets generated for all considered states of the ^{7}Li isotope are subsequently used to obtain the energies and the corresponding wave functions of ^{6}Li and $^\infty$Li. The nonrelativistic variational calculations yield basis sets of progressively larger size (i.e. length of the expansion) in a process that involves growing the basis set from a small number of functions to its final size. The growing of the basis set for each particular state is performed independently from other states. The growing procedure involves adding new functions to the set and variationally optimizing their nonlinear parameters using a procedure that employs the analytical energy gradient determined with respect to these parameters. More details about the basis set enlargement procedure can be found in our previous works [80,110–112].

It should be noted that the generation of the basis set for each considered state is by far the most time consuming part of the calculations. It required over a year of continuous computing using several hundred cores in total. Parallel computer systems equipped with Intel Xeon E5-2695v3 and AMD EPYC 7642 central processing units (CPUs) were used. The code is written in FORTRAN and makes use of MPI (Message Passing Interface) library to facilitate parallelism. In order to maintain high accuracy in all calculations and generate large ECG basis sets, in particular for higher excited states, we used extended precision arithmetic (80-bit format), which has a hardware implementation in floating-point modules on the x86 architecture. The use of extended precision, as compared to standard double precision (64-bit format), typically slows down calculations by a factor of 2–3. However, the four extra decimal figures in the mantissa provided by the extended precision, make a significant difference in the numerical accuracy and stability of the calculations. That, in turn, leads to more efficient basis set optimization.

3.1. Nonrelativistic energy

We start the presentation of the results with the survey of the energies of the ground $(1s^2\,2s)\,^2S$ state and the lowest excited $(1s^2\,2p)\,^2P$ state of $^\infty$Li available in the literature. These are shown in Table 1. Most results listed in the table are variational. The best results to date have been obtained using the variational method with explicitly correlated basis functions. As such functions explicitly depend on inter-electron distances, they allow for a very accurate description of the electronic correlation effects. Hylleraas-type (Hy) functions and explicitly correlated Gaussian (ECG) functions have been the most popular types used in high-accuracy atomic calculations. However, the Hylleraas basis set, despite its good performance for atoms, cannot be easily extended to the case of atomic systems with more than three electrons. The Gaussian functions do not have these limitations, but they are not as good as the Hy functions in describing the behavior of the wave function near the particle coalescence points. They also have less suitable long range behavior. These deficiencies can be largely overcome by using a larger number of basis functions.

As it can be deduced from Table 1, the most accurate to date nonrelativistic energies for the $^2S(1s^2\,2s)$ and $^2P(1s^2\,2p)$ states were reported by Wang et al. [67]. For the $^2S(1s^2\,2s)$ state, the energy value obtained with Hylleraas basis functions and extrapolated to an infinite number of functions of −7.478 060 323 910 150(5) hartree in slightly lower than the value of −7.478 060 323 906 57 hartree obtained in this work with 11 000 ECG basis functions. In order to assess the efficiency of the ECGs in calculating the lowest ^2S and ^2P bound states of lithium, additional calculations were performed for these states. For the ground ^2S state, the number of the ECGs were gradually increased from 11 000 to 12 000, which yielded the nonrelativistic energy of −7.478 060 323 907 70 hartree. This value can be compared with the energy of −7.478 060 323 910 044 374 hartree calculated by Wang et al. [64] using 12 168 Hylleraas basis functions.

For the $(1s^2\,2p)^2P$ state, Wang et al. [67] used 33 600 Hylleraas basis functions to expand the wave function. The energy extrapolated to an infinite number of functions was −7.410 156 532 652 41(3) hartree. In the present work, using 17 500 ECGs, we obtain the energy of −7.410 156 532 650 37 hartree. This energy agrees in 12 decimal figures with the Wang's et al. value.

In Table 3, some key expectation values are listed for the S- and P-states considered in this work. In recent years, states up to $9\,^2S$ and $10\,^2P$ were studied by Puchalski et al. [60] and Wang et al. [113] using Hylleraas type basis. Due to the high efficiency of the Hylleraas basis functions and very large number of terms employed in the calculations (15 952 and 22 302 for the S- and P states, respectively), the calculated nonrelativistic energies in the aforementioned works lie slightly below our values. Despite the rather significant difference in the number of basis functions we used, our expectation values are in good agreement with those obtained in [60,113]. For example, in the case of the $9\,^2S$ and $10\,^2P$ states (these are the highest one considered in [60,113], respectively) our values agree with those reported by Puchalski et al. and Wang et al. to 8 and 7 decimal figures, respectively.

3.2. Relativistic corrections

As discussed in Section 2, the relativistic correction is proportional to the sum of the expectation values $\langle H_{\rm MV}\rangle$, $\langle H_{\rm OO}\rangle$, $\langle H_{\rm D}\rangle$, $\langle H_{\rm SS}\rangle$, and $\langle H_{\rm SO}\rangle$. All of them are evaluated in the present work. The first two expectation values are shown in Table 3 for all 24 states of the ^{6}Li, ^{7}Li, and $^\infty$Li isotopes considered in this work. For comparison we also list the values obtained by Wang et al. [67] and by Puchalski and Pachucki [56] for the lowest three states, namely $2\,^2S$, $2\,^2P$, and $3\,^2S$. For these three states our values are in good agreement with those taken from Refs. [56,67]. For example, the expectation values of a singular operator $H_{\rm MV}$ (for which we adopted the regularization technique mentioned in the end of Section 2.2) agree to more than five digits after decimal point. It can be noted that there are some observable differences between the calculated values of $\langle H_{\rm OO}\rangle$ for ^{6}Li and ^{7}Li. For example, in the case of $^\infty$Li, one can compare the values of −0.435 597 832 5(4), −0.435 597 832 4(3), and −0.435 597 905(5) hartree obtained for the ground state by us, Wang et al. and Puchalski and Pachucki, respectively. As one can see, the values agree to nine and six decimal figures, respectively, with those from the previous works. Worse agreement with the value calculated by Puchalski and Pachucki can be due to a smaller number of the basis functions used in their calculations. In the case of ^{6}Li and ^{7}Li isotopes, the values calculated in the present work match very well (within the estimated uncertainties) the values presented in Ref. [67] (see Table 3), but not with the values reported in Ref. [56]. For example, in the present work, we obtain the value of −0.447 137 155 9(4) hartree for the ground state of ^{6}Li which agrees only up to only three decimal figures with the value of −0.447 259 957(5) hartree reported by Puchalski and Pachucki [56] but up to nine decimal figures with the result of −0.447 137 155 8(3) hartree reported by Wang et al. [67]. Wang et al. included the contribution due to the finite mass of the nucleus in their orbit–orbit Hamiltonian, $H_{\rm OO}$, and calculated the corresponding contribution to the energy perturbatively up to the first order. They also calculated the effect of the finite nuclear

Table 3
Convergence of the nonrelativistic variational energy (E_{nr}) and the expectation values of the mass–velocity Hamiltonian (H_{MV}), orbit–orbit Hamiltonian (H_{OO}), and one- and two-electron Dirac δ-functions with the number of the basis functions for the lowest twelve ^2S and ^2P states of the lithium atom. The numbers in parentheses are estimated uncertainties due to the basis truncation. The tilde symbol indicates that a regularization approach improving convergence [75,100–102] was used in the calculations of the corresponding expectation values. For comparison we provide some reference values from works [56,60,67,113], in which the variational calculations were performed using the Hylleraas-type basis functions. All expectation values are given in atomic units.

	Basis	E_{nr}	$\langle\tilde{H}_{MV}\rangle$	$\langle H_{OO}\rangle$	$\langle\tilde{\delta}(\mathbf{r}_i)\rangle$	$\langle\tilde{\delta}(\mathbf{r}_{ij})\rangle$	$\langle\mathcal{P}\left(1/r_i^3\right)\rangle$
$2\,^2S$							
^{6}Li	11000	−7.477350681409	−78.526998	−0.4471371560	4.61292633955	0.181394391275	−102.7347
	∞	−7.477350681412(3)	−78.526995(3)	−0.4471371559(4)	4.61292633961(6)	0.181394391281(6)	−102.7349(2)
[67]	∞	−7.477350681412340(5)	−78.5269952(1)	−0.4471371558(3)[a]	4.6129263405(1)	0.18139439125(2)	
[56]	10000	−7.477350681393					
[56]	∞	−7.477350681410(8)	−78.5556583(5)	−0.447259957(5)[b]	4.614188861(2)	0.1814440376(2)	
^{7}Li	11000	−7.477451930729	−78.531153	−0.4454910339	4.61310856432	0.181401118411	−102.7395
	∞	−7.477451930732(3)	−78.531150(3)	−0.4454910338(4)	4.61310856437(6)	0.181401118417(6)	−102.7397(2)
[67]	∞	−7.477451930732360(5)	−78.5311506(1)	−0.4454910338(3)[a]	4.6131085653(1)	0.18140111839(2)	
[56]	10000	−7.477451930713					
[56]	∞	−7.477451930729(8)	−78.5557252(5)	−0.445595893(5)[b]	4.614190964(2)	0.1814436818(2)	
$^\infty$Li	11000	−7.478060323907	−78.556126	−0.4355978322	4.61420361873	0.181441544287	−102.7684
	∞	−7.478060323910(3)	−78.556123(3)	−0.4355978325(4)	4.61420361878(6)	0.181441544293(6)	−102.7686(2)
[67]	∞	−7.478060323910150(6)	−78.5561228(1)	−0.4355978324(3)	4.6142036197(1)	0.18144154429(2)	
[56]	10000	−7.4780603238897					
[56]	∞	−7.478060323906(8)	−78.5561278(5)	−0.435597905(5)	4.614203596(2)	0.1814415440(2)	
[60]	30632	−7.478060323910097					
[60]	∞	−7.4780603239102(2)					
$2\,^2P$							
^{6}Li	12000	−7.409458110572	−77.476813	−0.4077728961	4.5574652832	0.17737818141	−101.4695
	∞	−7.409458110578(2)	−77.476810(3)	−0.4077728960(6)	4.5574652834(2)	0.17737818144(3)	−101.4709(14)
[67]	∞	−7.409458110578580(4)	−77.47680728(9)	−0.4077728986(4)[a]	4.55746528329(2)	0.1773296463(1)	
[56]	14000	−7.409458110554					
[56]	∞	−7.409458110593(8)	−77.5051589(10)	−0.40788491(2)[b]	4.558712653(2)	0.1774267284(1)	
^{7}Li	12000	−7.409557758967	−77.480923	−0.4061541891	4.5576460511	0.17738481802	−101.4742
	∞	−7.409557758973(2)	−77.480920(3)	−0.4061541890(6)	4.5576460513(2)	0.17738481805(3)	−101.4757(14)
[67]	∞	−7.409557758973640(3)	−77.48091724(9)	−0.4061541910(4)[a]	4.55764605111(2)	0.1773432058(1)	
[56]	14000	−7.409557758949					
[56]	∞	−7.409557758987(14)	−77.5052250(10)	−0.40624980(2)[b]	4.558715464(2)	0.1774264390(1)	
$^\infty$Li	12000	−7.410156532646	−77.505622	−0.3964257411	4.5587323501	0.17742469993	−101.5029
	∞	−7.410156532652(2)	−77.505619(3)	−0.3964257417(6)	4.5587323502(2)	0.17742469996(3)	−101.5044(14)
[67]	∞	−7.41015653265241(3)	−77.50561673(9)	−0.3964257417(4)	4.55873235019(2)	0.17742469997(1)	
[56]	14000	−7.4101565326286					
[56]	∞	−7.410156532665(14)	−77.5056221(10)	−0.39642580(2)	4.558732353(2)	0.1774246996(1)	
$3\,^2S$							
^{6}Li	11000	−7.353400979505	−77.828561	−0.4413285218	4.5775666064	0.17867628717	−101.943
	∞	−7.353400979517(12)	−77.828558(3)	−0.4413285216(3)	4.5775666067(2)	0.17867628719(2)	−101.944(2)
[67]	∞	−7.353400979512100(3)	−77.828550(1)	−0.441328520(3)[a]	4.5775666072(1)	0.1786762872(1)	
[56]	10000	−7.353400979449					
[56]	∞	−7.353400979495(19)	−77.856962(3)	−0.44144975(9)[b]	4.57881945(2)	0.1787251903(1)	
^{7}Li	11000	−7.353500488185	−77.832679	−0.4396994321	4.5777474649	0.17868292381	−101.947
	∞	−7.353500488197(12)	−77.832676(3)	−0.4396994319(3)	4.5777474652(2)	0.17868292383(2)	−101.949(2)
[67]	∞	−7.353500488192230(3)	−77.832668(1)	−0.439699431(3)[a]	4.5777474657(1)	0.1786829239(1)	
[56]	10000	−7.353500488129					
[56]	∞	−7.353500488175(19)	−77.857028(3)	−0.43980296(9)[b]	4.57882156(2)	0.1787248501(1)	
$^\infty$Li	11000	−7.354098421437	−77.857427	−0.4299086059	4.5788343086	0.17872280587	−101.976
	∞	−7.354098421449(12)	−77.857424(3)	−0.4299086061(3)	4.5788343089(2)	0.17872280588(2)	−101.978(2)
[67]	∞	−7.354098421444367(3)	−77.857416(1)	−0.429908605(3)	4.5788343093(1)	0.1787228059(1)	
[56]	10000	−7.3540984213799					
[56]	∞	−7.354098421426(19)	−77.857425(3)	−0.42990872(9)	4.57883428(2)	0.1787228063(1)	
[60]	15952	−7.35409842144266					
[60]	∞	−7.3540984214432(4)					
$3\,^2P$							
^{6}Li	12000	−7.336457285729	−77.570007	−0.4294346390	4.5638735255	0.177719697275	−101.628
	∞	−7.336457285734(5)	−77.570005(2)	−0.4294346389(3)	4.5638735257(2)	0.177719697285(10)	−101.631(2)
^{7}Li	12000	−7.336556363657	−77.574114	−0.4278123984	4.5640540455	0.177726313677	−101.633
	∞	−7.336556363662(5)	−77.574112(2)	−0.4278123983(3)	4.5640540457(2)	0.177726313687(10)	−101.635(2)
$^\infty$Li	12000	−7.337151708587	−77.598797	−0.4180627327	4.5651388552	0.177766074097	−101.662
	∞	−7.337151708592(5)	−77.598795(2)	−0.4180627330(3)	4.5651388553(2)	0.177766074107(10)	−101.664(2)
$4\,^2S$							
^{6}Li	11500	−7.317836821409	−77.692282	−0.4401241680	4.5708357170	0.17816806483	−101.7886
	∞	−7.317836821427(18)	−77.692275(7)	−0.4401241674(6)	4.5708357173(3)	0.17816806493(10)	−101.7896(11)
^{7}Li	11500	−7.317935842552	−77.696393	−0.4384984319	4.5710163193	0.17817468487	−101.7933
	∞	−7.317935842570(18)	−77.696386(7)	−0.4384984312(6)	4.5710163196(3)	0.17817468497(10)	−101.7944(11)

(*continued on next page*)

Table 3 (*continued*).

	Basis	E_{nr}	$\langle\tilde{H}_{MV}\rangle$	$\langle H_{OO}\rangle$	$\langle\tilde{\delta}(\mathbf{r}_i)\rangle$	$\langle\tilde{\delta}(\mathbf{r}_{ij})\rangle$	$\langle\mathcal{P}\left(1/r_i^3\right)\rangle$
$^{\infty}$Li	11500	−7.318530845984	−77.721098	−0.4287277640	4.5721016234	0.17821446717	−101.8220
	∞	−7.318530846003(18)	−77.721091(7)	−0.4287277646(6)	4.5721016237(3)	0.17821446727(10)	−101.8230(11)
[60]	15952	−7.3185308459903					
[60]	∞	−7.318530845994(2)					
$4\,^2P$							
^{6}Li	12000	−7.311196254253	−77.5923929	−0.4351337113	4.5655234534	0.17780217155	−101.666
	∞	−7.311196254260(8)	−77.5923914(15)	−0.4351337108(6)	4.5655234538(4)	0.17780217158(3)	−101.669(3)
[113]	∞	−7.3111962542635(2)					
^{7}Li	12000	−7.311295101605	−77.5964996	−0.4335106343	4.5657039274	0.17780878405	−101.671
	∞	−7.311295101612(8)	−77.5964982(15)	−0.4335106338(6)	4.5657039278(4)	0.17780878407(3)	−101.674(3)
[113]	∞	−7.3112951016176(2)					
$^{\infty}$Li	12000	−7.311889060739	−77.6211797	−0.4237559470	4.5667884603	0.17784852098	−101.700
	∞	−7.311889060747(8)	−77.6211782(15)	−0.4237559476(6)	4.5667884607(4)	0.17784852101(3)	−101.703(3)
[113]	22302	−7.31188906075855					
[113]	∞	−7.3118890607587(2)					
$5\,^2S$							
^{6}Li	12000	−7.30285897585	−77.648722	−0.4397360622	4.568708201	0.1780083130	−101.737
	∞	−7.30285897598(13)	−77.648708(14)	−0.4397360606(16)	4.568708203(2)	0.1780083133(3)	−101.744(7)
^{7}Li	12000	−7.30295779423	−77.652830	−0.4381114021	4.568888723	0.1780149279	−101.742
	∞	−7.30295779437(13)	−77.652817(14)	−0.4381114005(16)	4.568888725(2)	0.1780149282(3)	−101.749(7)
$^{\infty}$Li	12000	−7.30355157919	−77.677522	−0.4283472030	4.569973544	0.1780546791	−101.771
	∞	−7.30355157932(13)	−77.677508(14)	−0.4283472045(16)	4.569973546(2)	0.1780546794(3)	−101.777(7)
[60]	15952	−7.3035515792190					
[60]	∞	−7.303551579222(3)					
$5\,^2P$							
^{6}Li	12000	−7.29959617064	−77.600174	−0.4371973043	4.5661174259	0.17783119515	−101.6797
	∞	−7.29959617066(2)	−77.600167(7)	−0.4371973035(8)	4.5661174263(4)	0.17783119523(9)	−101.6807(10)
[113]	∞	−7.29959617066065(5)					
^{7}Li	12000	−7.29969490232	−77.604281	−0.4355739401	4.5662978861	0.17783780642	−101.6844
	∞	−7.29969490234(2)	−77.604273(7)	−0.4355739393(8)	4.5662978864(4)	0.17783780650(9)	−101.6855(10)
[113]	∞	−7.29969490233930(6)					
$^{\infty}$Li	12000	−7.30028816623	−77.628960	−0.4258175286	4.5673823359	0.17787753601	−101.7130
	∞	−7.30028816625(2)	−77.628952(7)	−0.4258175293(8)	4.5673823362(4)	0.17787753610(9)	−101.7141(10)
[113]	22302	−7.30028816626505					
[113]	∞	−7.3002881662651(1)					
$6\,^2S$							
^{6}Li	12500	−7.2951676316	−77.63074	−0.439575208	4.567832912	0.1779427503	−101.711
	∞	−7.2951676320(3)	−77.63072(2)	−0.439575199(9)	4.567832920(8)	0.1779427513(10)	−101.720(9)
^{7}Li	12500	−7.2952663467	−77.63485	−0.437950994	4.568013401	0.1779493630	−101.716
	∞	−7.2952663470(3)	−77.63483(2)	−0.437950985(9)	4.568013409(8)	0.1779493641(10)	−101.725(9)
$^{\infty}$Li	12500	−7.2958595107	−77.65953	−0.428189478	4.569098024	0.1779891016	−101.744
	∞	−7.2958595111(3)	−77.65951(2)	−0.428189470(9)	4.569098032(8)	0.1779891026(10)	−101.753(9)
[60]	15952	−7.2958595108083					
[60]	∞	−7.295859510815(6)					
$6\,^2P$							
^{6}Li	12000	−7.29332852201	−77.603540	−0.4381138534	4.5663805939	0.1778439165	−101.680
	∞	−7.29332852213(12)	−77.603531(10)	−0.4381138524(10)	4.5663805950(10)	0.1778439167(2)	−101.681(1)
[113]	22302	−7.2933285220817(4)					
^{7}Li	12000	−7.29342718774	−77.607647	−0.4364903653	4.5665610486	0.1778505273	−101.685
	∞	−7.29342718785(12)	−77.607637(10)	−0.4364903643(10)	4.5665610496(10)	0.1778505275(2)	−101.686(1)
[113]	22302	−7.2934271878104(4)					
$^{\infty}$Li	11000	−7.29402005529	−77.632326	−0.4267332105	4.5676454657	0.1778902539	−101.714
	∞	−7.29402005541(12)	−77.632316(10)	−0.4267332115(10)	4.5676454667(10)	0.1778902541(2)	−101.715(1)
[113]	22302	−7.29402005537765					
[113]	∞	−7.2940200553779(3)					
$7\,^2S$							
^{6}Li	13000	−7.290700813	−77.62202	−0.43949698	4.56740869	0.177911015	−101.683
	∞	−7.290700815(2)	−77.62188(13)	−0.43949689(9)	4.56740876(7)	0.177911026(11)	−101.70(2)
^{7}Li	13000	−7.290799469	−77.62612	−0.43787298	4.56758916	0.177917626	−101.687
	∞	−7.290799471(2)	−77.62599(13)	−0.43787289(9)	4.56758923(7)	0.177917637(11)	−101.71(2)
$^{\infty}$Li	13000	−7.291392274	−77.65081	−0.42811278	4.56867369	0.177957359	−101.716
	∞	−7.291392276(2)	−77.65067(13)	−0.42811268(9)	4.56867376(7)	0.177957369(11)	−101.74(2)
[60]	15952	−7.291392274160					
[60]	∞	−7.29139227422(5)					

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mass on the wave function in their calculation of the $\langle H_{OO}\rangle$ expectation value. The calculation was also done perturbatively, but this time up to the second order level. Puchalski and Pachucki [56] included an equivalent nuclear term in their H_{OO}. However, they only included the first-order term in the expansion of $\langle H_{OO}\rangle$ in terms of the inverse nuclear mass. In spite of some difference between our $\langle H_{OO}\rangle$ values and those from Ref. [56], the values of the total relativistic correction are very close because the $\langle H_{OO}\rangle$

Table 3 (*continued*).

	Basis	E_{nr}	$\langle\tilde{H}_{MV}\rangle$	$\langle H_{OO}\rangle$	$\langle\tilde{\delta}(\mathbf{r}_i)\rangle$	$\langle\tilde{\delta}(\mathbf{r}_{ij})\rangle$	$\langle\mathcal{P}\left(1/r_i^3\right)\rangle$
$7\,^2P$							
^{6}Li	12000	−7.2895636671	−77.60526	−0.438580632	4.566514443	0.1778503475	−101.6738
	∞	−7.2895636673(2)	−77.60524(2)	−0.438580621(12)	4.566514454(11)	0.1778503488(13)	−101.687(13)
[113]	∞	−7.289563667321(2)					
^{7}Li	12000	−7.2896622918	−77.60936	−0.436957083	4.566694895	0.1778569580	−101.6785
	∞	−7.2896622920(2)	−77.60934(2)	−0.436957071(12)	4.566694906(11)	0.1778569593(13)	−101.692(13)
[113]	∞	−7.289662291990(2)					
$^\infty$Li	12000	−7.2902549126	−77.63404	−0.427199558	4.567779296	0.1778966832	−101.7071
	∞	−7.2902549128(2)	−77.63402(2)	−0.427199548(12)	4.567779307(11)	0.1778966844(13)	−101.720(13)
[113]	22302	−7.29025491279716					
[113]	∞	−7.290254912799(2)					
$8\,^2S$							
^{6}Li	13500	−7.287878634	−77.61735	−0.43945459	4.56717859	0.17789381	−101.64
	∞	−7.287878636(2)	−77.61731(3)	−0.43945448(11)	4.56717868(9)	0.17789384(3)	−101.67(3)
^{7}Li	13500	−7.287977252	−77.62145	−0.43783071	4.56735905	0.17790042	−101.65
	∞	−7.287977254(2)	−77.62142(3)	−0.43783060(11)	4.56735914(9)	0.17790045(3)	−101.68(3)
$^\infty$Li	13500	−7.288569831	−77.64613	−0.42807121	4.56844352	0.17794015	−101.68
	∞	−7.288569833(2)	−77.64610(3)	−0.42807110(11)	4.56844361(9)	0.17794018(3)	−101.71(3)
[60]	15952	−7.288569832747					
[60]	∞	−7.28856983276(9)					
$8\,^2P$							
^{6}Li	14000	−7.2871270258	−77.6062	−0.4388427	4.56658951	0.17785394	−101.652
	∞	−7.2871270264(6)	−77.6060(3)	−0.4388425(3)	4.56658954(3)	0.17785396(2)	−101.662(10)
[113]	22302	−7.2871270262255(6)					
^{7}Li	14000	−7.2872256232	−77.6103	−0.4372191	4.56676996	0.17786055	−101.657
	∞	−7.2872256238(6)	−77.6101(3)	−0.4372189(3)	4.56676999(3)	0.17786057(2)	−101.667(10)
[113]	22302	−7.2872256236354(6)					
$^\infty$Li	14000	−7.2878180802	−77.6350	−0.4274614	4.56785436	0.17790028	−101.685
	∞	−7.2878180807(6)	−77.6348(3)	−0.4274611(3)	4.56785438(3)	0.17790030(2)	−101.696(10)
[113]	22302	−7.28781808061515					
[113]	∞	−7.2878180806158(6)					
$9\,^2S$							
^{6}Li	14000	−7.285982562	−77.61448	−0.4394295	4.56704318	0.17788370	−101.63
	∞	−7.285982565(3)	−77.61440(8)	−0.4394292(3)	4.56704329(11)	0.17788375(5)	−101.67(4)
^{7}Li	14000	−7.286081155	−77.61858	−0.4378057	4.56722364	0.17789031	−101.64
	∞	−7.286081158(3)	−77.61850(8)	−0.4378054(3)	4.56722375(11)	0.17789036(5)	−101.68(4)
$^\infty$Li	14000	−7.286673583	−77.64326	−0.4280466	4.56830808	0.17793004	−101.66
	∞	−7.286673586(3)	−77.64318(8)	−0.4280463(3)	4.56830819(11)	0.17793009(5)	−101.70(4)
[60]	15952	−7.28667358671					
[60]	∞	−7.2866735871(3)					
$9\,^2P$							
^{6}Li	15000	−7.285460105	−77.60709	−0.4390014	4.5666348	0.17785606	−101.63
	∞	−7.285460112(7)	−77.60700(9)	−0.4390011(3)	4.5666351(3)	0.17785609(3)	−101.71(9)
[113]	∞	−7.2854601072730(5)					
^{7}Li	15000	−7.285558683	−77.61120	−0.4373778	4.5668152	0.17786267	−101.63
	∞	−7.285558690(7)	−77.61111(9)	−0.4373775(3)	4.5668155(3)	0.17786270(3)	−101.72(9)
[113]	∞	−7.2855586856755(5)					
$^\infty$Li	15000	−7.286151026	−77.63588	−0.4276199	4.5678996	0.17790239	−101.66
	∞	−7.286151033(7)	−77.63579(9)	−0.4276196(3)	4.5678999(3)	0.17790243(3)	−101.75(9)
[113]	22302	−7.28615102842333					
[113]	∞	−7.2861510284238(5)					
$10\,^2S$							
^{6}Li	16000	−7.284647589	−77.6129	−0.4394143	4.5669580	0.17787732	−101.560
	∞	−7.284647601(13)	−77.6126(3)	−0.4394135(7)	4.5669583(3)	0.17787741(9)	−101.61(5)
^{7}Li	16000	−7.284746164	−77.6170	−0.4377905	4.5671384	0.17788393	−101.565
	∞	−7.284746176(13)	−77.6167(3)	−0.4377898(7)	4.5671387(3)	0.17788402(9)	−101.62(5)
$^\infty$Li	16000	−7.285338485	−77.6417	−0.4280316	4.5682228	0.17792365	−101.594
	∞	−7.285338498(13)	−77.6413(3)	−0.4280309(7)	4.5682232(3)	0.17792374(9)	−101.64(5)
$10\,^2P$							
^{6}Li	16000	−7.284269824	−77.60732	−0.43910226	4.56666367	0.177857468	−101.619
	∞	−7.284269829(5)	−77.60726(6)	−0.43910215(10)	4.56666373(6)	0.177857481(13)	−101.625(6)
[113]	∞	−7.2842698285171(9)					
^{7}Li	16000	−7.284368389	−77.61142	−0.43747864	4.56684412	0.177864079	−101.624
	∞	−7.284368393(5)	−77.61136(6)	−0.43747854(10)	4.56684418(6)	0.177864091(13)	−101.629(6)
[113]	∞	−7.2843683931451(9)					
$^\infty$Li	16000	−7.284960649	−77.63610	−0.42772069	4.56792851	0.177903802	−101.652
	∞	−7.284960653(5)	−77.63604(6)	−0.42772061(10)	4.56792857(6)	0.177903815(13)	−101.658(6)
[113]	22302	−7.28496065310864					
[113]	∞	−7.2849606531095(9)					

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Table 3 (*continued*).

	Basis	E_{nr}	$\langle\tilde{H}_{MV}\rangle$	$\langle H_{OO}\rangle$	$\langle\tilde{\delta}(\mathbf{r}_i)\rangle$	$\langle\tilde{\delta}(\mathbf{r}_{ij})\rangle$	$\langle\mathcal{P}\left(1/r_i^3\right)\rangle$
$11\,^2S$							
^{6}Li	16000	−7.28367220	−77.6127	−0.439410	4.566896	0.1778724	−101.2
	∞	−7.28367229(9)	−77.6123(4)	−0.439406(4)	4.566903(7)	0.1778730(6)	−101.4(2)
^{7}Li	16000	−7.28377077	−77.6168	−0.437786	4.567076	0.1778790	−101.2
	∞	−7.28377086(9)	−77.6164(4)	−0.437782(4)	4.567083(7)	0.1778796(6)	−101.4(2)
$^\infty$Li	16000	−7.28436301	−77.6415	−0.428027	4.568161	0.1779187	−101.2
	∞	−7.28436310(9)	−77.6411(4)	−0.428023(4)	4.568168(7)	0.1779193(6)	−101.4(2)
$11\,^2P$							
^{6}Li	16000	−7.28339037	−77.60762	−0.43917016	4.5666825	0.17785834	−101.55
	∞	−7.28339039(2)	−77.60758(4)	−0.43917000(16)	4.5666830(4)	0.17785837(3)	−101.59(4)
^{7}Li	16000	−7.28348892	−77.61173	−0.43754653	4.5668630	0.17786495	−101.55
	∞	−7.28348894(2)	−77.61168(4)	−0.43754638(16)	4.5668634(4)	0.17786498(3)	−101.59(4)
$^\infty$Li	16000	−7.28408112	−77.63640	−0.42778849	4.5679474	0.17790468	−101.58
	∞	−7.28408114(2)	−77.63636(4)	−0.42778836(16)	4.5679478(4)	0.17790471(3)	−101.62(4)
$12\,^2S$							
^{6}Li	16000	−7.2829380	−77.6112	−0.439399	4.566856	0.1778698	−101.26
	∞	−7.2829383(3)	−77.6114(3)	−0.439398(1)	4.566865(9)	0.1778700(2)	−101.30(4)
^{7}Li	16000	−7.2830365	−77.6154	−0.437775	4.567037	0.1778765	−101.26
	∞	−7.2830368(3)	−77.6155(3)	−0.437774(1)	4.567046(9)	0.1778766(2)	−101.30(4)
$^\infty$Li	16000	−7.2836287	−77.6400	−0.428016	4.568121	0.1779162	−101.29
	∞	−7.2836290(3)	−77.6402(3)	−0.428015(1)	4.568130(9)	0.1779164(2)	−101.33(4)
$12\,^2P$							
^{6}Li	16000	−7.28272222	−77.60797	−0.43921748	4.5666942	0.17785886	−101.43
	∞	−7.28272229(7)	−77.60793(4)	−0.43921735(14)	4.5666959(17)	0.17785897(11)	−101.52(9)
^{7}Li	16000	−7.28282077	−77.61208	−0.43759383	4.5668747	0.17786548	−101.44
	∞	−7.28282084(7)	−77.61204(4)	−0.43759372(14)	4.5668764(17)	0.17786558(11)	−101.52(9)
$^\infty$Li	16000	−7.28341292	−77.63676	−0.42783569	4.5679591	0.17790520	−101.46
	∞	−7.28341299(7)	−77.63672(4)	−0.42783563(14)	4.5679608(17)	0.17790531(11)	−101.55(9)
$13\,^2S$							
^{6}Li	17000	−7.2823708	−77.61158	−0.439401	4.566818	0.1778665	−101.04
	∞	−7.2823716(8)	−77.61171(12)	−0.439395(6)	4.566828(10)	0.1778671(6)	−101.19(15)
^{7}Li	17000	−7.2824693	−77.61569	−0.437778	4.566998	0.1778732	−101.05
	∞	−7.2824701(8)	−77.61581(12)	−0.437771(6)	4.567008(10)	0.1778737(6)	−101.19(15)
$^\infty$Li	17000	−7.2830615	−77.64037	−0.428018	4.568082	0.1779129	−101.08
	∞	−7.2830623(8)	−77.64049(12)	−0.428012(6)	4.568093(10)	0.1779135(6)	−101.22(15)
$13\,^2P$							
^{6}Li	17000	−7.2822019	−77.6093	−0.439259	4.566691	0.177858	−101.1
	∞	−7.2822023(5)	−77.6080(13)	−0.439247(12)	4.566704(13)	0.177860(2)	−101.3(2)
^{7}Li	17000	−7.2823004	−77.6134	−0.437635	4.566872	0.177864	−101.1
	∞	−7.2823009(5)	−77.6121(13)	−0.437623(12)	4.566885(13)	0.177866(2)	−101.3(2)
$^\infty$Li	17000	−7.2828925	−77.6381	−0.427875	4.567956	0.177904	−101.1
	∞	−7.2828930(5)	−77.6368(13)	−0.427864(12)	4.567969(13)	0.177906(2)	−101.3(2)

[a]In Ref. [67], the orbit–orbit energy correction (H_{OO}) includes both electronic (B_2, Eq. (10)) and nuclear ($\tilde{\Delta}_2$, Eq.(15)) terms. The effect due to the finite mass of the nucleus and the effect of the finite nuclear mass on the wave function are computed perturbatively up to the first and second order, respectively. The corresponding values shown in the table for ^{6}Li and ^{7}Li have been obtained using Eq.(21), $B_2(\mu/m_0) = B_2^0 + (\mu/m_0)B_2^1 + (\mu/m_0)^2 B_2^2$, and Eq. (25), $(m_e/m_0)\,\tilde{\Delta}_2 = -(\mu/m_0)\,\tilde{\Delta}_2^{(0)} - (\mu/m_0)^2\,(\tilde{\Delta}_2^{(1)} + 2\tilde{\Delta}_2^{(0)})$ taken from Ref. [67]. Note that the sign in the second term of the above equations employed here is different than the sign used in Ref. [67]. The authors of Ref. [67] confirmed to us that there was a typo in their paper and the sign we now quote is correct.
In this work, H_{OO} contains the contributions from both the electrons and the nucleus (the latter contribution is proportional to the inverse of the nuclear mass), as can be seen in Eq. (9).

[b]In Ref. [56], the orbit–orbit Hamiltonian includes a term due to the finite mass of the nucleus. However, the effect of the finite nuclear mass on the wave function in that work is only computed at the first order level which may explain a slight difference between their result and the present result.

expectation value is more than two orders of magnitude smaller than the contributions from the H_{MV} and H_D terms.

The energy corrections originating from the scalar relativistic effect represented by the H_{MV}, H_{OO}, H_D, and H_{SS} effective Hamiltonians uniformly shift the energies of all states for a particular ^2P level. In order to obtain the fine structure splitting of the states, a spin-dependent effective Hamiltonian, $\langle H_{SO}\rangle$, has to be considered.

As discussed in Section 2, the spin-dependent energy corrections are calculated as the expectation values of the respective Hamiltonian. These expectation values are shown in Table 4. The results include the expectation values of the H_{SO_1}, H_{SO_2} (see Eq. (11)), and H_{AMM} (Eq. (12)). The effects represented by the two former operators are of the order α^2 while those by the latter operator include terms higher than α^2. The spin–orbit corrections have been calculated using the following equation (for more information, see equations (24-26) in Ref. [120]):

$$E_{SO} = \alpha^2\left[C_J^{SO}(E_{SO_1} + E_{SO_2})\right] + 2\kappa\alpha^2\left[E_{AMM}\right], \tag{23}$$

where $C_J^{SO} = 3$ and E_{AMM} is equal to:

$$E_{AMM} = \frac{1}{\pi}\left[C_J^{SO}(E_{AMM_1} + E_{AMM_2})\right]. \tag{24}$$

Tables 5 and 6 show the calculated fine structure splitting values (in cm^{-1}) for ^2P states. Recently, the lowest $2\,^2P$ state was studied by Wang et al. [67] and Puchalski et al. [114–116] using the variational expansion in terms of the Hylleraas basis functions. A comparison with our results obtained at the same level (i.e. $\alpha^2 + \delta_{AMM}$) shows that the values in present work are in good agreement with the values reported by the other two groups. However, these values do not match very well the experimental data [117–119]. In order to improve the agreement,

Table 4
Expectation values $\langle H_{SO_1}\rangle$, $\langle H_{SO_2}\rangle$ and $\langle H_{AMM_2}\rangle$ that appear in Eq. (11) and (12) for the states $|n\,^2P, M_S = \frac{1}{2}, M_L = 1\rangle$ $(n = 2 - 13)$. Note that $\langle H_{AMM_1}\rangle = \langle H_{SO_1}\rangle_{INM}$, where $\langle H_{SO_1}\rangle_{INM}$ is the expectation value of the H_{SO_1} operator calculated for the case of the infinite nuclear mass. All expectation values are in atomic units. The numbers in parentheses are estimated uncertainties due to the basis truncation.

	Basis	$\langle H_{SO_1}\rangle$	$\langle H_{SO_2}\rangle$	$\langle H_{AMM_2}\rangle$
$2\,^2P$				
^{6}Li	12000	4.72384514×10^{-2}	-3.7709703×10^{-2}	
	∞	$4.72384522(8)\times10^{-2}$	$-3.7709706(3)\times10^{-2}$	
^{7}Li	12000	4.72372286×10^{-2}	-3.7708103×10^{-2}	
	∞	$4.72372294(8)\times10^{-2}$	$-3.7708105(3)\times10^{-2}$	
$^\infty$Li	12000	4.72298828×10^{-2}	-3.7698488×10^{-2}	$-3.288929050\times10^{-2}$
	∞	$4.72298836(8)\times10^{-2}$	$-3.7698490(3)\times10^{-2}$	$-3.288929048(2)\times10^{-2}$
$3\,^2P$				
^{6}Li	12000	1.41214621×10^{-2}	-1.13895851×10^{-2}	
	∞	$1.41214611(10)\times10^{-2}$	$-1.13895862(12)\times10^{-2}$	
^{7}Li	12000	1.41211266×10^{-2}	-1.13891162×10^{-2}	
	∞	$1.41211256(10)\times10^{-2}$	$-1.13891173(12)\times10^{-2}$	
$^\infty$Li	12000	1.41191112×10^{-2}	-1.13862991×10^{-2}	-9.80823045×10^{-3}
	∞	$1.41191122(10)\times10^{-2}$	$-1.13862979(12)\times10^{-2}$	$-9.80823040(5)\times10^{-3}$
$4\,^2P$				
^{6}Li	12000	5.9407856×10^{-3}	-4.804337×10^{-3}	
	∞	$5.9407861(10)\times10^{-3}$	$-4.804339(2)\times10^{-3}$	
^{7}Li	12000	5.9406523×10^{-3}	-4.804145×10^{-3}	
	∞	$5.9406528(10)\times10^{-3}$	$-4.804147(2)\times10^{-3}$	
$^\infty$Li	12000	5.9398517×10^{-3}	-4.802990×10^{-3}	-4.12095018×10^{-3}
	∞	$5.9398512(10)\times10^{-3}$	$-4.802992(2)\times10^{-3}$	$-4.12095006(12)\times10^{-3}$
$5\,^2P$				
^{6}Li	12000	3.0314162×10^{-3}	-2.454194×10^{-3}	
	∞	$3.0314153(9)\times10^{-3}$	$-2.454196(2)\times10^{-3}$	
^{7}Li	12000	3.0313506×10^{-3}	-2.454097×10^{-3}	
	∞	$3.0313498(9)\times10^{-3}$	$-2.454099(2)\times10^{-3}$	
$^\infty$Li	12000	3.0309566×10^{-3}	-2.453517×10^{-3}	-2.10142101×10^{-3}
	∞	$3.0309574(9)\times10^{-3}$	$-2.453520(2)\times10^{-3}$	$-2.10142094(7)\times10^{-3}$
$6\,^2P$				
^{6}Li	12000	1.7492957×10^{-3}	-1.417000×10^{-3}	
	∞	$1.7492959(2)\times10^{-3}$	$-1.417004(5)\times10^{-3}$	
^{7}Li	12000	1.7492590×10^{-3}	-1.416944×10^{-3}	
	∞	$1.7492588(2)\times10^{-3}$	$-1.416949(5)\times10^{-3}$	
$^\infty$Li	12000	1.7490379×10^{-3}	-1.416613×10^{-3}	-1.21218744×10^{-3}
	∞	$1.7490381(2)\times10^{-3}$	$-1.416618(5)\times10^{-3}$	$-1.21218735(10)\times10^{-3}$
$7\,^2P$				
^{6}Li	12000	1.0990681×10^{-3}	-0.890582×10^{-3}	
	∞	$1.0990693(12)\times10^{-3}$	$-0.890579(3)\times10^{-3}$	
^{7}Li	12000	1.0990457×10^{-3}	-0.890546×10^{-3}	
	∞	$1.0990469(12)\times10^{-3}$	$-0.890543(3)\times10^{-3}$	
$^\infty$Li	12000	1.0989110×10^{-3}	-0.890335×10^{-3}	-7.614338×10^{-4}
	∞	$1.0989122(12)\times10^{-3}$	$-0.890332(3)\times10^{-3}$	$-7.614334(3)\times10^{-4}$
$8\,^2P$				
^{6}Li	14000	7.34926×10^{-4}	-5.95635×10^{-4}	
	∞	$7.34928(2)\times10^{-4}$	$-5.95632(3)\times10^{-4}$	
^{7}Li	14000	7.34911×10^{-4}	-5.95612×10^{-4}	
	∞	$7.34913(2)\times10^{-4}$	$-5.95609(3)\times10^{-4}$	
$^\infty$Li	14000	7.34820×10^{-4}	-5.95473×10^{-4}	-5.090790×10^{-4}
	∞	$7.34822(2)\times10^{-4}$	$-5.95470(3)\times10^{-4}$	$-5.090786(4)\times10^{-4}$
$9\,^2P$				
^{6}Li	15000	5.15379×10^{-4}	-4.17760×10^{-4}	
	∞	$5.15383(4)\times10^{-4}$	$-4.17752(8)\times10^{-4}$	
^{7}Li	15000	5.15368×10^{-4}	-4.17744×10^{-4}	
	∞	$5.15371(4)\times10^{-4}$	$-4.17736(8)\times10^{-4}$	
$^\infty$Li	15000	5.15301×10^{-4}	-4.17645×10^{-4}	-3.56963×10^{-4}
	∞	$5.15305(4)\times10^{-4}$	$-4.17637(8)\times10^{-4}$	$-3.56957(6)\times10^{-4}$
$10\,^2P$				
^{6}Li	16000	3.75242×10^{-4}	-3.04195×10^{-4}	
	∞	$3.75233(9)\times10^{-4}$	$-3.04192(3)\times10^{-4}$	
^{7}Li	16000	3.75232×10^{-4}	-3.04181×10^{-4}	
	∞	$3.75223(9)\times10^{-4}$	$-3.04178(3)\times10^{-4}$	
$^\infty$Li	16000	3.75172×10^{-4}	-3.04100×10^{-4}	-2.59871×10^{-4}
	∞	$3.75181(9)\times10^{-4}$	$-3.04103(3)\times10^{-4}$	$-2.59873(15)\times10^{-4}$

(*continued on next page*)

Table 4 (*continued*).

	Basis	$\langle H_{SO_1}\rangle$	$\langle H_{SO_2}\rangle$	$\langle H_{AMM_2}\rangle$
$11\,^2P$				
^{6}Li	16000	2.81637×10^{-4}	-2.28331×10^{-4}	
	∞	$2.81629(8)\times10^{-4}$	$-2.28319(12)\times10^{-4}$	
^{7}Li	16000	2.81624×10^{-4}	-2.28317×10^{-4}	
	∞	$2.81616(8)\times10^{-4}$	$-2.28304(12)\times10^{-4}$	
$^\infty$Li	16000	2.81549×10^{-4}	-2.28232×10^{-4}	-1.950118×10^{-4}
	∞	$2.81557(8)\times10^{-4}$	$-2.28220(12)\times10^{-4}$	$-1.950109(9)\times10^{-4}$
$12\,^2P$				
^{6}Li	16000	2.16753×10^{-4}	-1.7574×10^{-4}	
	∞	$2.16737(16)\times10^{-4}$	$-1.7571(3)\times10^{-4}$	
^{7}Li	16000	2.16742×10^{-4}	-1.7573×10^{-4}	
	∞	$2.16726(16)\times10^{-4}$	$-1.7570(3)\times10^{-4}$	
$^\infty$Li	16000	2.16679×10^{-4}	-1.7566×10^{-4}	-1.50077×10^{-4}
	∞	$2.16663(16)\times10^{-4}$	$-1.7563(3)\times10^{-4}$	$-1.50063(14)\times10^{-4}$
$13\,^2P$				
^{6}Li	17000	1.7062×10^{-4}	-1.3837×10^{-4}	
	∞	$1.7072(11)\times10^{-4}$	$-1.3827(10)\times10^{-4}$	
^{7}Li	17000	1.7058×10^{-4}	-1.3834×10^{-4}	
	∞	$1.7069(11)\times10^{-4}$	$-1.3824(10)\times10^{-4}$	
$^\infty$Li	17000	1.7038×10^{-4}	-1.3816×10^{-4}	-1.18031×10^{-4}
	∞	$1.7049(11)\times10^{-4}$	$-1.3806(10)\times10^{-4}$	$-1.18022(9)\times10^{-4}$

Table 5
Fine-structure splittings of the states $|2\,^2P, M_S = \frac{1}{2}, M_L = 1\rangle$ of lithium, in cm^{-1}. The α^2 contribution is calculated as the expectation value of H_{SO} Hamiltonian shown in Eq. (11). The δ_{AMM} is the $2\kappa\alpha^2(\approx \frac{\alpha^3}{\pi})$ contribution representing the anomalous magnetic moment term calculated as the expectation value of the H_{AMM} operator given in Eq. (12). Reference values of Wang *et al.* [67] were obtained in calculations with the Hylleraas-type basis set, while the calculations of Puchalski *et al.* used both the Hylleraas-type and Gaussian basis sets [114–116]. The numbers in parentheses are estimated uncertainties due to the basis truncation.

	Basis		^{6}Li	^{7}Li	$^\infty$Li
Theory					
This work	12000	α^2	0.33409663	0.33410987	0.33418943
This work	∞	α^2	0.33409657(6)	0.33410981(6)	0.33418937(6)
This work	12000	$\alpha^2+\delta_{AMM}$	0.33526280	0.33527604	0.33535560
This work	∞	$\alpha^2+\delta_{AMM}$	0.33526274(6)	0.33527598(6)	0.33535554(6)
This work	12000	$\alpha^2+\delta_{AMM}+\delta_{QED}$	0.335323(3)	0.335341(3)	
This work	∞	$\alpha^2+\delta_{AMM}+\delta_{QED}$	**0.335323(3)**	**0.335341(3)**	
Wang *et al.* [67]		$\alpha^2(\mu/m_0)^0$			0.33418947(7)
Wang *et al.* [67]		$\alpha^2((\mu/m_0)^0+(\mu/m_0)^1)$	0.33409938(7)	0.33411223(7)	
Wang *et al.* [67]		$\alpha^2((\mu/m_0)^0+(\mu/m_0)^1+(\mu/m_0)^2)$	0.33409636(7)	0.33411002(8)	
Wang *et al.* [67]		$\alpha^2((\mu/m_0)^0+(\mu/m_0)^1+(\mu/m_0)^2)+\delta_{AMM}$	0.33526252(7)	0.33527617(8)	
Wang *et al.* [67]		$\alpha^2((\mu/m_0)^0+(\mu/m_0)^1+(\mu/m_0)^2)+\delta_{AMM}+\delta_{QED}$	**0.335322(3)**	**0.335341(3)**	
Puchalski *et al.* [114]		$\alpha^2(\mu/m_0)^0+\delta_{AMM}$			0.33535575(4)
Puchalski *et al.* [114,115]		$\alpha^2((\mu/m_0)^0+(\mu/m_0)^1+(\mu/m_0)^2)+\delta_{AMM}$	0.33526282(4)	0.33527608(4)	
Puchalski *et al.* [114–116]		$\alpha^2((\mu/m_0)^0+(\mu/m_0)^1+(\mu/m_0)^2)+\delta_{AMM}+\delta_{QED}$	**0.335323(3)**	**0.335340(3)**	
Experiment					
Brown *et al.* [117]			0.3353246(6)	0.3353423(6)	
Noble *et al.* [118]			0.335331(2)	0.335336(2)	
Das *et al.* [119]			0.33532738(14)	0.33529860(14)	

Puchalski et al. considered corrections up to the order $\alpha^5 \ln\alpha$. They also considered the hyperfine mixing correction (δE_{fs}) in the fine structure splitting calculations. After including these corrections, their calculated values are in good agreement with the experimental measurements (see Table 5).

In contrast to the lowest ^2P state, higher states have not been studied either theoretically or experimentally. To the best of our knowledge, the only previous high-accuracy calculations of these states were reported by Wang et al. [67] who used the Hylleraas basis functions. Experimental results were only reported for the $3\,^2P$ and $4\,^2P$ states [121]. Wang et al. included corrections up to the order of α^4 in their fine-structure splitting calculations. However, in determining these corrections, they used the approximate Dirac formula. In spite of that, the fine-structure splittings calculated in the present work at the α^3 level are in good agreement with the results of Wang et al. as can be seen from Table 6.

3.3. The total energy

Table 7 shows the total energies of the considered states calculated by summing up the nonrelativistic energies and the relativistic, QED, and HQED corrections ($E_{nr}+\alpha^2E_{rel}+\alpha^3E_{QED}+\alpha^4E_{HQED}$) calculated in the present work. The value of the fine structure constant used in the calculations, $\alpha = 7.297\,352\,569\,3\times10^{-3}$, is taken from CODATA 2018 [86].

3.4. Transition energies

The $^2S_{1/2}\rightarrow\,^2P_{1/2,\,3/2}$ and $^2P_{1/2,\,3/2}\rightarrow\,^2S_{1/2}$ transitions energies for ^{6}Li, ^{7}Li and $^\infty$Li calculated using E_{total} taken from Table 7 are shown in Table 8. The values derived from experimental data are also included for comparison. Most of the experimental transition energies of the lithium atom have been reported for the natural mixture of the ^{6}Li (7.59%) and ^{7}Li (92.41%) isotopes. Thus, in the present work, we calculate the weighted averages of

Table 6
Fine-structure splittings of states $|n\,^2P, M_S = \frac{1}{2}, M_L = 1\rangle\,(3 \le n \le 13)$ of lithium in cm^{-1}. The α^2 contribution is calculated as the expectation value of $\langle H_{\mathrm{SO}}\rangle$ Hamiltonian shown in Eq. (11). The δ_{AMM} is the $2\kappa\alpha^2(\approx \frac{\alpha^3}{\pi})$ contribution representing the anomalous magnetic moment term calculated as the expectation value of the $\langle H_{\mathrm{AMM}}\rangle$ shown in Eq. (12). The calculation in Ref. [67] are performed using Hylleraas-type basis functions. The numbers in parentheses are estimated uncertainties due to the basis truncation.

Isotope		Basis		Splitting	Isotope		Basis		Splitting
$3\,^2P$					$4\,^2P$				
^{6}Li	This work	12000	α^2	0.09578497	^{6}Li	This work	12000	α^2	0.03984613
	This work	∞	α^2	0.09578490(8)		This work	∞	α^2	0.03984607(10)
	This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.09613553		This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.03999404
	This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.09613546(8)		This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.03999398(10)
						Wang *et al.* (theo)[113]		α^2	0.039846242(12)
						Wang *et al.* (theo)[113]		$\alpha^2+\alpha^3+\alpha^4$	0.039996(2)
^{7}Li	This work	12000	α^2	0.09578965	^{7}Li	This work	12000	α^2	0.03984820
	This work	∞	α^2	0.09578958(8)		This work	∞	α^2	0.03984813(10)
	This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.09614021		This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.03999611
	This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.09614014(8)		This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.03999605(10)
	Isler *et al.* (exp)[121]			0.0962		Wang *et al.* (theo)[113]	∞	α^2	0.039848307(12)
						Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.039998(2)
						Isler *et al.* (exp)[121]			0.04
$^\infty$Li	This work	12000	α^2	0.09581776	$^\infty$Li	This work	12000	α^2	0.03986061
	This work	∞	α^2	0.09581784(8)		This work	∞	α^2	0.03986052(10)
	This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.09616832		This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.04000853
	This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.09616839(8)		This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.04000843(10)
						Wang *et al.* (theo)[113]	∞	α^2	0.039860719(10)
						Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.040010(2)
$5\,^2P$					$6\,^2P$				
^{6}Li	This work	12000	α^2	0.02023856	^{6}Li	This work	12000	α^2	0.0116510
	This work	∞	α^2	0.02023845(11)		This work	∞	α^2	0.0116508(2)
	This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.02031414		This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0116946
	This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.02031404(11)		This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0116944(2)
	Wang *et al.* (theo)[113]	∞	α^2	0.020238505(12)		Wang *et al.* (theo)[113]	∞	α^2	0.011651274(13)
	Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.0203148(4)		Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.0116954(12)
^{7}Li	This work	12000	α^2	0.02023964	^{7}Li	This work	12000	α^2	0.0116516
	This work	∞	α^2	0.02023953(11)		This work	∞	α^2	0.0116514(2)
	This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.02031523		This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0116953
	This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.02031512(11)		This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0116951(2)
	Wang *et al.* (theo)[113]	∞	α^2	0.020239585(12)		Wang *et al.* (theo)[113]	∞	α^2	0.011651903(13)
	Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.0203159(4)		Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.0116960(12)
$^\infty$Li	This work	12000	α^2	0.02024615	$^\infty$Li	This work	12000	α^2	0.0116555
	This work	∞	α^2	0.02024611(11)		This work	∞	α^2	0.0116553(2)
	This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.02032174		This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0116991
	This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.02032169(11)		This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0116990(2)
	Wang *et al.* (theo)[113]	∞	α^2	0.020246073(10)		Wang *et al.* (theo)[113]	∞	α^2	0.011655677(13)
	Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.0203224(4)		Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.01169977(10)
$7\,^2P$					$8\,^2P$				
^{6}Li	This work	12000	α^2	0.00730995	^{6}Li	This work	14000	α^2	0.0048838
	This work	∞	α^2	0.00731009(15)		This work	∞	α^2	0.0048840(2)
	This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.00733739		This work	14000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0049022
	This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.00733754(15)		This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0049024(2)
	Wang *et al.* (theo)[113]	∞	α^2	0.007310239(7)		Wang *et al.* (theo)[113]	∞	α^2	0.004883936(7)
	Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00733793(7)		Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00490246(7)
^{7}Li	This work	12000	α^2	0.00731040	^{7}Li	This work	14000	α^2	0.0048841
	This work	∞	α^2	0.00731054(15)		This work	∞	α^2	0.0048843(2)
	This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.00733784		This work	14000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0049025
	This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.00733799(15)		This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0049026(2)
	Wang *et al.* (theo)[113]	∞	α^2	0.007310636(7)		Wang *et al.* (theo)[113]	∞	α^2	0.004884204(7)
	Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00733833(7)		Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00490276(5)
$^\infty$Li	This work	12000	α^2	0.00731309	$^\infty$Li	This work	14000	α^2	0.0048858
	This work	∞	α^2	0.00731323(15)		This work	∞	α^2	0.0048860(2)
	This work	12000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.00734053		This work	14000	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0049041
	This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.00734068(15)		This work	∞	$\alpha^2+\delta_{\mathrm{AMM}}$	0.0049043(2)
	Wang *et al.* (theo)[113]	∞	α^2	0.007313026(7)		Wang *et al.* (theo)[113]	∞	α^2	0.004885817(7)
	Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00734073(6)		Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00490276(5)

(*continued on next page*)

the transition energies for the naturally occurring mixture of the two isotopes. These averages are also shown in Table 7.

For all studied states, the calculated transition energy values are within the experimental error bars. As can be seen, the FNM effects provide a significant contribution to the transition energies, in particular for the $2\,^2S_{1/2} \rightarrow 2\,^2P_{1/2,\,3/2}$ transition. For instance, the transition energies for ^{6}Li and ^{7}Li isotopes are shifted by up to 2.5 cm^{-1} when FNM effects are included in the calculations. The shift becomes smaller for the transition energies involving higher states.

As discussed previously, the lowest S- and P-states have been studied quite extensively both experimentally and computationally, so we can examine the accuracy of the transition energies calculated in this work by comparing them with the literature

Table 6 (*continued*).

Isotope		Basis		Splitting	Isotope		Basis		Splitting
$9\,^2P$					$10\,^2P$				
^{6}Li	This work	15000	α^2	0.0034227	^{6}Li	This work	16000	α^2	0.0024910
	This work	∞	α^2	0.0034231(4)		This work	∞	α^2	0.0024909(2)
	This work	15000	$\alpha^2+\delta_{\rm AMM}$	0.0034356		This work	16000	$\alpha^2+\delta_{\rm AMM}$	0.0025004
	This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0034360(4)		This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0025002(2)
	Wang *et al.* (theo)[113]	∞	α^2	0.003422935(7)		Wang *et al.* (theo)[113]	∞	α^2	0.0024911502(9)
	Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00343592(4)		Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00250061(2)
^{7}Li	This work	15000	α^2	0.0034229	^{7}Li	This work	16000	α^2	0.0024912
	This work	∞	α^2	0.0034233(4)		This work	∞	α^2	0.0024910(2)
	This work	15000	$\alpha^2+\delta_{\rm AMM}$	0.0034358		This work	16000	$\alpha^2+\delta_{\rm AMM}$	0.0025005
	This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0034362(4)		This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0025003(2)
	Wang *et al.* (theo)[113]	∞	α^2	0.003423124(7)		Wang *et al.* (theo)[113]	∞	α^2	0.0024912878(9)
	Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00343611(4)		Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00250075(2)
$^\infty$Li	This work	15000	α^2	0.0034240	$^\infty$Li	This work	16000	α^2	0.0024919
	This work	∞	α^2	0.0034244(4)		This work	∞	α^2	0.0024921(2)
	This work	15000	$\alpha^2+\delta_{\rm AMM}$	0.0034369		This work	16000	$\alpha^2+\delta_{\rm AMM}$	0.0025013
	This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0034373(4)		This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0025015(2)
	Wang *et al.* (theo)[113]	∞	α^2	0.003424262(7)		Wang *et al.* (theo)[113]	∞	α^2	0.0024921147(7)
	Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00343726(3)		Wang *et al.* (theo)[113]	∞	$\alpha^2+\alpha^3+\alpha^4$	0.00250157(2)
$11\,^2P$					$12\,^2P$				
^{6}Li	This work	16000	α^2	0.0018690	^{6}Li	This work	16000	α^2	0.0014380
	This work	∞	α^2	0.0018692(7)		This work	∞	α^2	0.0014383(3)
	This work	16000	$\alpha^2+\delta_{\rm AMM}$	0.0018761		This work	16000	$\alpha^2+\delta_{\rm AMM}$	0.0014434
	This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0018762(7)		This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0014438(3)
^{7}Li	This work	16000	α^2	0.0018691	^{7}Li	This work	16000	α^2	0.0014380
	This work	∞	α^2	0.0018692(7)		This work	∞	α^2	0.0014384(3)
	This work	16000	$\alpha^2+\delta_{\rm AMM}$	0.0018761		This work	16000	$\alpha^2+\delta_{\rm AMM}$	0.0014435
	This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0018763(7)		This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0014438(3)
$^\infty$Li	This work	16000	α^2	0.0018694	$^\infty$Li	This work	16000	α^2	0.0014383
	This work	∞	α^2	0.0018701(7)		This work	∞	α^2	0.0014386(3)
	This work	16000	$\alpha^2+\delta_{\rm AMM}$	0.0018764		This work	16000	$\alpha^2+\delta_{\rm AMM}$	0.0014437
	This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0018771(7)		This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.0014440(3)
$13\,^2P$									
^{6}Li	This work	17000	α^2	0.001131					
	This work	∞	α^2	0.001138(8)					
	This work	17000	$\alpha^2+\delta_{\rm AMM}$	0.001135					
	This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.001142(8)					
^{7}Li	This work	17000	α^2	0.001130					
	This work	∞	α^2	0.001138(8)					
	This work	17000	$\alpha^2+\delta_{\rm AMM}$	0.001135					
	This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.001142(8)					
$^\infty$Li	This work	17000	α^2	0.001130					
	This work	∞	α^2	0.001137(8)					
	This work	17000	$\alpha^2+\delta_{\rm AMM}$	0.001134					
	This work	∞	$\alpha^2+\delta_{\rm AMM}$	0.001141(8)					

results. For instance, 14 903.519 6(13) cm^{-1} is obtained for ^{6}Li $2\,^2S_{1/2} \rightarrow 2\,^2P_J$, $J = 1/2, 3/2$, centroid (i.e., center of gravity) in the present work which is in excellent agreement with the 14 903.519 6(9) and 14 903.520 6(9) cm^{-1} values reported by Wang et al. [67] and by Puchalski et al. [104], respectively. These theoretical values are in good agreement with the highly accurate experimental value of 14 903.520 282 2(7) cm^{-1} [122]. The small difference between the theoretical values in [67,104] can be attributed to the inclusion of the $\alpha^5 \ln\alpha$ and hyperfine mixing corrections in the latter calculations (for more information see Refs. [104,116]).

3.5. Isotope shift

Table 9 shows the isotope shifts of the transition energies determined based on the results of the present calculations. The experimental data [117,122,124] and previously reported theoretical calculations [67,104] are shown for comparison. Most of the previous studies investigated only the transitions between the lowest S- and P-states [67,104,117,122]. There is only one experimental study by Radziemski et al. [124] where some higher excitations were considered. In previous theoretical studies by Wang et al. [67] and by Puchalski et al. [104] the Hylleraas-type basis functions were used. The isotope shift value of 0.351 322(8) cm^{-1} for the lowest S–P transition calculated in the present work is in a good agreement with the values obtained by the other two theoretical studies (0.351 322 60(7) and 0.351 322 65(10) cm^{-1}, respectively). The larger uncertainty of our result compared to the uncertainties of the other two theoretical values is due to the different number of the basis functions employed in the calculations. In the present work, we use up to 11 000 and 12 000 ECG basis functions for the lowest S- and P-states, respectively, while up to 33 600 Hylleraas-type basis functions were used in the other calculations [67,104,125,126]. Most isotope shift values reported here for the transitions involving higher states have not been calculated before. The reported values are in good agreement with the available experimental results of Radziemski et al. [124].

3.6. Oscillator strength

Table 10 shows how the oscillator strength obtained in the length and velocity formalisms converge with the size of the ECG basis in the case of the $2\,^2S \rightarrow 2\,^2P$ and $9\,^2S \rightarrow 9\,^2P$ transitions. These two cases provide a good representation of the convergence behavior that is observed for all transitions calculated in

Table 7
The calculated total energy values ($E_{\text{total}} = E_{\text{nr}} + \alpha^2 E_{\text{rel}} + \alpha^3 E_{\text{QED}} + \alpha^4 E_{\text{HQED}}$) of S- and P- states, in atomic units. The values are shown in ascending order. The numbers in parentheses are estimated uncertainties due to the basis truncation.

	J	Basis	$E_{\text{total}}(^6\text{Li})$	$E_{\text{total}}(^7\text{Li})$	$E_{\text{total}}(^\infty\text{Li})$
$2\,^2S$	1/2	11000	−7.47787764512	−7.47797888750	−7.47858723898
	1/2	∞	−7.47787764496(16)	−7.47797888734(16)	−7.47858723882(16)
$2\,^2P$	1/2	12000	−7.40997323189	−7.41007287358	−7.41067160692
	1/2	∞	−7.40997323179(11)	−7.41007287347(11)	−7.41067160681(11)
	3/2	12000	−7.40997170433	−7.41007134595	−7.41067007892
	3/2	∞	−7.40997170422(11)	−7.41007134584(11)	−7.41067007882(11)
$3\,^2S$	1/2	11000	−7.35391930237	−7.35401880411	−7.35461669565
	1/2	∞	−7.35391930223(15)	−7.35401880396(15)	−7.35461669551(15)
$3\,^2P$	1/2	12000	−7.33697263261	−7.33707170366	−7.33766700727
	1/2	∞	−7.33697263251(10)	−7.33707170356(10)	−7.33766700717(10)
	3/2	12000	−7.33697219459	−7.33707126562	−7.33766656909
	3/2	∞	−7.33697219449(10)	−7.33707126552(10)	−7.33766656899(10)
$4\,^2S$	1/2	11500	−7.3183533119	−7.3184523261	−7.3190472878
	1/2	∞	−7.3183533116(3)	−7.3184523258(3)	−7.3190472875(3)
$4\,^2P$	1/2	12000	−7.31171159934	−7.31181043977	−7.31240435733
	1/2	∞	−7.31171159929(5)	−7.31181043972(5)	−7.31240435728(5)
	3/2	12000	−7.31171141711	−7.31181025754	−7.31240417504
	3/2	∞	−7.31171141706(5)	−7.31181025748(5)	−7.31240417499(5)
$5\,^2S$	1/2	12000	−7.3033748614	−7.3034736729	−7.3040674161
	1/2	∞	−7.3033748610(4)	−7.3034736725(4)	−7.3040674157(4)
$5\,^2P$	1/2	12000	−7.3001115028	−7.3002102276	−7.3008034498
	1/2	∞	−7.3001115025(3)	−7.3002102273(3)	−7.3008034495(3)
	3/2	12000	−7.3001114103	−7.3002101350	−7.3008033572
	3/2	∞	−7.3001114100(3)	−7.3002101347(3)	−7.3008033570(3)
$6\,^2S$	1/2	12500	−7.2956832644	−7.2957819725	−7.2963750948
	1/2	∞	−7.2956832639(5)	−7.2957819720(5)	−7.2963750943(5)
$6\,^2P$	1/2	12000	−7.2938438448	−7.2939425035	−7.2945353294
	1/2	∞	−7.2938438443(4)	−7.2939425031(4)	−7.2945353290(4)
	3/2	12000	−7.2938437915	−7.2939424503	−7.2945352761
	3/2	∞	−7.2938437910(4)	−7.2939424498(4)	−7.2945352757(4)
$7\,^2S$	1/2	13000	−7.291216323	−7.291314971	−7.291907735
	1/2	∞	−7.291216319(4)	−7.291314967(4)	−7.291907731(4)
$7\,^2P$	1/2	12000	−7.2900789851	−7.2901776028	−7.2907701819
	1/2	∞	−7.2900789844(6)	−7.2901776022(6)	−7.2907701812(6)
	3/2	12000	−7.2900789516	−7.2901775693	−7.2907701484
	3/2	∞	−7.2900789510(6)	−7.2901775687(6)	−7.2907701478(6)
$8\,^2S$	1/2	13500	−7.2883940794	−7.2884926902	−7.2890852280
	1/2	∞	−7.2883940800(6)	−7.2884926908(6)	−7.2890852285(6)
$8\,^2P$	1/2	14000	−7.287642342	−7.287740932	−7.288333348
	1/2	∞	−7.287642331(11)	−7.287740921(11)	−7.288333337(11)
	3/2	14000	−7.287642319	−7.287740910	−7.288333325
	3/2	∞	−7.287642309(11)	−7.287740899(11)	−7.288333314(11)
$9\,^2S$	1/2	14000	−7.28649796419	−7.28659654987	−7.28718893632
	1/2	∞	−7.28649796413(6)	−7.28659654980(6)	−7.28718893626(6)
$9\,^2P$	1/2	15000	−7.285975431	−7.286074003	−7.286666304
	1/2	∞	−7.285975434(3)	−7.286074006(3)	−7.286666307(3)
	3/2	15000	−7.285975416	−7.286073987	−7.286666288
	3/2	∞	−7.285975419(3)	−7.286073990(3)	−7.286666291(3)
$10\,^2S$	1/2	16000	−7.2851629721	−7.2852615401	−7.2858538203
	1/2	∞	−7.2851629707(14)	−7.2852615387(14)	−7.2858538188(14)
$10\,^2P$	1/2	16000	−7.2847851434	−7.2848837011	−7.2854759193
	1/2	∞	−7.2847851452(18)	−7.2848837029(18)	−7.2854759211(18)
	3/2	16000	−7.2847851320	−7.2848836897	−7.2854759079
	3/2	∞	−7.2847851338(18)	−7.2848836915(18)	−7.2854759097(18)
$11\,^2S$	1/2	16000	−7.28418762	−7.28428618	−7.28487838
	1/2	∞	−7.28418769(7)	−7.28428624(7)	−7.28487845(7)
$11\,^2P$	1/2	16000	−7.283905691	−7.284004239	−7.284596395
	1/2	∞	−7.283905709(18)	−7.284004256(18)	−7.284596413(18)
	3/2	16000	−7.283905683	−7.284004230	−7.284596386
	3/2	∞	−7.283905701(18)	−7.284004248(18)	−7.284596404(18)
$12\,^2S$	1/2	16000	−7.2834534	−7.2835519	−7.2841440
	1/2	∞	−7.2834537(3)	−7.2835522(3)	−7.2841443(3)

(*continued on next page*)

Table 7 (*continued*).

	J	Basis	$E_{total}(^6Li)$	$E_{total}(^7Li)$	$E_{total}(^\infty Li)$
$12\,^2P$	1/2	16000	−7.28323755	−7.28333609	−7.28392820
	1/2	∞	−7.28323762(7)	−7.28333616(7)	−7.28392826(7)
	3/2	16000	−7.28323754	−7.28333608	−7.28392819
	3/2	∞	−7.28323761(7)	−7.28333615(7)	−7.28392826(7)
$13\,^2S$	1/2	17000	−7.2828862	−7.2829847	−7.2835768
	1/2	∞	−7.2828870(8)	−7.2829855(8)	−7.2835776(8)
$13\,^2P$	1/2	17000	−7.2827173	−7.2828158	−7.2834079
	1/2	∞	−7.2827177(4)	−7.2828162(4)	−7.2834083(4)
	3/2	17000	−7.2827173	−7.2828158	−7.2834079
	3/2	∞	−7.2827177(4)	−7.2828162(4)	−7.2834083(4)

Table 8
$n\,^2S_{1/2} \rightarrow m\,^2P_{1/2,\,3/2}$ and $n\,^2P_{1/2,\,3/2} \rightarrow m\,^2S_{1/2}$, $(2 \le n, m \le 13)$ transition energies for ^{6}Li, ^{7}Li, $^\infty$Li, and the natural isotope mixture (NM) calculated in this work in comparison with NIST ASD values (Ref. [123]) and some literature data. All values are in cm^{-1}. The numbers in parentheses of are estimated root-mean-square uncertainties due to the basis truncation and neglecting higher order relativistic and QED corrections.

		$2\,^2S_{1/2} \rightarrow 2\,^2P_{1/2}$	$2\,^2S_{1/2} \rightarrow 2\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \rightarrow 3\,^2S_{1/2}$	$2\,^2P_{3/2} \rightarrow 3\,^2S_{1/2}$	Centroid
^{6}Li		14903.2961(13)	14903.6313(13)	14903.5196(13)	^{6}Li		12302.4155(5)	12302.0803(5)	12302.1920(5)
	theo. [67]			14903.5196(9)		exp. [124]	12302.4152(10)	12302.0799(10)	12302.1917(10)[a]
	theo. [104]	14903.2965(7)	14903.6318(7)	14903.5206(9)					
	exp. [124]	14903.2973(5)	14903.6327(5)	14903.5209(5)[a]					
	exp. [122]	14903.2967320(2)	14903.6320573(7)	14903.5202822(7)[a]					
^{7}Li		14903.6474(13)	14903.9826(13)	14903.8709(13)	^{7}Li		12302.4462(5)	12302.1110(5)	12302.2227(5)
	theo. [104]	14903.6479(7)	14903.9832(7)	14903.8719(9)		exp. [124]	12302.4463(10)	12302.1110(10)	12302.2228(10)[a]
	theo. [54]	14903.6479(10)	14903.9832(10)	14903.8714(10)[a]					
	exp. [124]	14903.6483(5)	14903.9838(5)	14903.8720(5)[a]					
	exp. [122]	14903.6481005(2)	14903.9834456(7)	14903.8716639(7)[a]					
$^\infty$Li		14905.7583(13)	14906.0937(13)	14905.9819(13)	$^\infty$Li		12302.6310(5)	12302.2956(5)	12302.4074(5)
	theo. [67]			14905.9825(9)					
	theo. [104]			14905.9834(9)					
NM		14903.6207(13)	14903.9560(13)	14903.8442(13)	NM		12302.4439(5)	12302.1086(5)	12302.4439(5)
	NIST	14903.66(10)	14904.00(10)	14903.89(10)[a]		NIST	12302.46(14)	12302.12(14)	12302.23(14)[a]
		$2\,^2S_{1/2} \rightarrow 3\,^2P_{1/2}$	$2\,^2S_{1/2} \rightarrow 3\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \rightarrow 4\,^2S_{1/2}$	$2\,^2P_{3/2} \rightarrow 4\,^2S_{1/2}$	Centroid
^{6}Li		30925.0757(12)	30925.1718(12)	30925.1398(12)	^{6}Li		20108.2482(3)	20107.9129(3)	20108.0246(3)
	exp. [124]	30925.08(2)	30925.17(2)	30925.14(2)[a]		exp. [124]	20108.2460(10)	20107.9107(10)	20108.0225(10)[a]
^{7}Li		30925.5522(12)	30925.6484(12)	30925.6163(12)	^{7}Li		20108.3859(3)	20108.0506(3)	20108.1624(3)
	exp. [124]	30925.55(2)	30925.65(2)	30925.62(2)[a]		exp. [124]	20108.3843(10)	20108.0490(10)	20108.1605(10)[a]
$^\infty$Li		30928.4159(12)	30928.5121(12)	30928.4800(12)	$^\infty$Li		20109.2137(3)	20108.8783(3)	20108.9901(3)
NM		30925.5161(12)	30925.6122(12)	30925.5802(12)	NM		20108.3754(3)	20108.0401(3)	20108.3754(3)
	NIST	30925.38(10)	30925.38(10)			NIST	20108.40(14)	20108.06(14)	20108.17(14)[a]
		$2\,^2S_{1/2} \rightarrow 4\,^2P_{1/2}$	$2\,^2S_{1/2} \rightarrow 4\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \rightarrow 5\,^2S_{1/2}$	$2\,^2P_{3/2} \rightarrow 5\,^2S_{1/2}$	Centroid
^{6}Li		36469.2316(11)	36469.2716(11)	36469.2583(11)	^{6}Li		23395.6381(3)	23395.3028(3)	23395.4146(3)
^{7}Li		36469.7588(11)	36469.7988(11)	36469.7855(11)		exp. [124]	23395.6326(15)	23395.2974(15)	23395.4091(15)[a]
$^\infty$Li		36472.9267(11)	36472.9667(11)	36472.9534(11)	^{7}Li		23395.8203(3)	23395.4850(3)	23395.5968(3)
NM		36469.7188(11)	36469.7588(11)	36469.7455(11)		exp. [124]	23395.8158(15)	23395.4805(15)	23395.5923(15)[a]
	NIST	36469.55(10)	36469.55(10)		$^\infty$Li		23396.9155(3)	23396.5801(3)	23396.6919(3)
					NM		23395.8065(3)	23395.4712(3)	23395.8065(3)
						NIST	23395.84(14)	23395.50(14)	23395.61(14)[a]
		$2\,^2S_{1/2} \rightarrow 5\,^2P_{1/2}$	$2\,^2S_{1/2} \rightarrow 5\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \rightarrow 6\,^2S_{1/2}$	$2\,^2P_{3/2} \rightarrow 6\,^2S_{1/2}$	Centroid
^{6}Li		39015.1585(11)	39015.1789(11)	39015.1721(11)	^{6}Li		25083.7485(3)	25083.4132(3)	25083.5250(3)
^{7}Li		39015.7111(11)	39015.7314(11)	39015.7246(11)		exp. [124]	25083.744(10)	25083.408(10)	25083.520(10)[a]
$^\infty$Li		39019.0316(11)	39019.0519(11)	39019.0451(11)	^{7}Li		25083.9534(3)	25083.6181(3)	25083.7299(3)
NM		39015.6692(11)	39015.6895(11)	39015.6827(11)		exp. [124]	25083.945(10)	25083.610(10)	25083.722(10)[a]
	NIST	39015.56(10)	39015.56(10)		$^\infty$Li		25085.1849(3)	25084.8495(3)	25084.9613(3)
					NM		25083.9378(3)	25083.6026(3)	25083.9378(3)
						NIST	25083.98(14)	25083.64(14)	25083.75(14)[a]
		$2\,^2S_{1/2} \rightarrow 6\,^2P_{1/2}$	$2\,^2S_{1/2} \rightarrow 6\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \rightarrow 7\,^2S_{1/2}$	$2\,^2P_{3/2} \rightarrow 7\,^2S_{1/2}$	Centroid
^{6}Li		40390.7505(11)	40390.7622(11)	40390.7583(11)	^{6}Li		26064.1289(7)	26063.7936(7)	26063.9053(7)
^{7}Li		40391.3175(11)	40391.3292(11)	40391.3253(11)	^{7}Li		26064.3468(7)	26064.0116(7)	26064.1233(7)
$^\infty$Li		40394.7250(11)	40394.7367(11)	40394.7328(11)	$^\infty$Li		26065.6571(7)	26065.3217(7)	26065.4335(7)
NM		40391.2745(11)	40391.2862(11)	40391.2823(11)	NM		26064.3303(7)	26063.9950(7)	26064.3303(7)
	NIST	40390.84(10)	40390.84(10)			NIST	26064.2(10)	26063.9(10)	26064.0(10)[a]
		$2\,^2S_{1/2} \rightarrow 7\,^2P_{1/2}$	$2\,^2S_{1/2} \rightarrow 7\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \rightarrow 8\,^2S_{1/2}$	$2\,^2P_{3/2} \rightarrow 8\,^2S_{1/2}$	Centroid
^{6}Li		41217.0417(13)	41217.0490(13)	41217.0466(13)	^{6}Li		26683.5397(4)	26683.2044(4)	26683.3162(4)
^{7}Li		41217.6177(13)	41217.6251(13)	41217.6226(13)	^{7}Li		26683.7659(4)	26683.4306(4)	26683.5424(4)
$^\infty$Li		41221.0794(13)	41221.0867(13)	41221.0843(13)	$^\infty$Li		26685.1257(4)	26684.7903(4)	26684.9021(4)
NM		41217.5740(13)	41217.5813(13)	41217.5789(13)	NM		26683.7487(4)	26683.4135(4)	26683.7487(4)
	NIST	41217.35(10)	41217.35(10)			NIST	26683.4(10)	26683.1(10)	26683.2(10)[a]

(*continued on next page*)

Table 8 (*continued*).

		$2\,^2S_{1/2} \to 8\,^2P_{1/2}$	$2\,^2S_{1/2} \to 8\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \to 9\,^2S_{1/2}$	$2\,^2P_{3/2} \to 9\,^2S_{1/2}$	Centroid
^{6}Li		41751.8231(18)	41751.8280(18)	41751.8263(18)	^{6}Li		27099.6889(8)	27099.3536(8)	27099.4654(8)
^{7}Li		41752.4051(18)	41752.4100(18)	41752.4084(18)	^{7}Li		27099.9206(8)	27099.5854(8)	27099.6971(8)
$^\infty$Li		41755.9027(18)	41755.9076(18)	41755.9060(18)	$^\infty$Li		27101.3136(8)	27100.9783(8)	27101.0900(8)
NM		41752.3609(18)	41752.3658(18)	41752.3642(18)	NM		27099.9030(8)	27099.5678(8)	27099.9030(8)
	NIST	41751.63(10)	41751.63(10)			NIST	27099.6(10)	27099.3(10)	27099.4(10)[a]
		$2\,^2S_{1/2} \to 9\,^2P_{1/2}$	$2\,^2S_{1/2} \to 9\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \to 10\,^2S_{1/2}$	$2\,^2P_{3/2} \to 10\,^2S_{1/2}$	Centroid
^{6}Li		42117.6676(12)	42117.6710(12)	42117.6699(12)	^{6}Li		27392.6858(6)	27392.3505(6)	27392.4622(6)
^{7}Li		42118.2538(12)	42118.2572(12)	42118.2561(12)	^{7}Li		27392.9214(6)	27392.5861(6)	27392.6979(6)
$^\infty$Li		42121.7765(12)	42121.7799(12)	42121.7788(12)	$^\infty$Li		27394.3377(6)	27394.0024(6)	27394.1141(6)
NM		42118.2093(12)	42118.2127(12)	42118.2116(12)	NM		27392.9035(6)	27392.5682(6)	27392.9035(6)
	NIST	42118.27(10)	42118.27(10)			NIST	27394(10)	27394(10)	
		$2\,^2S_{1/2} \to 10\,^2P_{1/2}$	$2\,^2S_{1/2} \to 10\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \to 11\,^2S_{1/2}$	$2\,^2P_{3/2} \to 11\,^2S_{1/2}$	Centroid
^{6}Li		42378.9056(11)	42378.9081(11)	42378.9073(11)	^{6}Li		27606.75(6)	27606.42(6)	27606.53(6)
^{7}Li		42379.4948(11)	42379.4973(11)	42379.4965(11)	^{7}Li		27606.99(6)	27606.65(6)	27606.77(6)
$^\infty$Li		42383.0357(11)	42383.0382(11)	42383.0374(11)	$^\infty$Li		27608.42(6)	27608.09(6)	27608.20(6)
NM		42379.4501(11)	42379.4526(11)	42379.4518(11)	NM		27606.97(6)	27606.64(6)	27606.97(6)
	NIST	42379.16(10)	42379.16(10)			NIST	27606(10)	27606(10)	
		$2\,^2S_{1/2} \to 11\,^2P_{1/2}$	$2\,^2S_{1/2} \to 11\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \to 12\,^2S_{1/2}$	$2\,^2P_{3/2} \to 12\,^2S_{1/2}$	Centroid
^{6}Li		42571.923(3)	42571.925(3)	42571.924(3)	^{6}Li		27767.90(4)	27767.57(4)	27767.68(4)
^{7}Li		42572.515(3)	42572.516(3)	42572.516(3)	^{7}Li		27768.15(4)	27767.81(4)	27767.92(4)
$^\infty$Li		42576.069(3)	42576.071(3)	42576.070(3)	$^\infty$Li		27769.60(4)	27769.27(4)	27769.38(4)
NM		42572.470(3)	42572.472(3)	42572.471(3)	NM		27768.13(4)	27767.79(4)	27768.13(4)
	NIST	42569.1(10)	42569.1(10)						
		$2\,^2S_{1/2} \to 12\,^2P_{1/2}$	$2\,^2S_{1/2} \to 12\,^2P_{3/2}$	Centroid			$2\,^2P_{1/2} \to 13\,^2S_{1/2}$	$2\,^2P_{3/2} \to 13\,^2S_{1/2}$	Centroid
^{6}Li		42718.563(7)	42718.565(7)	42718.564(7)	^{6}Li		27892.38(6)	27892.04(6)	27892.15(6)
^{7}Li		42719.156(7)	42719.158(7)	42719.157(7)	^{7}Li		27892.62(6)	27892.28(6)	27892.40(6)
$^\infty$Li		42722.721(7)	42722.723(7)	42722.722(7)	$^\infty$Li		27894.08(6)	27893.74(6)	27893.85(6)
NM		42719.111(7)	42719.113(7)	42719.112(7)	NM		27892.60(6)	27892.27(6)	27892.60(6)
	NIST	42719.14(10)	42719.14(10)						
		$2\,^2S_{1/2} \to 13\,^2P_{1/2}$	$2\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		42832.75(3)	42832.75(3)	42832.75(3)					
^{7}Li		42833.35(3)	42833.35(3)	42833.35(3)					
$^\infty$Li		42836.92(3)	42836.92(3)	42836.92(3)					
NM		42833.30(3)	42833.30(3)	42833.30(3)					
	NIST	42832.92(10)	42832.92(10)						
		$3\,^2S_{1/2} \to 3\,^2P_{1/2}$	$3\,^2S_{1/2} \to 3\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 4\,^2S_{1/2}$	$3\,^2P_{3/2} \to 4\,^2S_{1/2}$	Centroid
^{6}Li		3719.3641(3)	3719.4602(3)	3719.4282(3)	^{6}Li		4086.46854(17)	4086.37240(17)	4086.40445(17)
	exp. [124]	3719.3626(10)	3719.4593(10)	3719.4271(10)[a]		exp. [124]	4086.4670(10)	4086.3708(10)	4086.4029(10)[a]
^{7}Li		3719.4586(3)	3719.5548(3)	3719.5227(3)	^{7}Li		4086.48102(17)	4086.38488(17)	4086.41692(17)
	exp. [124]	3719.4569(10)	3719.5536(10)	3719.5214(10)[a]		exp. [124]	4086.4797(10)	4086.3835(10)	4086.4156(10)[a]
$^\infty$Li		3720.0266(3)	3720.1228(3)	3720.0907(3)	$^\infty$Li		4086.55606(17)	4086.45989(17)	4086.49194(17)
NM		3719.4514(3)	3719.5476(3)	3719.5155(3)	NM		4086.48007(17)	4086.38393(17)	4086.48007(17)
	NIST	3719.26(14)	3719.26(14)			NIST	4086.68(14)	4086.68(14)	
		$3\,^2S_{1/2} \to 4\,^2P_{1/2}$	$3\,^2S_{1/2} \to 4\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 5\,^2S_{1/2}$	$3\,^2P_{3/2} \to 5\,^2S_{1/2}$	Centroid
^{6}Li		9263.5201(3)	9263.5601(3)	9263.5467(3)	^{6}Li		7373.85845(13)	7373.76231(13)	7373.79436(13)
^{7}Li		9263.6652(3)	9263.7052(3)	9263.6919(3)		exp. [124]	7373.8512(10)	7373.7550(10)	7373.7871(10)[a]
$^\infty$Li		9264.5374(3)	9264.5774(3)	9264.5641(3)	^{7}Li		7373.91543(13)	7373.81929(13)	7373.85133(13)
NM		9263.6542(3)	9263.6942(3)	9263.6809(3)		exp. [124]	7373.9091(10)	7373.8129(10)	7373.8450(10)[a]
	NIST	9263.43(14)	9263.43(14)		$^\infty$Li		7374.25789(13)	7374.16172(13)	7374.19378(13)
					NM		7373.91110(13)	7373.81496(13)	7373.91110(13)
						NIST	7374.12(14)	7374.12(14)	
		$3\,^2S_{1/2} \to 5\,^2P_{1/2}$	$3\,^2S_{1/2} \to 5\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 6\,^2S_{1/2}$	$3\,^2P_{3/2} \to 6\,^2S_{1/2}$	Centroid
^{6}Li		11809.4470(3)	11809.4673(3)	11809.4605(3)	^{6}Li		9061.96887(12)	9061.87273(12)	9061.90478(12)
^{7}Li		11809.6175(3)	11809.6378(3)	11809.6310(3)		exp. [124]	9061.950(6)	9061.853(6)	9061.885(6)[a]
$^\infty$Li		11810.6423(3)	11810.6626(3)	11810.6558(3)	^{7}Li		9062.04852(12)	9061.95238(12)	9061.98443(12)
NM		11809.6046(3)	11809.6249(3)	11809.6181(3)		exp. [124]	9062.030(6)	9061.930(6)	9061.963(6)[a]
	NIST	11809.44(14)	11809.44(14)		$^\infty$Li		9062.52726(12)	9062.43109(12)	9062.46315(12)
					NM		9062.04248(12)	9061.94634(12)	9062.04248(12)
						NIST	9062.26(14)	9062.26(14)	
		$3\,^2S_{1/2} \to 6\,^2P_{1/2}$	$3\,^2S_{1/2} \to 6\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 7\,^2S_{1/2}$	$3\,^2P_{3/2} \to 7\,^2S_{1/2}$	Centroid
^{6}Li		13185.0389(3)	13185.0506(3)	13185.0467(3)	^{6}Li		10042.3492(7)	10042.2531(7)	10042.2851(7)
^{7}Li		13185.2239(3)	13185.2356(3)	13185.2317(3)	^{7}Li		10042.4420(7)	10042.3458(7)	10042.3779(7)
$^\infty$Li		13186.3357(3)	13186.3474(3)	13186.3435(3)	$^\infty$Li		10042.9995(7)	10042.9033(7)	10042.9354(7)
NM		13185.2099(3)	13185.2216(3)	13185.2177(3)	NM		10042.4349(7)	10042.3388(7)	10042.4349(7)
	NIST	13184.72(14)	13184.72(14)			NIST	10042.5(10)	10042.5(10)	

(*continued on next page*)

Table 8 (*continued*).

		$3\,^2S_{1/2} \to 7\,^2P_{1/2}$	$3\,^2S_{1/2} \to 7\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 8\,^2S_{1/2}$	$3\,^2P_{3/2} \to 8\,^2S_{1/2}$	Centroid
^{6}Li		14011.3301(6)	14011.3374(6)	14011.3350(6)	^{6}Li		10661.7601(3)	10661.6639(3)	10661.6960(3)
^{7}Li		14011.5241(6)	14011.5315(6)	14011.5290(6)	^{7}Li		10661.8611(3)	10661.7649(3)	10661.7970(3)
$^\infty$Li		14012.6901(6)	14012.6974(6)	14012.6950(6)	$^\infty$Li		10662.4681(3)	10662.3719(3)	10662.4040(3)
NM		14011.5094(6)	14011.5167(6)	14011.5143(6)	NM		10661.8534(3)	10661.7573(3)	10661.8534(3)
	NIST	14011.23(14)	14011.23(14)			NIST	10661.7(10)	10661.7(10)	
		$3\,^2S_{1/2} \to 8\,^2P_{1/2}$	$3\,^2S_{1/2} \to 8\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 9\,^2S_{1/2}$	$3\,^2P_{3/2} \to 9\,^2S_{1/2}$	Centroid
^{6}Li		14546.1115(14)	14546.1164(14)	14546.1148(14)	^{6}Li		11077.9092(7)	11077.8131(7)	11077.8452(7)
^{7}Li		14546.3115(14)	14546.3164(14)	14546.3148(14)	^{7}Li		11078.0158(7)	11077.9196(7)	11077.9517(7)
$^\infty$Li		14547.5134(14)	14547.5183(14)	14547.5167(14)	$^\infty$Li		11078.6560(7)	11078.5598(7)	11078.5919(7)
NM		14546.2963(14)	14546.3012(14)	14546.2996(14)	NM		11078.0077(7)	11077.9115(7)	11078.0077(7)
	NIST	14545.51(14)	14545.51(14)			NIST	11077.9(10)	11077.9(10)	
		$3\,^2S_{1/2} \to 9\,^2P_{1/2}$	$3\,^2S_{1/2} \to 9\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 10\,^2S_{1/2}$	$3\,^2P_{3/2} \to 10\,^2S_{1/2}$	Centroid
^{6}Li		14911.9560(5)	14911.9595(5)	14911.9583(5)	^{6}Li		11370.9061(6)	11370.8100(6)	11370.8420(6)
^{7}Li		14912.1602(5)	14912.1636(5)	14912.1625(5)	^{7}Li		11371.0165(6)	11370.9204(6)	11370.9524(6)
$^\infty$Li		14913.3872(5)	14913.3906(5)	14913.3895(5)	$^\infty$Li		11371.6801(6)	11371.5839(6)	11371.6160(6)
NM		14912.1447(5)	14912.1481(5)	14912.1470(5)	NM		11371.0082(6)	11370.9120(6)	11371.0082(6)
	NIST	14912.15(14)	14912.15(14)			NIST	11373(10)	11373(10)	
		$3\,^2S_{1/2} \to 10\,^2P_{1/2}$	$3\,^2S_{1/2} \to 10\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 11\,^2S_{1/2}$	$3\,^2P_{3/2} \to 11\,^2S_{1/2}$	Centroid
^{6}Li		15173.1940(3)	15173.1965(3)	15173.1957(3)	^{6}Li		11584.97(6)	11584.99(6)	11584.91(6)
^{7}Li		15173.4012(3)	15173.4037(3)	15173.4029(3)	^{7}Li		11585.08(6)	11584.99(6)	11585.02(6)
$^\infty$Li		15174.6464(3)	15174.6489(3)	15174.6481(3)	$^\infty$Li		11585.76(6)	11585.67(6)	11585.70(6)
NM		15173.3855(3)	15173.3880(3)	15173.3872(3)	NM		11585.08(6)	11584.99(6)	11585.08(6)
	NIST	15173.04(14)	15173.04(14)			NIST	11585(10)	11585(10)	
		$3\,^2S_{1/2} \to 11\,^2P_{1/2}$	$3\,^2S_{1/2} \to 11\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 12\,^2S_{1/2}$	$3\,^2P_{3/2} \to 12\,^2S_{1/2}$	Centroid
^{6}Li		15366.211(2)	15366.213(2)	15366.213(2)	^{6}Li		11746.12(4)	11746.02(4)	11746.06(4)
^{7}Li		15366.421(2)	15366.423(2)	15366.422(2)	^{7}Li		11746.24(4)	11746.15(4)	11746.18(4)
$^\infty$Li		15367.680(2)	15367.682(2)	15367.681(2)	$^\infty$Li		11746.95(4)	11746.85(4)	11746.88(4)
NM		15366.405(2)	15366.407(2)	15366.406(2)	NM		11746.23(4)	11746.14(4)	11746.23(4)
	NIST	15363.0(10)	15363.0(10)						
		$3\,^2S_{1/2} \to 12\,^2P_{1/2}$	$3\,^2S_{1/2} \to 12\,^2P_{3/2}$	Centroid			$3\,^2P_{1/2} \to 13\,^2S_{1/2}$	$3\,^2P_{3/2} \to 13\,^2S_{1/2}$	Centroid
^{6}Li		15512.852(7)	15512.853(7)	15512.8526(7)	^{6}Li		11870.60(6)	11870.50(6)	11870.53(6)
^{7}Li		15513.063(7)	15513.064(7)	15513.0638(7)	^{7}Li		11870.71(6)	11870.62(6)	11870.65(6)
$^\infty$Li		15514.332(7)	15514.333(7)	15514.3330(7)	$^\infty$Li		11871.42(6)	11871.32(6)	11871.35(6)
NM		15513.047(7)	15513.048(7)	15513.0478(7)	NM		11870.71(6)	11870.61(6)	11870.71(6)
	NIST	15513.02(14)	15513.02(14)						
		$3\,^2S_{1/2} \to 13\,^2P_{1/2}$	$3\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		15627.04(3)	15627.04(3)	15627.04(3)					
^{7}Li		15627.25(3)	15627.25(3)	15627.25(3)					
$^\infty$Li		15628.53(3)	15628.53(3)	15628.53(3)					
NM		15627.24(3)	15627.24(3)	15627.24(3)					
	NIST	15626.80(14)	15626.80(14)						
		$4\,^2S_{1/2} \to 4\,^2P_{1/2}$	$4\,^2S_{1/2} \to 4\,^2P_{3/2}$	Centroid			$4\,^2P_{1/2} \to 5\,^2S_{1/2}$	$4\,^2P_{3/2} \to 5\,^2S_{1/2}$	Centroid
^{6}Li		1457.68743(13)	1457.72742(13)	1457.71409(13)	^{6}Li		1829.70248(10)	1829.66249(10)	1829.67582(10)
^{7}Li		1457.72556(13)	1457.76556(13)	1457.75223(13)		exp. [124]	1829.703(2)	1829.663(2)	1829.676(2)[a]
$^\infty$Li		1457.95472(13)	1457.99473(13)	1457.98140(13)	^{7}Li		1829.70885(10)	1829.66885(10)	1829.68218(10)
NM		1457.72267(13)	1457.76266(13)	1457.74933(13)		exp. [124]	1829.708(2)	1829.668(2)	1829.681(2)[a]
	NIST	1457.49(14)	1457.49(14)		$^\infty$Li		1829.74711(10)	1829.70710(10)	1829.72044(10)
					NM		1829.70836(10)	1829.66837(10)	1829.70836(10)
						NIST	1829.95(14)	1829.95(14)	
		$4\,^2S_{1/2} \to 5\,^2P_{1/2}$	$4\,^2S_{1/2} \to 5\,^2P_{3/2}$	Centroid			$4\,^2P_{1/2} \to 6\,^2S_{1/2}$	$4\,^2P_{3/2} \to 6\,^2S_{1/2}$	Centroid
^{6}Li		4003.61433(12)	4003.63464(12)	5379.21412(12)	^{6}Li		3517.81290(11)	3517.77291(11)	3517.78624(11)
^{7}Li		4003.67786(12)	4003.69817(12)	5379.29212(12)		exp. [124]	3517.800(3)	3517.760(3)	3517.773(3)[a]
$^\infty$Li		4004.05962(12)	4004.07994(12)	5379.76089(12)	^{7}Li		3517.84194(11)	3517.80194(11)	3517.81528(11)
NM		4003.67304(12)	4003.69335(12)	5379.28620(12)		exp. [124]	3517.832(3)	3517.792(3)	3517.805(2)[a]
	NIST	4003.50(14)	4003.50(14)		$^\infty$Li		3518.01648(11)	3517.97647(11)	3517.98981(11)
					NM		3517.83974(11)	3517.79974(11)	3517.83974(11)
						NIST	3518.09(14)	3518.09(14)	
		$4\,^2S_{1/2} \to 6\,^2P_{1/2}$	$4\,^2S_{1/2} \to 6\,^2P_{3/2}$	Centroid			$4\,^2P_{1/2} \to 7\,^2S_{1/2}$	$4\,^2P_{3/2} \to 7\,^2S_{1/2}$	Centroid
^{6}Li		5379.20628(11)	5379.21797(11)	5379.21408(11)	^{6}Li		4498.1933(7)	4498.1533(7)	4498.1666(7)
^{7}Li		5379.28429(11)	5379.29597(11)	5379.29209(11)	^{7}Li		4498.2354(7)	4498.1954(7)	4498.2087(7)
$^\infty$Li		5379.75305(11)	5379.76474(11)	5379.76085(11)	$^\infty$Li		4498.4887(7)	4498.4487(7)	4498.4620(7)
NM		5379.27837(11)	5379.29005(11)	5379.28616(11)	NM		4498.2322(7)	4498.1922(7)	4498.2322(7)
	NIST	5378.78(14)	5378.78(14)			NIST	4498.4(10)	4498.4(10)	

(*continued on next page*)

the present work. In Tables 11 and 12 we show the calculated values of the transition matrix elements and the oscillator strengths of the $S \to P$ and $P \to S$ transitions for ^{6}Li, ^{7}Li, and $^\infty$Li, respectively. The oscillator strengths are calculated for all states considered in this work. In these two tables, only the values obtained with the largest basis sets are presented. In Table 11,

Table 8 (*continued*).

		$4\,^2S_{1/2} \to 7\,^2P_{1/2}$	$4\,^2S_{1/2} \to 7\,^2P_{3/2}$	Centroid			$4\,^2P_{1/2} \to 8\,^2S_{1/2}$	$4\,^2P_{3/2} \to 8\,^2S_{1/2}$	Centroid
^{6}Li		6205.4975(6)	6205.5048(6)	6205.5024(6)	^{6}Li		5117.6041(3)	5117.5641(3)	5117.5774(3)
^{7}Li		6205.5845(6)	6205.5918(6)	6205.5894(6)	^{7}Li		5117.6545(3)	5117.6145(3)	5117.6278(3)
$^\infty$Li		6206.1074(6)	6206.1148(6)	6206.1123(6)	$^\infty$Li		5117.9573(3)	5117.9173(3)	5117.9306(3)
NM		6205.5779(6)	6205.5852(6)	6205.5828(6)	NM		5117.6507(3)	5117.6107(3)	5117.6507(3)
	NIST	6205.29(14)	6205.29(14)			NIST	5117.6(10)	5117.6(10)	
		$4\,^2S_{1/2} \to 8\,^2P_{1/2}$	$4\,^2S_{1/2} \to 8\,^2P_{3/2}$	Centroid			$4\,^2P_{1/2} \to 9\,^2S_{1/2}$	$4\,^2P_{3/2} \to 9\,^2S_{1/2}$	Centroid
^{6}Li		6740.2788(14)	6740.2838(14)	6740.2821(14)	^{6}Li		5533.7533(7)	5533.7133(7)	5533.7266(7)
^{7}Li		6740.3718(14)	6740.3767(14)	6740.3751(14)	^{7}Li		5533.8092(7)	5533.7692(7)	5533.7825(7)
$^\infty$Li		6740.9307(14)	6740.9356(14)	6740.9340(14)	$^\infty$Li		5534.1452(7)	5534.1052(7)	5534.1186(7)
NM		6740.3648(14)	6740.3697(14)	6740.3681(14)	NM		5533.8049(7)	5533.7650(7)	5533.8049(7)
	NIST	6739.57(14)	6739.57(14)			NIST	5533.8(10)	5533.8(10)	
		$4\,^2S_{1/2} \to 9\,^2P_{1/2}$	$4\,^2S_{1/2} \to 9\,^2P_{3/2}$	Centroid			$4\,^2P_{1/2} \to 10\,^2S_{1/2}$	$4\,^2P_{3/2} \to 10\,^2S_{1/2}$	Centroid
^{6}Li		7106.1234(4)	7106.1268(4)	7106.1257(4)	^{6}Li		5826.7502(6)	5826.7102(6)	5826.7235(6)
^{7}Li		7106.2206(4)	7106.2240(4)	7106.2229(4)	^{7}Li		5826.8100(6)	5826.7700(6)	5826.7833(6)
$^\infty$Li		7106.8045(4)	7106.8080(4)	7106.8068(4)	$^\infty$Li		5827.1693(6)	5827.1293(6)	5827.1427(6)
NM		7106.2132(4)	7106.2166(4)	7106.2155(4)	NM		5826.8054(6)	5826.7654(6)	5826.8054(6)
	NIST	7106.21(14)	7106.21(14)			NIST	5828(10)	5828(10)	
		$4\,^2S_{1/2} \to 10\,^2P_{1/2}$	$4\,^2S_{1/2} \to 10\,^2P_{3/2}$	Centroid			$4\,^2P_{1/2} \to 11\,^2S_{1/2}$	$4\,^2P_{3/2} \to 11\,^2S_{1/2}$	Centroid
^{6}Li		7367.3614(2)	7367.3639(2)	7367.3631(2)	^{6}Li		6040.82(6)	6040.89(6)	6040.79(6)
^{7}Li		7367.4616(2)	7367.4641(2)	7367.4633(2)	^{7}Li		6040.88(6)	6040.84(6)	6040.85(6)
$^\infty$Li		7368.0637(2)	7368.0662(2)	7368.0654(2)	$^\infty$Li		6041.25(6)	6041.21(6)	6041.23(6)
NM		7367.4540(2)	7367.4565(2)	7367.4557(2)	NM		6040.87(6)	6040.84(6)	6040.87(6)
	NIST	7367.10(14)	7367.10(14)			NIST	6040(10)	6040(10)	
		$4\,^2S_{1/2} \to 11\,^2P_{1/2}$	$4\,^2S_{1/2} \to 11\,^2P_{3/2}$	Centroid			$4\,^2P_{1/2} \to 12\,^2S_{1/2}$	$4\,^2P_{3/2} \to 12\,^2S_{1/2}$	Centroid
^{6}Li		7560.379(2)	7560.381(2)	7560.380(2)	^{6}Li		6201.97(4)	6201.93(4)	6201.94(4)
^{7}Li		7560.481(2)	7560.483(2)	7560.483(2)	^{7}Li		6202.03(4)	6201.99(4)	6202.01(4)
$^\infty$Li		7561.097(2)	7561.099(2)	7561.098(2)	$^\infty$Li		6202.43(4)	6202.39(4)	6202.41(4)
NM		7560.474(2)	7560.475(2)	7560.475(2)	NM		6202.03(4)	6201.99(4)	6202.03(4)
	NIST	7557.0(10)	7557.0(10)						
		$4\,^2S_{1/2} \to 12\,^2P_{1/2}$	$4\,^2S_{1/2} \to 12\,^2P_{3/2}$	Centroid			$4\,^2P_{1/2} \to 13\,^2S_{1/2}$	$4\,^2P_{3/2} \to 13\,^2S_{1/2}$	Centroid
^{6}Li		7707.019(7)	7707.020(7)	7707.020(7)	^{6}Li		6326.44(6)	6326.40(6)	6326.41(6)
^{7}Li		7707.123(7)	7707.125(7)	7707.124(7)	^{7}Li		6326.51(6)	6326.47(6)	6326.48(6)
$^\infty$Li		7707.749(7)	7707.751(7)	7707.750(7)	$^\infty$Li		6326.91(6)	6326.87(6)	6326.88(6)
NM		7707.115(7)	7707.117(7)	7707.116(7)	NM		6326.50(6)	6326.46(6)	6326.50(6)
	NIST	7707.08(14)	7707.08(14)						
		$4\,^2S_{1/2} \to 13\,^2P_{1/2}$	$4\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		7821.21(3)	7821.21(3)	7821.21(3)					
^{7}Li		7821.31(3)	7821.31(3)	7821.31(3)					
$^\infty$Li		7821.95(3)	7821.95(3)	7821.95(3)					
NM		7821.30(3)	7821.31(3)	7821.31(3)					
	NIST	7820.86(14)	7820.86(14)						
		$5\,^2S_{1/2} \to 5\,^2P_{1/2}$	$5\,^2S_{1/2} \to 5\,^2P_{3/2}$	Centroid			$5\,^2P_{1/2} \to 6\,^2S_{1/2}$	$5\,^2P_{3/2} \to 6\,^2S_{1/2}$	Centroid
^{6}Li		716.22442(8)	716.24474(8)	716.23796(8)	^{6}Li		971.88600(9)	971.86568(9)	971.87245(9)
^{7}Li		716.24345(8)	716.26376(8)	716.25699(8)	^{7}Li		971.88965(9)	971.86933(9)	971.87610(9)
$^\infty$Li		716.35779(8)	716.37811(8)	716.37133(8)	$^\infty$Li		971.91158(9)	971.89126(9)	971.89804(9)
NM		716.24200(8)	716.26232(8)	716.25555(8)	NM		971.88937(9)	971.86905(9)	971.88937(9)
	NIST	716.06(14)	716.06(14)			NIST	972.08(14)	972.08(14)	
		$5\,^2S_{1/2} \to 6\,^2P_{1/2}$	$5\,^2S_{1/2} \to 6\,^2P_{3/2}$	Centroid			$5\,^2P_{1/2} \to 7\,^2S_{1/2}$	$5\,^2P_{3/2} \to 7\,^2S_{1/2}$	Centroid
^{6}Li		2091.81637(8)	2091.82806(8)	2091.82417(8)	^{6}Li		1952.2664(6)	1952.2460(6)	1952.2528(6)
^{7}Li		2091.84988(8)	2091.86157(8)	2091.85768(8)	^{7}Li		1952.2831(6)	1952.2628(6)	1952.2696(6)
$^\infty$Li		2092.05122(8)	2092.06291(8)	2092.05902(8)	$^\infty$Li		1952.3838(6)	1952.3635(6)	1952.3702(6)
NM		2091.84734(8)	2091.85902(8)	2091.85513(8)	NM		1952.2818(6)	1952.2615(6)	1952.2818(6)
	NIST	2091.34(14)	2091.34(14)			NIST	1952.3(10)	1952.3(10)	
		$5\,^2S_{1/2} \to 7\,^2P_{1/2}$	$5\,^2S_{1/2} \to 7\,^2P_{3/2}$	Centroid			$5\,^2P_{1/2} \to 8\,^2S_{1/2}$	$5\,^2P_{3/2} \to 8\,^2S_{1/2}$	Centroid
^{6}Li		2918.1076(6)	2918.1149(6)	2918.1125(6)	^{6}Li		2571.6772(3)	2571.6569(3)	2571.6636(3)
^{7}Li		2918.1501(6)	2918.1574(6)	2918.1550(6)	^{7}Li		2571.7022(3)	2571.6819(3)	2571.6886(3)
$^\infty$Li		2918.4056(6)	2918.4129(6)	2918.4105(6)	$^\infty$Li		2571.8524(3)	2571.8321(3)	2571.8389(3)
NM		2918.1469(6)	2918.1542(6)	2918.1517(6)	NM		2571.7003(3)	2571.6800(3)	2571.7003(3)
	NIST	2917.85(14)	2917.85(14)			NIST	2571.5(10)	2571.5(10)	
		$5\,^2S_{1/2} \to 8\,^2P_{1/2}$	$5\,^2S_{1/2} \to 8\,^2P_{3/2}$	Centroid			$5\,^2P_{1/2} \to 9\,^2S_{1/2}$	$5\,^2P_{3/2} \to 9\,^2S_{1/2}$	Centroid
^{6}Li		3452.8889(14)	3452.8938(14)	3452.8922(14)	^{6}Li		2987.8264(7)	2987.8061(7)	2987.8128(7)
^{7}Li		3452.9374(14)	3452.9423(14)	3452.9407(14)	^{7}Li		2987.8569(7)	2987.8366(7)	2987.8434(7)
$^\infty$Li		3453.2289(14)	3453.2338(14)	3453.2322(14)	$^\infty$Li		2988.0403(7)	2988.0200(7)	2988.0268(7)
NM		3452.9338(14)	3452.9387(14)	3452.9370(14)	NM		2987.8546(7)	2987.8343(7)	2987.8546(7)
	NIST	3452.13(14)	3452.13(14)			NIST	2987.7(10)	2987.7(10)	

(*continued on next page*)

Table 8 (*continued*).

		$5\,^2S_{1/2} \to 9\,^2P_{1/2}$	$5\,^2S_{1/2} \to 9\,^2P_{3/2}$	Centroid			$5\,^2P_{1/2} \to 10\,^2S_{1/2}$	$5\,^2P_{3/2} \to 10\,^2S_{1/2}$	Centroid
^{6}Li		3818.7335(5)	3818.7369(5)	3818.7358(5)	^{6}Li		3280.8233(6)	3280.8029(6)	3280.8097(6)
^{7}Li		3818.7862(5)	3818.7896(5)	3818.7884(5)	^{7}Li		3280.8577(6)	3280.8374(6)	3280.8441(6)
$^\infty$Li		3819.1027(5)	3819.1061(5)	3819.1050(5)	$^\infty$Li		3281.0644(6)	3281.0441(6)	3281.0509(6)
NM		3818.7822(5)	3818.7856(5)	3818.7844(5)	NM		3280.8551(6)	3280.8347(6)	3280.8551(6)
	NIST	3818.77(14)	3818.77(14)			NIST	3282(10)	3282(10)	
		$5\,^2S_{1/2} \to 10\,^2P_{1/2}$	$5\,^2S_{1/2} \to 10\,^2P_{3/2}$	Centroid			$5\,^2P_{1/2} \to 11\,^2S_{1/2}$	$5\,^2P_{3/2} \to 11\,^2S_{1/2}$	Centroid
^{6}Li		4079.9715(3)	4079.9740(3)	4079.9732(3)	^{6}Li		3494.89(6)	3494.98(6)	3494.87(6)
^{7}Li		4080.0272(3)	4080.0297(3)	4080.0289(3)	^{7}Li		3494.93(6)	3494.91(6)	3494.91(6)
$^\infty$Li		4080.3619(3)	4080.3644(3)	4080.3636(3)	$^\infty$Li		3495.15(6)	3495.13(6)	3495.14(6)
NM		4080.0230(3)	4080.0255(3)	4080.0246(3)	NM		3494.92(6)	3494.91(6)	3494.92(6)
	NIST	4079.66(14)	4079.66(14)			NIST	3494(10)	3494(10)	
		$5\,^2S_{1/2} \to 11\,^2P_{1/2}$	$5\,^2S_{1/2} \to 11\,^2P_{3/2}$	Centroid			$5\,^2P_{1/2} \to 12\,^2S_{1/2}$	$5\,^2P_{3/2} \to 12\,^2S_{1/2}$	Centroid
^{6}Li		4272.989(3)	4272.991(3)	4272.990(3)	^{6}Li		3656.04(4)	3656.02(4)	3656.02(4)
^{7}Li		4273.047(3)	4273.049(3)	4273.048(3)	^{7}Li		3656.08(4)	3656.06(4)	3656.07(4)
$^\infty$Li		4273.395(3)	4273.397(3)	4273.396(3)	$^\infty$Li		3656.33(4)	3656.31(4)	3656.32(4)
NM		4273.042(3)	4273.044(3)	4273.044(3)	NM		3656.08(4)	3656.06(4)	3656.08(4)
	NIST	4269.6(10)	4269.6(10)						
		$5\,^2S_{1/2} \to 12\,^2P_{1/2}$	$5\,^2S_{1/2} \to 12\,^2P_{3/2}$	Centroid			$5\,^2P_{1/2} \to 13\,^2S_{1/2}$	$5\,^2P_{3/2} \to 13\,^2S_{1/2}$	Centroid
^{6}Li		4419.629(7)	4419.631(7)	4419.6301(7)	^{6}Li		3780.51(6)	3780.49(6)	3780.50(6)
^{7}Li		4419.689(7)	4419.690(7)	4419.6898(7)	^{7}Li		3780.56(6)	3780.54(6)	3780.54(6)
$^\infty$Li		4420.048(7)	4420.049(7)	4420.0485(7)	$^\infty$Li		3780.80(6)	3780.78(6)	3780.79(6)
NM		4419.684(7)	4419.686(7)	4419.6852(7)	NM		3780.55(6)	3780.53(6)	3780.55(6)
	NIST	4419.64(14)	4419.64(14)						
		$5\,^2S_{1/2} \to 13\,^2P_{1/2}$	$5\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		4533.82(3)	4533.82(3)	4533.82(3)					
^{7}Li		4533.88(3)	4533.88(3)	4533.88(3)					
$^\infty$Li		4534.25(3)	4534.25(3)	4534.25(3)					
NM		4533.87(3)	4533.87(3)	4533.87(3)					
	NIST	4533.42(14)	4533.42(14)						
		$6\,^2S_{1/2} \to 6\,^2P_{1/2}$	$6\,^2S_{1/2} \to 6\,^2P_{3/2}$	Centroid			$6\,^2P_{1/2} \to 7\,^2S_{1/2}$	$6\,^2P_{3/2} \to 7\,^2S_{1/2}$	Centroid
^{6}Li		403.70595(9)	403.71764(9)	403.71375(9)	^{6}Li		576.6744(7)	576.6627(7)	576.6666(7)
^{7}Li		403.71679(9)	403.72847(9)	403.72458(9)	^{7}Li		576.6767(7)	576.6650(7)	576.6689(7)
$^\infty$Li		403.78185(9)	403.79354(9)	403.78964(9)	$^\infty$Li		576.6904(7)	576.6787(7)	576.6826(7)
NM		403.71596(9)	403.72765(9)	403.72376(9)	NM		576.6765(7)	576.6648(7)	576.6765(7)
	NIST	403.20(14)	403.20(14)			NIST	577.1(10)	577.1(10)	
		$6\,^2S_{1/2} \to 7\,^2P_{1/2}$	$6\,^2S_{1/2} \to 7\,^2P_{3/2}$	Centroid			$6\,^2P_{1/2} \to 8\,^2S_{1/2}$	$6\,^2P_{3/2} \to 8\,^2S_{1/2}$	Centroid
^{6}Li		1229.9971(6)	1230.0045(6)	1230.0020(6)	^{6}Li		1196.0852(3)	1196.0736(3)	1196.0774(3)
^{7}Li		1230.0170(6)	1230.0243(6)	1230.0219(6)	^{7}Li		1196.0958(3)	1196.0841(3)	1196.0880(3)
$^\infty$Li		1230.1362(6)	1230.1435(6)	1230.1411(6)	$^\infty$Li		1196.1590(3)	1196.1473(3)	1196.1512(3)
NM		1230.0155(6)	1230.0228(6)	1230.0204(6)	NM		1196.0950(3)	1196.0833(3)	1196.0950(3)
	NIST	1229.71(14)	1229.71(14)			NIST	1196.3(10)	1196.3(10)	
		$6\,^2S_{1/2} \to 8\,^2P_{1/2}$	$6\,^2S_{1/2} \to 8\,^2P_{3/2}$	Centroid			$6\,^2P_{1/2} \to 9\,^2S_{1/2}$	$6\,^2P_{3/2} \to 9\,^2S_{1/2}$	Centroid
^{6}Li		1764.7785(14)	1764.7834(14)	1764.7818(14)	^{6}Li		1612.2344(7)	1612.2227(7)	1612.2266(7)
^{7}Li		1764.8043(14)	1764.8092(14)	1764.8076(14)	^{7}Li		1612.2505(7)	1612.2388(7)	1612.2427(7)
$^\infty$Li		1764.9595(14)	1764.9644(14)	1764.9628(14)	$^\infty$Li		1612.3469(7)	1612.3352(7)	1612.3391(7)
NM		1764.8024(14)	1764.8073(14)	1764.8057(14)	NM		1612.2492(7)	1612.2376(7)	1612.2492(7)
	NIST	1763.99(14)	1763.99(14)			NIST	1612.5(10)	1612.5(10)	
		$6\,^2S_{1/2} \to 9\,^2P_{1/2}$	$6\,^2S_{1/2} \to 9\,^2P_{3/2}$	Centroid			$6\,^2P_{1/2} \to 10\,^2S_{1/2}$	$6\,^2P_{3/2} \to 10\,^2S_{1/2}$	Centroid
^{6}Li		2130.6231(5)	2130.6265(5)	2130.6254(5)	^{6}Li		1905.2313(5)	1905.2196(5)	1905.2235(5)
^{7}Li		2130.6531(5)	2130.6565(5)	2130.6553(5)	^{7}Li		1905.2512(5)	1905.2396(5)	1905.2434(5)
$^\infty$Li		2130.8333(5)	2130.8367(5)	2130.8356(5)	$^\infty$Li		1905.3710(5)	1905.3593(5)	1905.3632(5)
NM		2130.6508(5)	2130.6542(5)	2130.6531(5)	NM		1905.2497(5)	1905.2380(5)	1905.2497(5)
	NIST	2130.63(14)	2130.63(14)			NIST	1907(10)	1907(10)	
		$6\,^2S_{1/2} \to 10\,^2P_{1/2}$	$6\,^2S_{1/2} \to 10\,^2P_{3/2}$	Centroid			$6\,^2P_{1/2} \to 11\,^2S_{1/2}$	$6\,^2P_{3/2} \to 11\,^2S_{1/2}$	Centroid
^{6}Li		2391.8611(3)	2391.8636(3)	2391.8628(3)	^{6}Li		2119.30(6)	2119.40(6)	2119.29(6)
^{7}Li		2391.8941(3)	2391.8966(3)	2391.8958(3)	^{7}Li		2119.32(6)	2119.31(6)	2119.31(6)
$^\infty$Li		2392.0925(3)	2392.0950(3)	2392.0942(3)	$^\infty$Li		2119.46(6)	2119.44(6)	2119.45(6)
NM		2391.8916(3)	2391.8941(3)	2391.8933(3)	NM		2119.32(6)	2119.31(6)	2119.32(6)
	NIST	2391.52(14)	2391.52(14)			NIST	2119(10)	2119(10)	
		$6\,^2S_{1/2} \to 11\,^2P_{1/2}$	$6\,^2S_{1/2} \to 11\,^2P_{3/2}$	Centroid			$6\,^2P_{1/2} \to 12\,^2S_{1/2}$	$6\,^2P_{3/2} \to 12\,^2S_{1/2}$	Centroid

(*continued on next page*)

the uncertainties shown are due to the basis set truncation error. In Table 12, the uncertainties are calculated as root mean squares of the uncertainties of $|\mu_{if}|^2$ and ΔE. The oscillator strengths are compared with the available literature results. All prior theoretical studies only considered transitions between the lowest states. Thus, for higher states, the oscillator strengths presented here are the first ever values obtained in direct calculations. The most accurate previous value of the oscillator strength for the lowest ($2\,^2S \to 2\,^2P$) transition was that by Yan and Drake [47]. They calculated it in the length and velocity formalisms for the ^{7}Li and

Table 8 (*continued*).

^{6}Li		2584.879(3)	2584.880(3)	2584.880(3)	^{6}Li		2280.45(4)	2280.43(4)	2280.44(4)
^{7}Li		2584.914(3)	2584.916(3)	2584.915(3)	^{7}Li		2280.48(4)	2280.46(4)	2280.47(4)
$^\infty$Li		2585.126(3)	2585.128(3)	2585.127(3)	$^\infty$Li		2280.64(4)	2280.62(4)	2280.63(4)
NM		2584.911(3)	2584.913(3)	2584.912(3)	NM		2280.47(4)	2280.46(4)	2280.47(4)
	NIST	2581.5(10)	2581.5(10)						
		$6\,^2S_{1/2} \rightarrow 12\,^2P_{1/2}$	$6\,^2S_{1/2} \rightarrow 12\,^2P_{3/2}$	Centroid			$6\,^2P_{1/2} \rightarrow 13\,^2S_{1/2}$	$6\,^2P_{3/2} \rightarrow 13\,^2S_{1/2}$	Centroid
^{6}Li		2731.519(7)	2731.520(7)	2731.520(7)	^{6}Li		2404.92(6)	2404.91(6)	2404.91(6)
^{7}Li		2731.556(7)	2731.557(7)	2731.557(7)	^{7}Li		2404.95(6)	2404.94(6)	2404.94(6)
$^\infty$Li		2731.778(7)	2731.780(7)	2731.779(7)	$^\infty$Li		2405.11(6)	2405.10(6)	2405.10(6)
NM		2731.553(7)	2731.554(7)	2731.554(7)	NM		2404.95(6)	2404.94(6)	2404.95(6)
	NIST	2731.50(14)	2731.50(14)						
		$6\,^2S_{1/2} \rightarrow 13\,^2P_{1/2}$	$6\,^2S_{1/2} \rightarrow 13\,^2P_{3/2}$	Centroid					
^{6}Li		2845.71(3)	2845.71(3)	2845.71(3)					
^{7}Li		2845.75(3)	2845.75(3)	2845.75(3)					
$^\infty$Li		2845.98(3)	2845.98(3)	2845.98(3)					
NM		2845.74(3)	2845.74(3)	2845.74(3)					
	NIST	2845.28(14)	2845.28(14)						
		$7\,^2S_{1/2} \rightarrow 7\,^2P_{1/2}$	$7\,^2S_{1/2} \rightarrow 7\,^2P_{3/2}$	Centroid			$7\,^2P_{1/2} \rightarrow 8\,^2S_{1/2}$	$7\,^2P_{3/2} \rightarrow 8\,^2S_{1/2}$	Centroid
^{6}Li		249.6168(12)	249.6241(12)	249.6217(12)	^{6}Li		369.7941(9)	369.7867(9)	369.7892(9)
^{7}Li		249.6235(12)	249.6309(12)	249.6284(12)	^{7}Li		369.7956(9)	369.7882(9)	369.7907(9)
$^\infty$Li		249.6640(12)	249.6713(12)	249.6689(12)	$^\infty$Li		369.8046(9)	369.7973(9)	369.7997(9)
NM		249.6230(12)	249.6303(12)	249.6279(12)	NM		369.7954(9)	369.7881(9)	369.7954(9)
	NIST	249.4(10)	249.4(10)			NIST	369.8(10)	369.8(10)	
		$7\,^2S_{1/2} \rightarrow 8\,^2P_{1/2}$	$7\,^2S_{1/2} \rightarrow 8\,^2P_{3/2}$	Centroid			$7\,^2P_{1/2} \rightarrow 9\,^2S_{1/2}$	$7\,^2P_{3/2} \rightarrow 9\,^2S_{1/2}$	Centroid
^{6}Li		784.3982(11)	784.4031(11)	784.4014(11)	^{6}Li		785.94323(15)	785.93590(15)	785.93834(15)
^{7}Li		784.4109(11)	784.4158(11)	784.4141(11)	^{7}Li		785.95027(15)	785.94293(15)	785.94538(15)
$^\infty$Li		784.4873(11)	784.4922(11)	784.4906(11)	$^\infty$Li		785.99255(15)	785.98521(15)	785.98765(15)
NM		784.4099(11)	784.4148(11)	784.4132(11)	NM		785.94973(15)	785.94240(15)	785.94973(15)
	NIST	783.7(10)	783.7(10)			NIST	786.0(10)	786.0(10)	
		$7\,^2S_{1/2} \rightarrow 9\,^2P_{1/2}$	$7\,^2S_{1/2} \rightarrow 9\,^2P_{3/2}$	Centroid			$7\,^2P_{1/2} \rightarrow 10\,^2S_{1/2}$	$7\,^2P_{3/2} \rightarrow 10\,^2S_{1/2}$	Centroid
^{6}Li		1150.2427(9)	1150.2461(9)	1150.2450(9)	^{6}Li		1078.9401(11)	1078.9328(11)	1078.9352(11)
^{7}Li		1150.2596(9)	1150.2630(9)	1150.2619(9)	^{7}Li		1078.9510(11)	1078.9437(11)	1078.9461(11)
$^\infty$Li		1150.3611(9)	1150.3645(9)	1150.3634(9)	$^\infty$Li		1079.0166(11)	1079.0093(11)	1079.0118(11)
NM		1150.2583(9)	1150.2617(9)	1150.2606(9)	NM		1078.9502(11)	1078.9429(11)	1078.9502(11)
	NIST	1150.4(10)	1150.4(10)			NIST	1081(10)	1081(10)	
		$7\,^2S_{1/2} \rightarrow 10\,^2P_{1/2}$	$7\,^2S_{1/2} \rightarrow 10\,^2P_{3/2}$	Centroid			$7\,^2P_{1/2} \rightarrow 11\,^2S_{1/2}$	$7\,^2P_{3/2} \rightarrow 11\,^2S_{1/2}$	Centroid
^{6}Li		1411.4807(8)	1411.4832(8)	1411.4824(8)	^{6}Li		1293.01(6)	1293.11(6)	1293.00(6)
^{7}Li		1411.5006(8)	1411.5031(8)	1411.5023(8)	^{7}Li		1293.02(6)	1293.01(6)	1293.01(6)
$^\infty$Li		1411.6203(8)	1411.6228(8)	1411.6220(8)	$^\infty$Li		1293.10(6)	1293.09(6)	1293.10(6)
NM		1411.4991(8)	1411.5016(8)	1411.5008(8)	NM		1293.02(6)	1293.02(6)	1293.02(6)
	NIST	1411.3(10)	1411.3(10)			NIST	1293(10)	1293(10)	
		$7\,^2S_{1/2} \rightarrow 11\,^2P_{1/2}$	$7\,^2S_{1/2} \rightarrow 11\,^2P_{3/2}$	Centroid			$7\,^2P_{1/2} \rightarrow 12\,^2S_{1/2}$	$7\,^2P_{3/2} \rightarrow 12\,^2S_{1/2}$	Centroid
^{6}Li		1604.498(3)	1604.500(3)	1604.499(3)	^{6}Li		1454.15(4)	1454.15(4)	1454.15(4)
^{7}Li		1604.520(3)	1604.522(3)	1604.522(3)	^{7}Li		1454.18(4)	1454.17(4)	1454.17(4)
$^\infty$Li		1604.654(3)	1604.655(3)	1604.655(3)	$^\infty$Li		1454.28(4)	1454.27(4)	1454.28(4)
NM		1604.519(3)	1604.521(3)	1604.520(3)	NM		1454.17(4)	1454.17(4)	1454.17(4)
	NIST	1601.2(14)	1601.2(14)						
		$7\,^2S_{1/2} \rightarrow 12\,^2P_{1/2}$	$7\,^2S_{1/2} \rightarrow 12\,^2P_{3/2}$	Centroid			$7\,^2P_{1/2} \rightarrow 13\,^2S_{1/2}$	$7\,^2P_{3/2} \rightarrow 13\,^2S_{1/2}$	Centroid
^{6}Li		1751.138(7)	1751.140(7)	1751.139(7)	^{6}Li		1578.63(6)	1578.62(6)	1578.63(6)
^{7}Li		1751.162(7)	1751.164(7)	1751.163(7)	^{7}Li		1578.65(6)	1578.64(6)	1578.64(6)
$^\infty$Li		1751.306(7)	1751.307(7)	1751.307(7)	$^\infty$Li		1578.75(6)	1578.75(6)	1578.75(6)
NM		1751.160(7)	1751.162(7)	1751.161(7)	NM		1578.65(6)	1578.64(6)	1578.65(6)
	NIST	1751.2(10)	1751.2(10)						
		$7\,^2S_{1/2} \rightarrow 13\,^2P_{1/2}$	$7\,^2S_{1/2} \rightarrow 13\,^2P_{3/2}$	Centroid					
^{6}Li		1865.33(3)	1865.33(3)	1865.33(3)					
^{7}Li		1865.35(3)	1865.35(3)	1865.35(3)					
$^\infty$Li		1865.50(3)	1865.50(3)	1865.50(3)					
NM		1865.35(3)	1865.35(3)	1865.35(3)					
	NIST	1865.0(10)	1865.0(10)						
		$8\,^2S_{1/2} \rightarrow 8\,^2P_{1/2}$	$8\,^2S_{1/2} \rightarrow 8\,^2P_{3/2}$	Centroid			$8\,^2P_{1/2} \rightarrow 9\,^2S_{1/2}$	$8\,^2P_{3/2} \rightarrow 9\,^2S_{1/2}$	Centroid
^{6}Li		164.9873(17)	164.9922(17)	164.9906(17)	^{6}Li		251.1619(12)	251.1570(12)	251.1586(12)
^{7}Li		164.9918(17)	164.9967(17)	164.9951(17)	^{7}Li		251.1629(12)	251.1580(12)	251.1596(12)
$^\infty$Li		165.0187(17)	165.0236(17)	165.0220(17)	$^\infty$Li		251.1692(12)	251.1643(12)	251.1660(12)
NM		164.9915(17)	164.9964(17)	164.9947(17)	NM		251.1628(12)	251.1579(12)	251.1628(12)
	NIST	164.5(10)	164.5(10)			NIST	251.7(10)	251.7(10)	
		$8\,^2S_{1/2} \rightarrow 9\,^2P_{1/2}$	$8\,^2S_{1/2} \rightarrow 9\,^2P_{3/2}$	Centroid			$8\,^2P_{1/2} \rightarrow 10\,^2S_{1/2}$	$8\,^2P_{3/2} \rightarrow 10\,^2S_{1/2}$	Centroid

(*continued on next page*)

Table 8 (*continued*).

^{6}Li		530.8319(5)	530.8353(5)	530.8342(5)	^{6}Li		544.159(2)	544.154(2)	544.155(2)
^{7}Li		530.8405(5)	530.8439(5)	530.8428(5)	^{7}Li		544.164(2)	544.159(2)	544.160(2)
$^\infty$Li		530.8925(5)	530.8959(5)	530.8948(5)	$^\infty$Li		544.193(2)	544.188(2)	544.190(2)
NM		530.8399(5)	530.8433(5)	530.8421(5)	NM		544.163(2)	544.158(2)	544.163(2)
	NIST	531.2(10)	531.2(10)			NIST	546(10)	546(10)	
		$8\,^2S_{1/2} \to 10\,^2P_{1/2}$	$8\,^2S_{1/2} \to 10\,^2P_{3/2}$	Centroid			$8\,^2P_{1/2} \to 11\,^2S_{1/2}$	$8\,^2P_{3/2} \to 11\,^2S_{1/2}$	Centroid
^{6}Li		792.0699(4)	792.0724(4)	792.0716(4)	^{6}Li		758.22(6)	758.33(6)	758.22(6)
^{7}Li		792.0816(4)	792.0841(4)	792.0832(4)	^{7}Li		758.23(6)	758.23(6)	758.23(6)
$^\infty$Li		792.1517(4)	792.1542(4)	792.1534(4)	$^\infty$Li		758.28(6)	758.27(6)	758.27(6)
NM		792.0807(4)	792.0832(4)	792.0823(4)	NM		758.23(6)	758.23(6)	758.23(6)
	NIST	792.1(10)	792.1(10)			NIST	758(10)	758(10)	
		$8\,^2S_{1/2} \to 11\,^2P_{1/2}$	$8\,^2S_{1/2} \to 11\,^2P_{3/2}$	Centroid			$8\,^2P_{1/2} \to 12\,^2S_{1/2}$	$8\,^2P_{3/2} \to 12\,^2S_{1/2}$	Centroid
^{6}Li		985.087(2)	985.089(2)	985.089(2)	^{6}Li		919.37(5)	919.37(5)	919.37(5)
^{7}Li		985.101(2)	985.103(2)	985.103(2)	^{7}Li		919.39(5)	919.38(5)	919.39(5)
$^\infty$Li		985.185(2)	985.187(2)	985.186(2)	$^\infty$Li		919.46(5)	919.45(5)	919.46(5)
NM		985.100(2)	985.102(2)	985.101(2)	NM		919.39(5)	919.38(5)	919.39(5)
	NIST	982.0(14)	982.0(14)						
		$8\,^2S_{1/2} \to 12\,^2P_{1/2}$	$8\,^2S_{1/2} \to 12\,^2P_{3/2}$	Centroid			$8\,^2P_{1/2} \to 13\,^2S_{1/2}$	$8\,^2P_{3/2} \to 13\,^2S_{1/2}$	Centroid
^{6}Li		1131.727(6)	1131.729(6)	1131.728(6)	^{6}Li		1043.85(6)	1043.85(6)	1043.85(6)
^{7}Li		1131.743(6)	1131.745(6)	1131.744(6)	^{7}Li		1043.86(6)	1043.86(6)	1043.86(6)
$^\infty$Li		1131.837(6)	1131.839(6)	1131.838(6)	$^\infty$Li		1043.93(6)	1043.93(6)	1043.93(6)
NM		1131.742(6)	1131.743(6)	1131.743(6)	NM		1043.86(6)	1043.86(6)	1043.86(6)
	NIST	1132.0(10)	1132.0(10)						
		$8\,^2S_{1/2} \to 13\,^2P_{1/2}$	$8\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		1245.92(3)	1245.92(3)	1245.92(3)					
^{7}Li		1245.93(3)	1245.93(3)	1245.93(3)					
$^\infty$Li		1246.04(3)	1246.04(3)	1246.04(3)					
NM		1245.93(3)	1245.93(3)	1245.93(3)					
	NIST	1245.8(10)	1245.8(10)						
		$9\,^2S_{1/2} \to 9\,^2P_{1/2}$	$9\,^2S_{1/2} \to 9\,^2P_{3/2}$	Centroid			$9\,^2P_{1/2} \to 10\,^2S_{1/2}$	$9\,^2P_{3/2} \to 10\,^2S_{1/2}$	Centroid
^{6}Li		114.6827(11)	114.6861(11)	114.6850(11)	^{6}Li		178.3142(4)	178.3108(4)	178.3119(4)
^{7}Li		114.6858(11)	114.6892(11)	114.6881(11)	^{7}Li		178.3150(4)	178.3115(4)	178.3127(4)
$^\infty$Li		114.7046(11)	114.7080(11)	114.7068(11)	$^\infty$Li		178.3195(4)	178.3161(4)	178.3173(4)
NM		114.6856(11)	114.6890(11)	114.6879(11)	NM		178.3149(4)	178.3115(4)	178.3149(4)
	NIST	115.0(10)	115.0(10)			NIST	180(10)	180(10)	
		$9\,^2S_{1/2} \to 10\,^2P_{1/2}$	$9\,^2S_{1/2} \to 10\,^2P_{3/2}$	Centroid			$9\,^2P_{1/2} \to 11\,^2S_{1/2}$	$9\,^2P_{3/2} \to 11\,^2S_{1/2}$	Centroid
^{6}Li		375.9207(7)	375.9232(7)	375.9224(7)	^{6}Li		392.38(6)	392.49(6)	392.38(6)
^{7}Li		375.9268(7)	375.9293(7)	375.9285(7)	^{7}Li		392.38(6)	392.38(6)	392.38(6)
$^\infty$Li		375.9638(7)	375.9663(7)	375.9654(7)	$^\infty$Li		392.40(6)	392.40(6)	392.40(6)
NM		375.9264(7)	375.9289(7)	375.9280(7)	NM		392.38(6)	392.39(6)	392.38(6)
	NIST	375.9(10)	375.9(10)			NIST	392(10)	392(10)	
		$9\,^2S_{1/2} \to 11\,^2P_{1/2}$	$9\,^2S_{1/2} \to 11\,^2P_{3/2}$	Centroid			$9\,^2P_{1/2} \to 12\,^2S_{1/2}$	$9\,^2P_{3/2} \to 12\,^2S_{1/2}$	Centroid
^{6}Li		568.938(3)	568.940(3)	568.939(3)	^{6}Li		553.53(4)	553.53(4)	553.53(4)
^{7}Li		568.947(3)	568.948(3)	568.948(3)	^{7}Li		553.54(4)	553.54(4)	553.54(4)
$^\infty$Li		568.997(3)	568.999(3)	568.998(3)	$^\infty$Li		553.58(4)	553.58(4)	553.58(4)
NM		568.946(3)	568.948(3)	568.947(3)	NM		553.54(4)	553.54(4)	553.54(4)
	NIST	565.8(14)	565.8(14)						
		$9\,^2S_{1/2} \to 12\,^2P_{1/2}$	$9\,^2S_{1/2} \to 12\,^2P_{3/2}$	Centroid			$9\,^2P_{1/2} \to 13\,^2S_{1/2}$	$9\,^2P_{3/2} \to 13\,^2S_{1/2}$	Centroid
^{6}Li		715.578(7)	715.580(7)	715.579(7)	^{6}Li		678.01(6)	678.00(6)	678.00(6)
^{7}Li		715.588(7)	715.590(7)	715.589(7)	^{7}Li		678.01(6)	678.01(6)	678.01(6)
$^\infty$Li		715.649(7)	715.651(7)	715.650(7)	$^\infty$Li		678.06(6)	678.05(6)	678.05(6)
NM		715.588(7)	715.589(7)	715.589(7)	NM		678.01(6)	678.01(6)	678.01(6)
	NIST	715.8(10)	715.8(10)						
		$9\,^2S_{1/2} \to 13\,^2P_{1/2}$	$9\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		829.77(3)	829.77(3)	829.77(3)					
^{7}Li		829.78(3)	829.78(3)	829.78(3)					
$^\infty$Li		829.85(3)	829.85(3)	829.85(3)					
NM		829.78(3)	829.78(3)	829.78(3)					
	NIST	829.6(10)	829.6(10)						

(*continued on next page*)

$^\infty$Li isotopes using Hylleraas-type basis sets. Despite a relatively small number of basis functions employed in their work (3502 functions for the S-state and 3463 functions for the P-state), our results are in good agreement with the values they obtained. Furthermore, the agreement between the two values obtained in the present work using two different formalisms is notably better than the agreement seen in other works. For instance, Yan and Drake [47] obtained the values of 0.746 956 939 6(98) and 0.746 959 7(50) for $2\,^2S \to 2\,^2P$ oscillator strength in the length and velocity forms, respectively. At the same time the values obtained in the present work using these two forms are 0.746 956 809 89(6) and 0.746 956 799(8), respectively. The two values agree to within nine digits after the decimal points. The oscillator strength calculation with the Hylleraas-type basis functions (less than

Table 8 (*continued*).

		$10\,^2S_{1/2} \to 10\,^2P_{1/2}$	$10\,^2S_{1/2} \to 10\,^2P_{3/2}$	Centroid			$10\,^2P_{1/2} \to 11\,^2S_{1/2}$	$10\,^2P_{3/2} \to 11\,^2S_{1/2}$	Centroid
^{6}Li		82.9238(6)	82.9263(6)	82.9255(6)	^{6}Li		131.14(6)	131.25(6)	131.14(6)
^{7}Li		82.9261(6)	82.9286(6)	82.9277(6)	^{7}Li		131.14(6)	131.14(6)	131.14(6)
$^\infty$Li		82.9397(6)	82.9422(6)	82.9413(6)	$^\infty$Li		131.15(6)	131.14(6)	131.14(6)
NM		82.9259(6)	82.9284(6)	82.9276(6)	NM		131.14(6)	131.15(6)	131.14(6)
	NIST	81(10)	81(10)			NIST	131(10)	131(10)	
		$10\,^2S_{1/2} \to 11\,^2P_{1/2}$	$10\,^2S_{1/2} \to 11\,^2P_{3/2}$	Centroid			$10\,^2P_{1/2} \to 12\,^2S_{1/2}$	$10\,^2P_{3/2} \to 12\,^2S_{1/2}$	Centroid
^{6}Li		275.941(2)	275.943(2)	275.943(2)	^{6}Li		292.29(4)	292.29(4)	292.29(4)
^{7}Li		275.946(2)	275.948(2)	275.947(2)	^{7}Li		292.30(4)	292.30(4)	292.30(4)
$^\infty$Li		275.973(2)	275.975(2)	275.974(2)	$^\infty$Li		292.33(4)	292.32(4)	292.32(4)
NM		275.945(2)	275.947(2)	275.947(2)	NM		292.30(4)	292.30(4)	292.30(4)
	NIST	271(10)	271(10)						
		$10\,^2S_{1/2} \to 12\,^2P_{1/2}$	$10\,^2S_{1/2} \to 12\,^2P_{3/2}$	Centroid			$10\,^2P_{1/2} \to 13\,^2S_{1/2}$	$10\,^2P_{3/2} \to 13\,^2S_{1/2}$	Centroid
^{6}Li		422.581(6)	422.583(6)	422.582(6)	^{6}Li		416.77(6)	416.76(6)	416.77(6)
^{7}Li		422.588(6)	422.589(6)	422.589(6)	^{7}Li		416.77(6)	416.77(6)	416.77(6)
$^\infty$Li		422.625(6)	422.627(6)	422.626(6)	$^\infty$Li		416.80(6)	416.80(6)	416.80(6)
NM		422.587(6)	422.589(6)	422.588(6)	NM		416.77(6)	416.77(6)	416.77(6)
	NIST	421(10)	421(10)						
		$10\,^2S_{1/2} \to 13\,^2P_{1/2}$	$10\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		536.77(3)	536.77(3)	536.77(3)					
^{7}Li		536.78(3)	536.78(3)	536.78(3)					
$^\infty$Li		536.82(3)	536.82(3)	536.82(3)					
NM		536.78(3)	536.78(3)	536.78(3)					
	NIST	535(10)	535(10)						
		$11\,^2S_{1/2} \to 11\,^2P_{1/2}$	$11\,^2S_{1/2} \to 11\,^2P_{3/2}$	Centroid			$11\,^2P_{1/2} \to 12\,^2S_{1/2}$	$11\,^2P_{3/2} \to 12\,^2S_{1/2}$	Centroid
^{6}Li		61.88(5)	61.76(5)	61.88(5)	^{6}Li		99.27(4)	99.27(4)	99.27(4)
^{7}Li		61.88(5)	61.88(5)	61.88(5)	^{7}Li		99.28(4)	99.28(4)	99.28(4)
$^\infty$Li		61.89(5)	61.89(5)	61.89(5)	$^\infty$Li		99.29(4)	99.29(4)	99.29(4)
NM		61.88(5)	61.87(5)	61.88(5)	NM		99.28(4)	99.28(4)	99.28(4)
	NIST	59(10)	59(10)						
		$11\,^2S_{1/2} \to 12\,^2P_{1/2}$	$11\,^2S_{1/2} \to 12\,^2P_{3/2}$	Centroid			$11\,^2P_{1/2} \to 13\,^2S_{1/2}$	$11\,^2P_{3/2} \to 13\,^2S_{1/2}$	Centroid
^{6}Li		208.52(5)	208.40(5)	208.52(5)	^{6}Li		223.75(6)	223.75(6)	223.75(6)
^{7}Li		208.52(5)	208.52(5)	208.52(5)	^{7}Li		223.75(6)	223.75(6)	223.75(6)
$^\infty$Li		208.54(5)	208.54(5)	208.54(5)	$^\infty$Li		223.76(6)	223.76(6)	223.76(6)
NM		208.52(5)	208.51(5)	208.52(5)	NM		223.75(6)	223.75(6)	223.75(6)
	NIST	209(10)	209(10)						
		$11\,^2S_{1/2} \to 13\,^2P_{1/2}$	$11\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		322.705(16)	322.706(16)	322.705(16)					
^{7}Li		322.710(16)	322.711(16)	322.710(16)					
$^\infty$Li		322.738(16)	322.739(16)	322.739(16)					
NM		322.709(16)	322.710(16)	322.710(16)					
	NIST	323(10)	323(10)						
		$12\,^2S_{1/2} \to 12\,^2P_{1/2}$	$12\,^2S_{1/2} \to 12\,^2P_{3/2}$	Centroid			$12\,^2P_{1/2} \to 13\,^2S_{1/2}$	$12\,^2P_{3/2} \to 13\,^2S_{1/2}$	Centroid
^{6}Li		47.37(4)	47.37(4)	47.37(4)	^{6}Li		77.11(5)	77.11(5)	77.11(5)
^{7}Li		47.36(4)	47.36(4)	47.36(4)	^{7}Li		77.11(5)	77.11(5)	77.11(5)
$^\infty$Li		47.36(4)	47.36(4)	47.36(4)	$^\infty$Li		77.11(5)	77.11(5)	77.11(5)
NM		47.36(4)	47.36(4)	47.36(4)	NM		77.11(5)	77.11(5)	77.11(5)
		$12\,^2S_{1/2} \to 13\,^2P_{1/2}$	$12\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		161.555(8)	161.556(8)	161.556(8)					
^{7}Li		161.552(8)	161.553(8)	161.553(8)					
$^\infty$Li		161.558(8)	161.559(8)	161.559(8)					
NM		161.553(8)	161.554(8)	161.553(8)					
		$13\,^2S_{1/2} \to 13\,^2P_{1/2}$	$13\,^2S_{1/2} \to 13\,^2P_{3/2}$	Centroid					
^{6}Li		37.079(2)	37.080(2)	37.079(2)					
^{7}Li		37.080(2)	37.081(2)	37.080(2)					
$^\infty$Li		37.086(2)	37.087(2)	37.086(2)					
NM		37.080(2)	37.081(2)	37.080(2)					

[a]We used the data for ^{6}Li and ^{7}Li taken from the corresponding Reference and computed the centroid value as the center of gravity.

400 terms were used) were also done by Pestka and Woźnicki [42]. Also, Froese Fischer [46] employed the multi-configuration Hartree–Fock method to study the oscillator strengths for the lower states ($n \leq 4$) of the lithium atom. The lithium oscillator strengths were also calculated using the full-core plus correlation (FCPC) method and a model potential method in Refs. [128,129]. The results of the mentioned calculations are compared with our values in the table.

In general, the agreement between the oscillator strengths calculated in the present work and the available literature values correlates with the accuracy of the method that was used to generate the wave function. The present work not only provides new benchmark values for the oscillator strengths, but reports them for a considerably wider range of S–P transitions compared to prior computational studies. Moreover, we computed the dipole moments and the corresponding oscillator strength for different

Table 9
The ^{6}Li–^{7}Li spin-independent isotope shift for the $n\,^2S_{1/2} \rightarrow m\,^2P_{1/2,\,3/2}$ and $n\,^2P_{1/2,\,3/2} \rightarrow m\,^2S_{1/2}$, $(2 \leq n, m \leq 13)$ transition frequencies. All values are in cm^{-1}. The numbers in parentheses of are estimated root-mean-square uncertainties due to the basis truncation and neglecting higher order relativistic and QED corrections.

Transition	IS	Transition	IS
$2\,^2S \rightarrow 2\,^2P$	0.351322(8)	$2\,^2P \rightarrow 3\,^2S$	0.0307052(6)
Wang *et al.* (theo) [67]	0.35132260(7)	Radziemski *et al.* (exp) [124]	0.0311(14)
Puchalski *et al.* (theo) [104]	0.35132265(10)	$2\,^2P \rightarrow 4\,^2S$	0.1377078(8)
Radziemski *et al.* (exp) [124]	0.3511(7)	Radziemski *et al.* (exp) [124]	0.1383(14)
Sansonetti *et al.* (exp) [122]	0.3513817(7)	$2\,^2P \rightarrow 5\,^2S$	0.1822082(13)
Brown *et al.* (exp) [117]	0.3513862(7)	Radziemski *et al.* (exp) [124]	0.1831(21)
$2\,^2S \rightarrow 3\,^2P$	0.476555(9)	$2\,^2P \rightarrow 6\,^2S$	0.2048845(14)
Radziemski *et al.* (exp) [124]	0.48(3)	Radziemski *et al.* (exp) [124]	0.2010(14)
$2\,^2S \rightarrow 4\,^2P$	0.527168(10)	$2\,^2P \rightarrow 7\,^2S$	0.2179859(15)
$2\,^2S \rightarrow 5\,^2P$	0.552558(10)	$2\,^2P \rightarrow 8\,^2S$	0.2262326(16)
$2\,^2S \rightarrow 6\,^2P$	0.567034(10)	$2\,^2P \rightarrow 9\,^2S$	0.2317575(16)
$2\,^2S \rightarrow 7\,^2P$	0.576046(10)	$2\,^2P \rightarrow 10\,^2S$	0.2356390(16)
$2\,^2S \rightarrow 8\,^2P$	0.582028(10)	$2\,^2P \rightarrow 11\,^2S$	0.2384698(16)
$2\,^2S \rightarrow 9\,^2P$	0.586200(10)	$2\,^2P \rightarrow 12\,^2S$	0.2458197(19)
$2\,^2S \rightarrow 10\,^2P$	0.589223(10)	$2\,^2P \rightarrow 13\,^2S$	0.2422281(19)
$2\,^2S \rightarrow 11\,^2P$	0.591484(10)		
$2\,^2S \rightarrow 12\,^2P$	0.593217(10)		
$2\,^2S \rightarrow 13\,^2P$	0.594578(10)		
$3\,^2S \rightarrow 3\,^2P$	0.094528(2)	$3\,^2P \rightarrow 4\,^2S$	0.0124744(5)
Radziemski *et al.* (exp) [124]	0.0943(14)	Radziemski *et al.* (exp) [124]	0.0127(14)
$3\,^2S \rightarrow 4\,^2P$	0.145141(2)	$3\,^2P \rightarrow 5\,^2S$	0.05697476(5)
$3\,^2S \rightarrow 5\,^2P$	0.170531(2)	Radziemski *et al.* (exp) [124]	0.0579(14)
$3\,^2S \rightarrow 6\,^2P$	0.185007(2)	$3\,^2P \rightarrow 6\,^2S$	0.07965113(14)
$3\,^2S \rightarrow 7\,^2P$	0.194019(2)	Radziemski *et al.* (exp) [124]	0.080(8)
$3\,^2S \rightarrow 8\,^2P$	0.200002(2)	$3\,^2P \rightarrow 7\,^2S$	0.0927525(2)
$3\,^2S \rightarrow 9\,^2P$	0.204173(2)	$3\,^2P \rightarrow 8\,^2S$	0.1009991(3)
$3\,^2S \rightarrow 10\,^2P$	0.207196(2)	$3\,^2P \rightarrow 9\,^2S$	0.1065241(3)
$3\,^2S \rightarrow 11\,^2P$	0.209457(2)	$3\,^2P \rightarrow 10\,^2S$	0.1104056(3)
$3\,^2S \rightarrow 12\,^2P$	0.211190(2)	$3\,^2P \rightarrow 11\,^2S$	0.1132364(4)
$3\,^2S \rightarrow 13\,^2P$	0.212551(3)	$3\,^2P \rightarrow 12\,^2S$	0.1205863(16)
		$3\,^2P \rightarrow 13\,^2S$	0.1169947(10)
$4\,^2S \rightarrow 4\,^2P$	0.0381384(7)	$4\,^2P \rightarrow 5\,^2S$	0.0063619(3)
$4\,^2S \rightarrow 5\,^2P$	0.0635289(8)	Radziemski *et al.* (exp) [124]	0.006(3)
$4\,^2S \rightarrow 6\,^2P$	0.0780043(8)	$4\,^2P \rightarrow 6\,^2S$	0.02903831(10)
$4\,^2S \rightarrow 7\,^2P$	0.0870161(8)	Radziemski *et al.* (exp) [124]	0.032(4)
$4\,^2S \rightarrow 8\,^2P$	0.0929990(9)	$4\,^2P \rightarrow 7\,^2S$	0.04213965(7)
$4\,^2S \rightarrow 9\,^2P$	0.0971704(8)	$4\,^2P \rightarrow 8\,^2S$	0.05038633(4)
$4\,^2S \rightarrow 10\,^2P$	0.1001939(8)	$4\,^2P \rightarrow 9\,^2S$	0.05591132(7)
$4\,^2S \rightarrow 11\,^2P$	0.1024541(8)	$4\,^2P \rightarrow 10\,^2S$	0.05979278(13)
$4\,^2S \rightarrow 12\,^2P$	0.1041875(8)	$4\,^2P \rightarrow 11\,^2S$	0.0626236(2)
$4\,^2S \rightarrow 13\,^2P$	0.105549(2)	$4\,^2P \rightarrow 12\,^2S$	0.0699735(17)
		$4\,^2P \rightarrow 13\,^2S$	0.0663819(10)
$5\,^2S \rightarrow 5\,^2P$	0.0190285(4)	$5\,^2P \rightarrow 6\,^2S$	0.00364787(17)
$5\,^2S \rightarrow 6\,^2P$	0.0335040(4)	$5\,^2P \rightarrow 7\,^2S$	0.01674921(11)
$5\,^2S \rightarrow 7\,^2P$	0.0425157(4)	$5\,^2P \rightarrow 8\,^2S$	0.02499589(5)
$5\,^2S \rightarrow 8\,^2P$	0.0484986(5)	$5\,^2P \rightarrow 9\,^2S$	0.03052087(3)
$5\,^2S \rightarrow 9\,^2P$	0.0526701(4)	$5\,^2P \rightarrow 10\,^2S$	0.03440234(11)
$5\,^2S \rightarrow 10\,^2P$	0.0556935(4)	$5\,^2P \rightarrow 11\,^2S$	0.0372332(2)
$5\,^2S \rightarrow 11\,^2P$	0.0579538(4)	$5\,^2P \rightarrow 12\,^2S$	0.0445830(17)
$5\,^2S \rightarrow 12\,^2P$	0.0596871(4)	$5\,^2P \rightarrow 13\,^2S$	0.0409915(10)
$5\,^2S \rightarrow 13\,^2P$	0.061048(2)		
$6\,^2S \rightarrow 6\,^2P$	0.0108276(2)	$6\,^2P \rightarrow 7\,^2S$	0.00227372(13)
$6\,^2S \rightarrow 7\,^2P$	0.0198394(2)	$6\,^2P \rightarrow 8\,^2S$	0.01052040(7)
$6\,^2S \rightarrow 8\,^2P$	0.0258223(3)	$6\,^2P \rightarrow 9\,^2S$	0.01604538(5)
$6\,^2S \rightarrow 9\,^2P$	0.0299937(2)	$6\,^2P \rightarrow 10\,^2S$	0.01992685(11)
$6\,^2S \rightarrow 10\,^2P$	0.0330171(2)	$6\,^2P \rightarrow 11\,^2S$	0.0227577(2)
$6\,^2S \rightarrow 11\,^2P$	0.0352774(2)	$6\,^2P \rightarrow 12\,^2S$	0.0301075(17)
$6\,^2S \rightarrow 12\,^2P$	0.0370108(3)	$6\,^2P \rightarrow 13\,^2S$	0.0265160(10)
$6\,^2S \rightarrow 13\,^2P$	0.038372(2)		
$7\,^2S \rightarrow 7\,^2P$	0.00673802(13)	$7\,^2P \rightarrow 8\,^2S$	0.00150867(8)
$7\,^2S \rightarrow 8\,^2P$	0.0127209(2)	$7\,^2P \rightarrow 9\,^2S$	0.00703365(5)
$7\,^2S \rightarrow 9\,^2P$	0.01689235(12)	$7\,^2P \rightarrow 10\,^2S$	0.01091511(7)
$7\,^2S \rightarrow 10\,^2P$	0.01991580(13)	$7\,^2P \rightarrow 11\,^2S$	0.0137459(3)
$7\,^2S \rightarrow 11\,^2P$	0.02217604(12)	$7\,^2P \rightarrow 12\,^2S$	0.0210958(15)
$7\,^2S \rightarrow 12\,^2P$	0.02390942(16)	$7\,^2P \rightarrow 13\,^2S$	0.0175042(11)
$7\,^2S \rightarrow 13\,^2P$	0.025271(2)		

(*continued on next page*)

Table 9 (*continued*).

Transition	IS	Transition	IS
$8\,^2S \to 8\,^2P$	0.0044742(2)	$8\,^2P \to 9\,^2S$	0.0010507(2)
$8\,^2S \to 9\,^2P$	0.00864566(10)	$8\,^2P \to 10\,^2S$	0.00493220(12)
$8\,^2S \to 10\,^2P$	0.01166911(11)	$8\,^2P \to 11\,^2S$	0.0077630(4)
$8\,^2S \to 11\,^2P$	0.01392936(6)	$8\,^2P \to 12\,^2S$	0.0151129(15)
$8\,^2S \to 12\,^2P$	0.01566274(18)	$8\,^2P \to 13\,^2S$	0.0115213(12)
$8\,^2S \to 13\,^2P$	0.017024(2)		
$9\,^2S \to 9\,^2P$	0.00312068(8)	$9\,^2P \to 10\,^2S$	0.00076078(2)
$9\,^2S \to 10\,^2P$	0.00614413(9)	$9\,^2P \to 11\,^2S$	0.0035916(3)
$9\,^2S \to 11\,^2P$	0.00840438(3)	$9\,^2P \to 12\,^2S$	0.0109415(17)
$9\,^2S \to 12\,^2P$	0.01013776(17)	$9\,^2P \to 13\,^2S$	0.0073499(11)
$9\,^2S \to 13\,^2P$	0.011499(2)		
$10\,^2S \to 10\,^2P$	0.00226267(3)	$10\,^2P \to 11\,^2S$	0.0005681(3)
$10\,^2S \to 11\,^2P$	0.00452292(9)	$10\,^2P \to 12\,^2S$	0.0079180(16)
$10\,^2S \to 12\,^2P$	0.00625629(9)	$10\,^2P \to 13\,^2S$	0.0043265(11)
$10\,^2S \to 13\,^2P$	0.007617(2)		
$11\,^2S \to 11\,^2P$	0.0016921(2)	$11\,^2P \to 12\,^2S$	0.0056578(16)
$11\,^2S \to 12\,^2P$	0.0034255(4)	$11\,^2P \to 13\,^2S$	0.0020662(10)
$11\,^2S \to 13\,^2P$	0.0047867(18)		
$12\,^2S \to 12\,^2P$	0.0012968(16)	$12\,^2P \to 13\,^2S$	0.0003328(12)
$12\,^2S \to 13\,^2P$	0.002660(2)		
$13\,^2S \to 13\,^2P$	0.0010284(10)		

Table 10
Nonrelativistic oscillator strengths in length (f_L) and velocity forms (f_V) for the $2\,^2S \to 2\,^2P$ and $9\,^2S \to 9\,^2P$ transitions and infinite nuclear mass ($^\infty$Li). The oscillator strength uncertainties (numbers in parentheses) are taken as root mean squares of the uncertainties of $|\mu_{if}|^2$ and ΔE, where ΔE is the difference between the non-relativistic energies of initial (i) and final (f) states. The calculation in Ref. [47,108,127] were performed using Hylleraas-type basis functions.

	Basis (^2S)	Basis (^2P)	f^L_{if}	f^V_{if}
$2\,^2S \to 2\,^2P$				
This work	8 000	9 000	0.74695680952	0.746956759
This work	9 000	10 000	0.74695680971	0.746956775
This work	11 000	12 000	0.74695680983	0.746956791
This work	∞	∞	0.74695680989(6)	0.746956799(8)
Yan and Drake [108]	∞	∞	0.7469572(10)	0.7469571(54)
Yan *et al.* [47]	3 502	3 463	0.7469569494	0.7469603
Yan *et al.* [47]	∞	∞	0.7469569396(98)	0.7469597(50)
Tang *et al.* [127]	∞	∞	0.7469563(5)	
$9\,^2S \to 9\,^2P$				
This work	14 000	14 000	3.65793496332	3.657654257
This work	15 000	15 000	3.65792321371	3.657682357
This work	16 000	16 000	3.65788546220	3.657720521
This work	∞	∞	3.657867(19)	3.65776(8)

isotopes. While currently the experimental determination of oscillator strengths cannot discriminate between different isotopes, this may become feasible in the future. The oscillator strengths for all transitions considered in this work are shown graphically in Fig. 1 in the form of a map that depicts their magnitude on a logarithmic scale. Both the tabulated values of the oscillator strengths and their depiction show that the largest values of the strengths correspond, as expected, to transitions between states with the same principal quantum number, i.e., for example, for the $n\,^2S \to n\,^2P$ transitions. One can notice that the calculated oscillator strengths are also quite sizable for the transitions of the type: $n\,^2P \to (n+1)\,^2S$. This indicates a possibility to use "cascade" excitations to prepare a lithium atom in a particular Rydberg state.

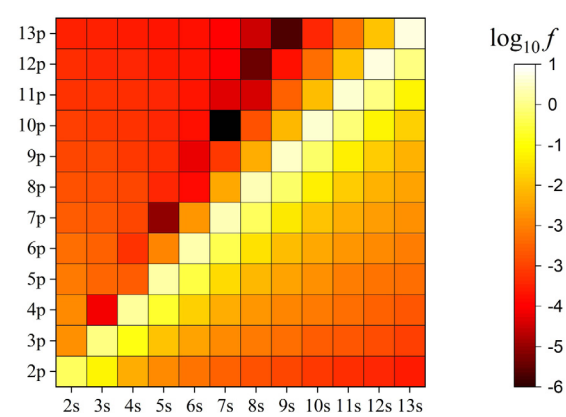

Fig. 1. The logarithmic map of the calculated absorption oscillator strengths for transitions between $S \to P$ and $P \to S$ states of the lithium atom.

4. Summary

In this work, the $1s^2$ ns and $1s^2\,np$ ($n = 2, \ldots, 13$) Rydberg states of the lithium atom were studied. In the framework of the Rayleigh–Ritz variational method with all-particle explicitly correlated Gaussian basis functions we performed very accurate calculations of the nonrelativistic energies and wave functions. The wave functions were then used to compute the leading relativistic and QED corrections to the energies of the studied states by means of the perturbation theory. The leading relativistic effects include the mass–velocity, orbit–orbit, Darwin, spin–spin, and spin–orbit correction. The calculated fine structure splittings are in very good agreement with previous studies and available

Table 11
The squares of the transition matrix elements, in length ($|\boldsymbol{\mu}_{if}|^2$) and velocity forms ($|\mathbf{p}_{if}|^2$) for the transitions involving ^2S and ^2P states. The numbers in parentheses are estimated uncertainties due to the basis truncation.

Transition	$\lvert\boldsymbol{\mu}_{if}\rvert^2(^6\mathrm{Li})$	$\lvert\boldsymbol{\mu}_{if}\rvert^2(^7\mathrm{Li})$	$\lvert\boldsymbol{\mu}_{if}\rvert^2(^\infty\mathrm{Li})$	$\lvert\mathbf{p}_{if}\rvert^2(^6\mathrm{Li})$	$\lvert\mathbf{p}_{if}\rvert^2(^7\mathrm{Li})$	$\lvert\mathbf{p}_{if}\rvert^2(^\infty\mathrm{Li})$
$2\,^2S \to 2\,^2P$	$3.3006378559(16)\times10^{1}$	$3.3005563700(16)\times10^{1}$	$3.3000667384(16)\times10^{1}$	$1.52056401(5)\times10^{-1}$	$1.52071691(5)\times10^{-1}$	$1.52163594(5)\times10^{-1}$
$2\,^2S \to 3\,^2P$	$1.0088016(3)\times10^{-1}$	$1.0085531(3)\times10^{-1}$	$1.0070609(3)\times10^{-1}$	$2.0014705(19)\times10^{-3}$	$2.0011961(19)\times10^{-3}$	$1.9995474(19)\times10^{-3}$
$2\,^2S \to 3\,^2P$ Ref. [46]			$1.003\ \times10^{-1}$			
$2\,^2S \to 4\,^2P$	$7.714123(4)\times10^{-2}$	$7.712936(4)\times10^{-2}$	$7.705810(4)\times10^{-2}$	$2.128494(10)\times10^{-3}$	$2.128397(10)\times10^{-3}$	$2.127810(10)\times10^{-3}$
$2\,^2S \to 4\,^2P$ Ref. [42]			$7.616\ \times10^{-2}$			
$2\,^2S \to 5\,^2P$	$4.31614(4)\times10^{-2}$	$4.31556(4)\times10^{-2}$	$4.31206(4)\times10^{-2}$	$1.363009(12)\times10^{-3}$	$1.362972(12)\times10^{-3}$	$1.362753(12)\times10^{-3}$
$2\,^2S \to 5\,^2P$ Ref. [128]			$4.420\ \times10^{-2}$			
$2\,^2S \to 6\,^2P$	$2.559332(9)\times10^{-2}$	$2.559008(9)\times10^{-2}$	$2.557059(9)\times10^{-2}$	$8.66218(3)\times10^{-4}$	$8.66202(3)\times10^{-4}$	$8.66106(3)\times10^{-4}$
$2\,^2S \to 6\,^2P$ Ref. [128]			$2.577\ \times10^{-2}$			
$2\,^2S \to 7\,^2P$	$1.625255(10)\times10^{-2}$	$1.625056(10)\times10^{-2}$	$1.623860(10)\times10^{-2}$	$5.72811(4)\times10^{-2}$	$5.72804(4)\times10^{-2}$	$5.72760(4)\times10^{-4}$
$2\,^2S \to 7\,^2P$ Ref. [128]			$1.617\ \times10^{-2}$			
$2\,^2S \to 8\,^2P$	$1.092184(13)\times10^{-2}$	$1.092053(13)\times10^{-2}$	$1.091266(13)\times10^{-2}$	$3.94988(6)\times10^{-2}$	$3.94984(6)\times10^{-2}$	$3.94959(6)\times10^{-4}$
$2\,^2S \to 8\,^2P$ Ref. [128]			$1.084\ \times10^{-2}$			
$2\,^2S \to 9\,^2P$	$7.67906(13)\times10^{-3}$	$7.67815(13)\times10^{-3}$	$7.67264(13)\times10^{-3}$	$2.82602(11)\times10^{-4}$	$2.82599(11)\times10^{-4}$	$2.82583(11)\times10^{-4}$
$2\,^2S \to 9\,^2P$ Ref. [128]			$7.599\ \times10^{-3}$			
$2\,^2S \to 10\,^2P$	$5.59933(12)\times10^{-3}$	$5.59864(12)\times10^{-3}$	$5.59448(12)\times10^{-3}$	$2.08630(4)\times10^{-4}$	$2.08626(4)\times10^{-4}$	$2.08604(4)\times10^{-4}$
$2\,^2S \to 11\,^2P$	$4.20637(9)\times10^{-3}$	$4.20578(9)\times10^{-3}$	$4.20222(9)\times10^{-3}$	$1.58162(6)\times10^{-4}$	$1.58156(6)\times10^{-4}$	$1.58120(6)\times10^{-4}$
$2\,^2S \to 12\,^2P$	$3.23920(11)\times10^{-3}$	$3.23873(11)\times10^{-3}$	$3.23590(11)\times10^{-3}$	$1.22645(16)\times10^{-4}$	$1.22639(16)\times10^{-4}$	$1.22607(16)\times10^{-4}$
$2\,^2S \to 13\,^2P$	$2.550902(4)\times10^{-3}$	$2.550153(4)\times10^{-3}$	$2.545658(4)\times10^{-3}$	$9.707(4)\times10^{-5}$	$9.705(4)\times10^{-5}$	$9.693(4)\times10^{-5}$
$2\,^2P \to 3\,^2S$	$1.774973778(16)\times10^{1}$	$1.774978750(16)\times10^{1}$	$1.775008538(16)\times10^{1}$	$5.5746291(10)\times10^{-2}$	$5.5751078(10)\times10^{-2}$	$5.5779852(10)\times10^{-2}$
$2\,^2P \to 3\,^2S$ Ref. [46]			$1.7743\ \times10^{1}$			
$2\,^2P \to 4\,^2S$	$1.2606738(15)$	$1.2606560(15)$	$1.2605489(15)$	$1.0576889(5)\times10^{-2}$	$1.0577710(5)\times10^{-2}$	$1.0582647(5)\times10^{-2}$
$2\,^2P \to 4\,^2S$ Ref. [46]			1.260			
$2\,^2P \to 5\,^2S$	$3.644750(11)\times10^{-1}$	$3.644686(11)\times10^{-1}$	$3.644302(11)\times10^{-1}$	$4.139397(4)\times10^{-3}$	$4.139712(4)\times10^{-3}$	$4.141604(4)\times10^{-3}$
$2\,^2P \to 5\,^2S$ Ref. [129]			$3.66\ \times10^{-1}$			
$2\,^2P \to 6\,^2S$	$1.602278(4)\times10^{-1}$	$1.602247(4)\times10^{-1}$	$1.602065(4)\times10^{-1}$	$2.091808(2)\times10^{-3}$	$2.091965(2)\times10^{-3}$	$2.092913(2)\times10^{-3}$
$2\,^2P \to 6\,^2S$ Ref. [129]			$1.62\ \times10^{-1}$			
$2\,^2P \to 7\,^2S$	$8.61750(12)\times10^{-2}$	$8.61732(12)\times10^{-2}$	$8.61630(12)\times10^{-2}$	$1.214688(2)\times10^{-3}$	$1.214779(2)\times10^{-3}$	$1.215325(2)\times10^{-3}$
$2\,^2P \to 7\,^2S$ Ref. [129]			$8.68\ \times10^{-2}$			
$2\,^2P \to 8\,^2S$	$5.22077(6)\times10^{-2}$	$5.22066(6)\times10^{-2}$	$5.22001(6)\times10^{-2}$	$7.712888(19)\times10^{-4}$	$7.713459(19)\times10^{-4}$	$7.716891(19)\times10^{-4}$
$2\,^2P \to 8\,^2S$ Ref. [129]			$5.26\ \times10^{-2}$			
$2\,^2P \to 9\,^2S$	$3.42295(3)\times10^{-2}$	$3.42286(3)\times10^{-2}$	$3.42237(3)\times10^{-2}$	$5.21584(7)\times10^{-4}$	$5.21620(7)\times10^{-4}$	$5.21842(7)\times10^{-4}$
$2\,^2P \to 10\,^2S$	$2.37474(8)\times10^{-2}$	$2.37465(8)\times10^{-2}$	$2.37413(8)\times10^{-2}$	$3.69725(7)\times10^{-4}$	$3.69747(7)\times10^{-4}$	$3.69876(7)\times10^{-4}$
$2\,^2P \to 11\,^2S$	$1.7195(20)\times10^{-2}$	$1.7194(20)\times10^{-2}$	$1.7185(20)\times10^{-2}$	$2.719(3)\times10^{-4}$	$2.719(3)\times10^{-4}$	$2.719(3)\times10^{-4}$
$2\,^2P \to 12\,^2S$	$1.289(3)\times10^{-2}$	$1.288(3)\times10^{-2}$	$1.288(3)\times10^{-2}$	$2.0601(11)\times10^{-4}$	$2.0600(11)\times10^{-4}$	$2.0597(11)\times10^{-4}$
$2\,^2P \to 13\,^2S$	$9.917(15)\times10^{-3}$	$9.915(15)\times10^{-3}$	$9.904(15)\times10^{-3}$	$1.601(2)\times10^{-4}$	$1.601(2)\times10^{-4}$	$1.600(2)\times10^{-4}$
$3\,^2S \to 3\,^2P$	$2.151180063(3)\times10^{2}$	$2.151117979(3)\times10^{2}$	$2.150744933(3)\times10^{2}$	$6.172418(3)\times10^{-2}$	$6.173035(3)\times10^{-2}$	$6.176745(3)\times10^{-2}$
$3\,^2S \to 3\,^2P$ Ref. [46]			$2.152\ \times10^{2}$			
$3\,^2S \to 4\,^2P$	$3.145447(14)\times10^{-3}$	$3.137321(14)\times10^{-3}$	$3.088734(14)\times10^{-3}$	$5.5995(15)\times10^{-6}$	$5.5859(15)\times10^{-6}$	$5.5043(15)\times10^{-6}$
$3\,^2S \to 4\,^2P$ Ref. [42]			$2.6\ \times10^{-3}$			
$3\,^2S \to 5\,^2P$	$7.18526(2)\times10^{-2}$	$7.18313(2)\times10^{-2}$	$7.17033(2)\times10^{-2}$	$2.07895(10)\times10^{-4}$	$2.07857(10)\times10^{-4}$	$2.07629(10)\times10^{-4}$
$3\,^2S \to 5\,^2P$ Ref. [129]			$7.26\ \times10^{-2}$			
$3\,^2S \to 6\,^2P$	$5.62174(12)\times10^{-2}$	$5.62049(12)\times10^{-2}$	$5.61300(12)\times10^{-2}$	$2.027588(20)\times10^{-4}$	$2.027371(20)\times10^{-4}$	$2.026067(20)\times10^{-4}$
$3\,^2S \to 6\,^2P$ Ref. [129]			$5.65\ \times10^{-2}$			
$3\,^2S \to 7\,^2P$	$3.8537(3)\times10^{-2}$	$3.8530(3)\times10^{-2}$	$3.8485(3)\times10^{-2}$	$1.569631(10)\times10^{-4}$	$1.569506(10)\times10^{-4}$	$1.568755(10)\times10^{-4}$
$3\,^2S \to 7\,^2P$ Ref. [129]			$3.88\ \times10^{-2}$			
$3\,^2S \to 8\,^2P$	$2.6663(2)\times10^{-2}$	$2.6658(2)\times10^{-2}$	$2.6628(2)\times10^{-2}$	$1.17048(7)\times10^{-4}$	$1.17040(7)\times10^{-4}$	$1.16993(7)\times10^{-4}$
$3\,^2S \to 8\,^2P$ Ref. [129]			$2.68\ \times10^{-2}$			
$3\,^2S \to 9\,^2P$	$1.89957(19)\times10^{-2}$	$1.89923(19)\times10^{-2}$	$1.89723(19)\times10^{-2}$	$8.7631(8)\times10^{-5}$	$8.7626(8)\times10^{-5}$	$8.7596(8)\times10^{-5}$
$3\,^2S \to 10\,^2P$	$1.39437(17)\times10^{-2}$	$1.39413(17)\times10^{-2}$	$1.39265(17)\times10^{-2}$	$6.6600(8)\times10^{-5}$	$6.6596(8)\times10^{-5}$	$6.6570(8)\times10^{-5}$
$3\,^2S \to 11\,^2P$	$1.05130(11)\times10^{-2}$	$1.05110(11)\times10^{-2}$	$1.04989(11)\times10^{-2}$	$5.1496(7)\times10^{-5}$	$5.1492(7)\times10^{-5}$	$5.1471(7)\times10^{-5}$
$3\,^2S \to 12\,^2P$	$8.1124(11)\times10^{-3}$	$8.1108(11)\times10^{-3}$	$8.1014(11)\times10^{-3}$	$4.0485(13)\times10^{-5}$	$4.0482(13)\times10^{-5}$	$4.0464(13)\times10^{-5}$
$3\,^2S \to 13\,^2P$	$6.39517(9)\times10^{-3}$	$6.39301(9)\times10^{-3}$	$6.38010(9)\times10^{-3}$	$3.23611(15)\times10^{-5}$	$3.23538(15)\times10^{-5}$	$3.23097(15)\times10^{-5}$
$3\,^2P \to 4\,^2S$	$1.078788943(6)\times10^{2}$	$1.078788568(6)\times10^{2}$	$1.078786264(6)\times10^{2}$	$3.738349(5)\times10^{-2}$	$3.738662(5)\times10^{-2}$	$3.740540(5)\times10^{-2}$
$3\,^2P \to 4\,^2S$ Ref. [46]			$1.078\ \times10^{2}$			
$3\,^2P \to 5\,^2S$	$6.946066(4)$	$6.945933(4)$	$6.945132(4)$	$7.836753(5)\times10^{-3}$	$7.837336(5)\times10^{-3}$	$7.840840(5)\times10^{-3}$
$3\,^2P \to 5\,^2S$ Ref. [129]			6.97			
$3\,^2P \to 6\,^2S$	$1.931349(7)$	$1.931305(7)$	$1.931037(7)$	$3.290832(10)\times10^{-3}$	$3.291071(10)\times10^{-3}$	$3.292509(10)\times10^{-3}$
$3\,^2P \to 6\,^2S$ Ref. [129]			1.94			
$3\,^2P \to 7\,^2S$	$8.37578(2)\times10^{-1}$	$8.37556(2)\times10^{-1}$	$8.37430(2)\times10^{-1}$	$1.752639(4)\times10^{-3}$	$1.752765(4)\times10^{-3}$	$1.753521(4)\times10^{-3}$
$3\,^2P \to 7\,^2S$ Ref. [129]			$8.40\ \times10^{-1}$			
$3\,^2P \to 8\,^2S$	$4.49419(4)\times10^{-1}$	$4.49407(4)\times10^{-1}$	$4.49335(4)\times10^{-1}$	$1.059993(3)\times10^{-3}$	$1.060069(3)\times10^{-3}$	$1.060520(3)\times10^{-3}$
$3\,^2P \to 8\,^2S$ Ref. [129]			$4.51\ \times10^{-1}$			
$3\,^2P \to 9\,^2S$	$2.73059(2)\times10^{-1}$	$2.73051(2)\times10^{-1}$	$2.73001(2)\times10^{-1}$	$6.95288(7)\times10^{-4}$	$6.95335(7)\times10^{-4}$	$6.95617(7)\times10^{-4}$
$3\,^2P \to 10\,^2S$	$1.79983(6)\times10^{-1}$	$1.79975(6)\times10^{-1}$	$1.79929(6)\times10^{-1}$	$4.82851(13)\times10^{-4}$	$4.82877(13)\times10^{-4}$	$4.83036(13)\times10^{-4}$
$3\,^2P \to 11\,^2S$	$1.2568(15)\times10^{-1}$	$1.2567(15)\times10^{-1}$	$1.2561(15)\times10^{-1}$	$3.500(4)\times10^{-4}$	$3.500(4)\times10^{-4}$	$3.500(4)\times10^{-4}$
$3\,^2P \to 12\,^2S$	$9.14(7)\times10^{-2}$	$9.14(7)\times10^{-2}$	$9.12(7)\times10^{-2}$	$2.6234(15)\times10^{-4}$	$2.6232(15)\times10^{-4}$	$2.6227(15)\times10^{-4}$
$3\,^2P \to 13\,^2S$	$6.917(14)\times10^{-2}$	$6.915(14)\times10^{-2}$	$6.908(14)\times10^{-2}$	$2.022(4)\times10^{-4}$	$2.022(4)\times10^{-4}$	$2.021(4)\times10^{-4}$

(*continued on next page*)

Table 11 (*continued*).

Transition	$\lvert\boldsymbol{\mu}_{if}\rvert^2(^6\mathrm{Li})$	$\lvert\boldsymbol{\mu}_{if}\rvert^2(^7\mathrm{Li})$	$\lvert\boldsymbol{\mu}_{if}\rvert^2(^\infty\mathrm{Li})$	$\lvert\mathbf{p}_{if}\rvert^2(^6\mathrm{Li})$	$\lvert\mathbf{p}_{if}\rvert^2(^7\mathrm{Li})$	$\lvert\mathbf{p}_{if}\rvert^2(^\infty\mathrm{Li})$
$4\,^2S \to 4\,^2P$	$7.41276708(7)\times10^{2}$	$7.41254071(7)\times10^{2}$	$7.41118055(7)\times10^{2}$	$3.267031(9)\times10^{-2}$	$3.267356(9)\times10^{-2}$	$3.269310(9)\times10^{-2}$
$4\,^2S \to 4\,^2P$ Ref. [42]			$7.422\ \times10^{2}$			
$4\,^2S \to 5\,^2P$	$1.611152(3)\times10^{-1}$	$1.612067(3)\times10^{-1}$	$1.617566(3)\times10^{-1}$	$5.3578(5)\times10^{-5}$	$5.36136(5)\times10^{-5}$	$5.3827(5)\times10^{-5}$
$4\,^2S \to 5\,^2P$ Ref. [129]			$1.57\ \times10^{-1}$			
$4\,^2S \to 6\,^2P$	$3.45027(6)\times10^{-2}$	$3.44797(6)\times10^{-2}$	$3.43414(6)\times10^{-2}$	$2.07122(10)\times10^{-5}$	$2.07012(10)\times10^{-5}$	$2.06354(10)\times10^{-5}$
$4\,^2S \to 6\,^2P$ Ref. [129]			$3.56\ \times10^{-2}$			
$4\,^2S \to 7\,^2P$	$5.0754(5)\times10^{-2}$	$5.0736(5)\times10^{-2}$	$5.0626(5)\times10^{-2}$	$4.05479(3)\times10^{-5}$	$4.05385(3)\times10^{-5}$	$4.04818(3)\times10^{-5}$
$4\,^2S \to 7\,^2P$ Ref. [129]			$5.15\ \times10^{-2}$			
$4\,^2S \to 8\,^2P$	$4.2062(9)\times10^{-2}$	$4.2050(9)\times10^{-2}$	$4.1977(9)\times10^{-2}$	$3.9652(4)\times10^{-5}$	$3.9645(4)\times10^{-5}$	$3.9606(4)\times10^{-5}$
$4\,^2S \to 8\,^2P$ Ref. [129]			$4.26\ \times10^{-2}$			
$4\,^2S \to 9\,^2P$	$3.20590(17)\times10^{-2}$	$3.20506(17)\times10^{-2}$	$3.20001(17)\times10^{-2}$	$3.359(2)\times10^{-5}$	$3.358(2)\times10^{-5}$	$3.356(2)\times10^{-5}$
$4\,^2S \to 10\,^2P$	$2.42719(9)\times10^{-2}$	$2.42658(9)\times10^{-2}$	$2.42292(9)\times10^{-2}$	$2.7326(4)\times10^{-5}$	$2.7322(4)\times10^{-5}$	$2.7302(4)\times10^{-5}$
$4\,^2S \to 11\,^2P$	$1.8593(2)\times10^{-2}$	$1.8588(2)\times10^{-2}$	$1.8559(2)\times10^{-2}$	$2.2039(8)\times10^{-5}$	$2.2036(8)\times10^{-5}$	$2.2022(8)\times10^{-5}$
$4\,^2S \to 12\,^2P$	$1.44749(19)\times10^{-2}$	$1.44712(19)\times10^{-2}$	$1.44490(19)\times10^{-2}$	$1.7820(4)\times10^{-5}$	$1.7819(4)\times10^{-5}$	$1.7808(4)\times10^{-5}$
$4\,^2S \to 13\,^2P$	$1.1467(3)\times10^{-2}$	$1.1463(3)\times10^{-2}$	$1.1436(3)\times10^{-2}$	$1.4535(3)\times10^{-5}$	$1.4531(3)\times10^{-5}$	$1.4508(3)\times10^{-5}$
$4\,^2P \to 5\,^2S$	$3.6253027(2)\times10^{2}$	$3.6252956(2)\times10^{2}$	$3.6252524(2)\times10^{2}$	$2.518575(10)\times10^{-2}$	$2.518786(10)\times10^{-2}$	$2.520055(10)\times10^{-2}$
$4\,^2P \to 5\,^2S$ Ref. [129]			$3.62\ \times10^{2}$			
$4\,^2P \to 6\,^2S$	$2.1684578(11)\times10^{1}$	$2.1684107(11)\times10^{1}$	$2.1681273(11)\times10^{1}$	$5.56808(4)\times10^{-3}$	$5.56849(4)\times10^{-3}$	$5.57097(4)\times10^{-3}$
$4\,^2P \to 6\,^2S$ Ref. [129]			$2.17\ \times10^{1}$			
$4\,^2P \to 7\,^2S$	$5.81268(4)$	$5.81253(4)$	$5.81162(4)$	$2.440353(20)\times10^{-3}$	$2.440527(20)\times10^{-3}$	$2.441576(20)\times10^{-3}$
$4\,^2P \to 7\,^2S$ Ref. [129]			5.82			
$4\,^2P \to 8\,^2S$	$2.47473(12)$	$2.47466(12)$	$2.47422(12)$	$1.344808(10)\times10^{-3}$	$1.344902(10)\times10^{-3}$	$1.345469(10)\times10^{-3}$
$4\,^2P \to 8\,^2S$ Ref. [129]			2.48			
$4\,^2P \to 9\,^2S$	$1.31607(10)$	$1.31603(10)$	$1.31578(10)$	$8.36220(7)\times10^{-4}$	$8.36276(7)\times10^{-4}$	$8.36611(7)\times10^{-4}$
$4\,^2P \to 10\,^2S$	$7.9681(4)\times10^{-1}$	$7.9677(4)\times10^{-1}$	$7.9656(4)\times10^{-1}$	$5.61272(16)\times10^{-4}$	$5.61303(16)\times10^{-4}$	$5.61485(16)\times10^{-4}$
$4\,^2P \to 11\,^2S$	$5.250(6)\times10^{-1}$	$5.250(6)\times10^{-1}$	$5.247(6)\times10^{-1}$	$3.975(5)\times10^{-4}$	$3.975(5)\times10^{-4}$	$3.975(5)\times10^{-4}$
$4\,^2P \to 12\,^2S$	$3.69(5)\times10^{-1}$	$3.69(5)\times10^{-1}$	$3.69(5)\times10^{-1}$	$2.9298(18)\times10^{-4}$	$2.9297(18)\times10^{-4}$	$2.9290(18)\times10^{-4}$
$4\,^2P \to 13\,^2S$	$2.686(5)\times10^{-1}$	$2.686(5)\times10^{-1}$	$2.683(5)\times10^{-1}$	$2.231(5)\times10^{-4}$	$2.230(5)\times10^{-4}$	$2.229(5)\times10^{-4}$
$5\,^2S \to 5\,^2P$	$1.88737174(11)\times10^{3}$	$1.88731233(11)\times10^{3}$	$1.88695536(11)\times10^{3}$	$2.008179(4)\times10^{-2}$	$2.008378(4)\times10^{-2}$	$2.009575(4)\times10^{-2}$
$5\,^2S \to 5\,^2P$ Ref. [129]			$1.890\ \times10^{3}$			
$5\,^2S \to 6\,^2P$	$1.09327(2)$	$1.09361(2)$	$1.09566(2)$	$9.9249(3)\times10^{-5}$	$9.9289(3)\times10^{-5}$	$9.9533(3)\times10^{-5}$
$5\,^2S \to 6\,^2P$ Ref. [129]			1.08			
$5\,^2S \to 7\,^2P$	$1.6483(3)\times10^{-3}$	$1.6412(3)\times10^{-3}$	$1.5984(3)\times10^{-3}$	$2.9103(3)\times10^{-7}$	$2.8989(3)\times10^{-7}$	$2.8306(3)\times10^{-7}$
$5\,^2S \to 8\,^2P$	$3.233(2)\times10^{-2}$	$3.231(2)\times10^{-2}$	$3.219(2)\times10^{-2}$	$7.996(3)\times10^{-6}$	$7.992(3)\times10^{-6}$	$7.970(3)\times10^{-6}$
$5\,^2S \to 8\,^2P$ Ref. [129]			$3.33\ \times10^{-2}$			
$5\,^2S \to 9\,^2P$	$3.687(2)\times10^{-2}$	$3.685(2)\times10^{-2}$	$3.675(2)\times10^{-2}$	$1.1143(8)\times10^{-5}$	$1.1140(8)\times10^{-5}$	$1.1123(8)\times10^{-5}$
$5\,^2S \to 10\,^2P$	$3.204(18)\times10^{-2}$	$3.202(18)\times10^{-2}$	$3.195(18)\times10^{-2}$	$1.10547(9)\times10^{-5}$	$1.10523(9)\times10^{-5}$	$1.10384(9)\times10^{-5}$
$5\,^2S \to 11\,^2P$	$2.604(7)\times10^{-2}$	$2.603(7)\times10^{-2}$	$2.598(7)\times10^{-2}$	$9.8826(16)\times10^{-6}$	$9.8808(16)\times10^{-6}$	$9.8700(16)\times10^{-6}$
$5\,^2S \to 12\,^2P$	$2.094(3)\times10^{-2}$	$2.093(3)\times10^{-2}$	$2.089(3)\times10^{-2}$	$8.498(3)\times10^{-6}$	$8.496(3)\times10^{-6}$	$8.488(3)\times10^{-6}$
$5\,^2S \to 13\,^2P$	$1.690(5)\times10^{-2}$	$1.689(5)\times10^{-2}$	$1.685(5)\times10^{-2}$	$7.213(2)\times10^{-6}$	$7.210(2)\times10^{-6}$	$7.196(2)\times10^{-6}$
$5\,^2P \to 6\,^2S$	$9.111229(3)\times10^{2}$	$9.111202(3)\times10^{2}$	$9.111039(3)\times10^{2}$	$1.785911(4)\times10^{-2}$	$1.786060(4)\times10^{-2}$	$1.786956(4)\times10^{-2}$
$5\,^2P \to 6\,^2S$ Ref. [129]			$9.12\ \times10^{2}$			
$5\,^2P \to 7\,^2S$	$5.159066(6)\times10^{1}$	$5.158946(6)\times10^{1}$	$5.158223(6)\times10^{1}$	$4.08000(3)\times10^{-3}$	$4.08030(3)\times10^{-3}$	$4.08208(3)\times10^{-3}$
$5\,^2P \to 7\,^2S$ Ref. [129]			$5.16\ \times10^{1}$			
$5\,^2P \to 8\,^2S$	$1.34099(3)\times10^{1}$	$1.34095(3)\times10^{1}$	$1.34072(3)\times10^{1}$	$1.840176(8)\times10^{-3}$	$1.840304(8)\times10^{-3}$	$1.841079(8)\times10^{-3}$
$5\,^2P \to 8\,^2S$ Ref. [129]			$1.35\ \times10^{1}$			
$5\,^2P \to 9\,^2S$	$5.60754(7)$	$5.60737(7)$	$5.60633(7)$	$1.038660(13)\times10^{-3}$	$1.038728(13)\times10^{-3}$	$1.039140(13)\times10^{-3}$
$5\,^2P \to 10\,^2S$	$2.9507(8)$	$2.9505(8)$	$2.9498(8)$	$6.59008(15)\times10^{-4}$	$6.59043(15)\times10^{-4}$	$6.59254(15)\times10^{-4}$
$5\,^2P \to 11\,^2S$	$1.776(2)$	$1.775(2)$	$1.774(2)$	$4.501(5)\times10^{-4}$	$4.501(5)\times10^{-4}$	$4.501(5)\times10^{-4}$
$5\,^2P \to 12\,^2S$	$1.160(19)$	$1.160(19)$	$1.156(19)$	$3.2358(10)\times10^{-4}$	$3.2357(10)\times10^{-4}$	$3.2352(10)\times10^{-4}$
$5\,^2P \to 13\,^2S$	$8.158(19)\times10^{-1}$	$8.156(19)\times10^{-1}$	$8.148(19)\times10^{-1}$	$2.419(5)\times10^{-4}$	$2.419(5)\times10^{-4}$	$2.417(5)\times10^{-4}$
$6\,^2S \to 6\,^2P$	$4.0097329(14)\times10^{3}$	$4.0096043(14)\times10^{3}$	$4.0088315(14)\times10^{3}$	$1.355483(7)\times10^{-2}$	$1.355616(7)\times10^{-2}$	$1.356417(7)\times10^{-2}$
$6\,^2S \to 6\,^2P$ Ref. [129]			$4.010\ \times10^{3}$			
$6\,^2S \to 7\,^2P$	$3.50957(12)$	$3.51040(12)$	$3.51541(12)$	$1.10162(4)\times10^{-4}$	$1.10198(4)\times10^{-4}$	$1.10413(4)\times10^{-4}$
$6\,^2S \to 7\,^2P$ Ref. [129]			3.46			
$6\,^2S \to 8\,^2P$	$2.6762(8)\times10^{-2}$	$2.6801(8)\times10^{-2}$	$2.7036(8)\times10^{-2}$	$1.7298(12)\times10^{-6}$	$1.7322(12)\times10^{-6}$	$1.7468(12)\times10^{-6}$
$6\,^2S \to 9\,^2P$	$1.080(3)\times10^{-2}$	$1.078(3)\times10^{-2}$	$1.069(3)\times10^{-2}$	$1.0161(20)\times10^{-6}$	$1.0150(20)\times10^{-6}$	$1.0086(20)\times10^{-6}$
$6\,^2S \to 10\,^2P$	$2.548(19)\times10^{-2}$	$2.546(19)\times10^{-2}$	$2.536(19)\times10^{-2}$	$3.0185(14)\times10^{-6}$	$3.0171(14)\times10^{-6}$	$3.0084(14)\times10^{-6}$
$6\,^2S \to 11\,^2P$	$2.739(8)\times10^{-2}$	$2.737(8)\times10^{-2}$	$2.728(8)\times10^{-2}$	$3.7779(19)\times10^{-6}$	$3.7766(19)\times10^{-6}$	$3.7688(19)\times10^{-6}$
$6\,^2S \to 12\,^2P$	$2.466(11)\times10^{-2}$	$2.465(11)\times10^{-2}$	$2.458(11)\times10^{-2}$	$3.8063(6)\times10^{-6}$	$3.8053(6)\times10^{-6}$	$3.7991(6)\times10^{-6}$
$6\,^2S \to 13\,^2P$	$2.104(11)\times10^{-2}$	$2.102(11)\times10^{-2}$	$2.095(11)\times10^{-2}$	$3.533(3)\times10^{-6}$	$3.531(3)\times10^{-6}$	$3.522(3)\times10^{-6}$
$6\,^2P \to 7\,^2S$	$1.920387(9)\times10^{3}$	$1.920380(9)\times10^{3}$	$1.920338(9)\times10^{3}$	$1.325274(11)\times10^{-2}$	$1.325383(11)\times10^{-2}$	$1.326037(11)\times10^{-2}$
$6\,^2P \to 7\,^2S$ Ref. [129]			$1.920\ \times10^{3}$			
$6\,^2P \to 8\,^2S$	$1.042787(3)\times10^{2}$	$1.042761(3)\times10^{2}$	$1.042604(3)\times10^{2}$	$3.095512(17)\times10^{-3}$	$3.095732(17)\times10^{-3}$	$3.097051(17)\times10^{-3}$
$6\,^2P \to 8\,^2S$ Ref. [129]			$1.04\ \times10^{2}$			
$6\,^2P \to 9\,^2S$	$2.64232(6)\times10^{1}$	$2.64224(6)\times10^{1}$	$2.64177(6)\times10^{1}$	$1.425110(16)\times10^{-3}$	$1.425203(16)\times10^{-3}$	$1.425761(16)\times10^{-3}$
$6\,^2P \to 10\,^2S$	$1.0872(2)\times10^{1}$	$1.0871(2)\times10^{1}$	$1.0869(2)\times10^{1}$	$8.18792(9)\times10^{-4}$	$8.18835(9)\times10^{-4}$	$8.19092(9)\times10^{-4}$
$6\,^2P \to 11\,^2S$	$5.663(5)$	$5.663(5)$	$5.660(5)$	$5.276(6)\times10^{-4}$	$5.276(6)\times10^{-4}$	$5.276(6)\times10^{-4}$
$6\,^2P \to 12\,^2S$	$3.41(6)$	$3.40(6)$	$3.41(6)$	$3.652(2)\times10^{-4}$	$3.652(2)\times10^{-4}$	$3.651(2)\times10^{-4}$
$6\,^2P \to 13\,^2S$	$2.216(4)$	$2.216(4)$	$2.213(4)$	$2.660(5)\times10^{-4}$	$2.660(5)\times10^{-4}$	$2.658(5)\times10^{-4}$

(*continued on next page*)

Table 11 (*continued*).

Transition	$\lvert\boldsymbol{\mu}_{if}\rvert^2(^6\mathrm{Li})$	$\lvert\boldsymbol{\mu}_{if}\rvert^2(^7\mathrm{Li})$	$\lvert\boldsymbol{\mu}_{if}\rvert^2(^\infty\mathrm{Li})$	$\lvert\mathbf{p}_{if}\rvert^2(^6\mathrm{Li})$	$\lvert\mathbf{p}_{if}\rvert^2(^7\mathrm{Li})$	$\lvert\mathbf{p}_{if}\rvert^2(^\infty\mathrm{Li})$
$7\,^2S \to 7\,^2P$	$7.54514(4)\times10^3$	$7.54490(4)\times10^3$	$7.54343(4)\times10^3$	$9.7514(2)\times10^{-3}$	$9.7523(2)\times10^{-3}$	$9.7580(2)\times10^{-3}$
$7\,^2S \to 7\,^2P$ Ref. [129]			$7.560\ \times10^3$			
$7\,^2S \to 8\,^2P$	8.3141(5)	8.3158(5)	8.3259(5)	$1.06144(4)\times10^{-4}$	$1.06173(4)\times10^{-4}$	$1.06346(4)\times10^{-4}$
$7\,^2S \to 8\,^2P$ Ref. [129]			8.23			
$7\,^2S \to 9\,^2P$	$0.1806(6)\times10^{-1}$	$0.1808(6)\times10^{-1}$	$1.8157(6)\times10^{-1}$	$4.963(3)\times10^{-6}$	$4.966(3)\times10^{-6}$	$4.986(3)\times10^{-6}$
$7\,^2S \to 10\,^2P$	$6(4)\times10^{-6}$	$7(4)\times10^{-6}$	$2(4)\times10^{-6}$	$1.9(11)\times10^{-11}$	$2.4(11)\times10^{-11}$	$6.4(11)\times10^{-11}$
$7\,^2S \to 11\,^2P$	$1.21(7)\times10^{-2}$	$1.21(7)\times10^{-2}$	$1.20(7)\times10^{-2}$	$6.37(3)\times10^{-7}$	$6.36(3)\times10^{-7}$	$6.32(3)\times10^{-7}$
$7\,^2S \to 12\,^2P$	$1.95(6)\times10^{-2}$	$1.95(6)\times10^{-2}$	$1.94(6)\times10^{-2}$	$1.225(5)\times10^{-6}$	$1.224(5)\times10^{-6}$	$1.220(5)\times10^{-6}$
$7\,^2S \to 13\,^2P$	$2.03(3)\times10^{-2}$	$2.03(3)\times10^{-2}$	$2.02(3)\times10^{-2}$	$1.469(3)\times10^{-6}$	$1.468(3)\times10^{-6}$	$1.462(3)\times10^{-6}$
$7\,^2P \to 8\,^2S$	$3.594365(15)\times10^3$	$3.594350(15)\times10^3$	$3.594259(15)\times10^3$	$1.020004(5)\times10^{-2}$	$1.020087(5)\times10^{-2}$	$1.020584(5)\times10^{-2}$
$7\,^2P \to 8\,^2S$ Ref. [129]			$3.600\ \times10^3$			
$7\,^2P \to 9\,^2S$	$1.88868(4)\times10^2$	$1.88863(4)\times10^2$	$1.88832(4)\times10^2$	$2.42076(4)\times10^{-3}$	$2.42092(4)\times10^{-3}$	$2.42189(4)\times10^{-3}$
$7\,^2P \to 10\,^2S$	$4.6856(5)\times10^1$	$4.6855(5)\times10^1$	$4.6844(5)\times10^1$	$1.131781(20)\times10^{-3}$	$1.131840(20)\times10^{-3}$	$1.132195(20)\times10^{-3}$
$7\,^2P \to 11\,^2S$	$1.901(3)\times10^1$	$1.901(3)\times10^1$	$1.900(3)\times10^1$	$6.593(8)\times10^{-4}$	$6.593(8)\times10^{-4}$	$6.594(8)\times10^{-4}$
$7\,^2P \to 12\,^2S$	9.75(15)	9.75(15)	9.72(15)	$4.302(3)\times10^{-4}$	$4.301(3)\times10^{-4}$	$4.301(3)\times10^{-4}$
$7\,^2P \to 13\,^2S$	5.828(4)	5.827(4)	5.821(4)	$3.013(5)\times10^{-4}$	$3.013(5)\times10^{-4}$	$3.011(5)\times10^{-4}$
$8\,^2S \to 8\,^2P$	$1.301085(5)\times10^4$	$1.301043(5)\times10^4$	$1.300789(5)\times10^4$	$7.34618(2)\times10^{-3}$	$7.34687(2)\times10^{-3}$	$7.35101(2)\times10^{-3}$
$8\,^2S \to 8\,^2P$ Ref. [129]			$1.3000\ \times10^4$			
$8\,^2S \to 9\,^2P$	$1.6605(2)\times10^1$	$1.6609(2)\times10^1$	$1.6627(2)\times10^1$	$9.7110(11)\times10^{-5}$	$9.7132(11)\times10^{-5}$	$9.7262(11)\times10^{-5}$
$8\,^2S \to 10\,^2P$	$5.516(4)\times10^{-1}$	$5.519(4)\times10^{-1}$	$5.535(4)\times10^{-1}$	$7.1867(5)\times10^{-6}$	$7.1900(5)\times10^{-6}$	$7.2104(5)\times10^{-6}$
$8\,^2S \to 11\,^2P$	$1.76(5)\times10^{-2}$	$1.76(5)\times10^{-2}$	$1.77(5)\times10^{-2}$	$3.566(6)\times10^{-7}$	$3.572(6)\times10^{-7}$	$3.606(6)\times10^{-7}$
$8\,^2S \to 12\,^2P$	$1.87(5)\times10^{-3}$	$1.86(5)\times10^{-3}$	$1.83(5)\times10^{-3}$	$4.65(5)\times10^{-8}$	$4.64(5)\times10^{-8}$	$4.55(5)\times10^{-8}$
$8\,^2S \to 13\,^2P$	$1.0(3)\times10^{-3}$	$1.0(3)\times10^{-3}$	$1.0(3)\times10^{-3}$	$3.25(3)\times10^{-7}$	$3.24(3)\times10^{-7}$	$3.22(3)\times10^{-7}$
$8\,^2P \to 9\,^2S$	$6.17441(6)\times10^3$	$6.17438(6)\times10^3$	$6.17420(6)\times10^3$	$8.08282(13)\times10^{-3}$	$8.08345(13)\times10^{-3}$	$8.08728(13)\times10^{-3}$
$8\,^2P \to 10\,^2S$	$3.15985(14)\times10^2$	$3.15975(14)\times10^2$	$3.15916(14)\times10^2$	$1.941438(18)\times10^{-3}$	$1.941549(18)\times10^{-3}$	$1.942221(18)\times10^{-3}$
$8\,^2P \to 11\,^2S$	$7.703(9)\times10^1$	$7.703(9)\times10^1$	$7.700(9)\times10^1$	$9.188(10)\times10^{-4}$	$9.188(10)\times10^{-4}$	$9.189(10)\times10^{-4}$
$8\,^2P \to 12\,^2S$	$3.10(4)\times10^1$	$3.10(4)\times10^1$	$3.10(4)\times10^1$	$5.412(3)\times10^{-4}$	$5.412(3)\times10^{-4}$	$5.411(3)\times10^{-4}$
$8\,^2P \to 13\,^2S$	$1.5790(9)\times10^1$	$1.5787(9)\times10^1$	$1.5772(9)\times10^1$	$3.569(6)\times10^{-4}$	$3.569(6)\times10^{-4}$	$3.568(6)\times10^{-4}$
$9\,^2S \to 9\,^2P$	$2.10046(2)\times10^4$	$2.10039(2)\times10^4$	$2.09999(2)\times10^4$	$5.73064(12)\times10^{-3}$	$5.73114(12)\times10^{-3}$	$5.73410(12)\times10^{-3}$
$9\,^2S \to 10\,^2P$	$2.9674(4)\times10^1$	$2.9680(4)\times10^1$	$2.9714(4)\times10^1$	$8.7038(14)\times10^{-5}$	$8.7054(14)\times10^{-5}$	$8.7149(14)\times10^{-5}$
$9\,^2S \to 11\,^2P$	$1.246(2)\times10^0$	$1.246(2)\times10^0$	1.247(2)	$8.3774(10)\times10^{-6}$	$8.3800(10)\times10^{-6}$	$8.3952(10)\times10^{-6}$
$9\,^2S \to 12\,^2P$	$8.51(9)\times10^{-2}$	$8.50(9)\times10^{-2}$	$8.47(9)\times10^{-2}$	$9.120(18)\times10^{-7}$	$9.127(18)\times10^{-7}$	$9.169(18)\times10^{-7}$
$9\,^2S \to 13\,^2P$	$1.64(13)\times10^{-3}$	$1.63(13)\times10^{-3}$	$1.63(13)\times10^{-3}$	$2.63(9)\times10^{-8}$	$2.64(9)\times10^{-8}$	$2.72(9)\times10^{-8}$
$9\,^2P \to 10\,^2S$	$9.9391(3)\times10^3$	$9.9390(3)\times10^3$	$9.9387(3)\times10^3$	$6.55795(18)\times10^{-3}$	$6.55842(18)\times10^{-3}$	$6.56126(18)\times10^{-3}$
$9\,^2P \to 11\,^2S$	$4.979(6)\times10^2$	$4.979(6)\times10^2$	$4.977(6)\times10^2$	$1.5903(16)\times10^{-3}$	$1.5903(16)\times10^{-3}$	$1.5905(16)\times10^{-3}$
$9\,^2P \to 12\,^2S$	$1.193(10)\times10^2$	$1.193(10)\times10^2$	$1.191(10)\times10^2$	$7.602(5)\times10^{-4}$	$7.601(5)\times10^{-4}$	$7.600(5)\times10^{-4}$
$9\,^2P \to 13\,^2S$	$4.745(5)\times10^1$	$4.744(5)\times10^1$	$4.740(5)\times10^1$	$4.523(7)\times10^{-4}$	$4.522(7)\times10^{-4}$	$4.520(7)\times10^{-4}$
$10\,^2S \to 10\,^2P$	$3.22051(14)\times10^4$	$3.22042(14)\times10^4$	$3.21988(14)\times10^4$	$4.5937(2)\times10^{-3}$	$4.5940(2)\times10^{-3}$	$4.5961(2)\times10^{-3}$
$10\,^2S \to 11\,^2P$	$4.899(4)\times10^1$	$4.900(4)\times10^1$	$4.907(4)\times10^1$	$7.7466(12)\times10^{-5}$	$7.7472(12)\times10^{-5}$	$7.7506(12)\times10^{-5}$
$10\,^2S \to 12\,^2P$	2.379(15)	2.378(15)	2.376(15)	$8.867(11)\times10^{-6}$	$8.867(11)\times10^{-6}$	$8.865(11)\times10^{-6}$
$10\,^2S \to 13\,^2P$	$2.339(7)\times10^{-1}$	$2.330(7)\times10^{-1}$	$2.278(7)\times10^{-1}$	$1.397(12)\times10^{-6}$	$1.397(12)\times10^{-6}$	$1.398(12)\times10^{-6}$
$10\,^2P \to 11\,^2S$	$1.520(3)\times10^4$	$1.520(3)\times10^4$	$1.520(3)\times10^4$	$5.425(2)\times10^{-3}$	$5.425(2)\times10^{-3}$	$5.427(2)\times10^{-3}$
$10\,^2P \to 12\,^2S$	$7.50(3)\times10^2$	$7.50(3)\times10^2$	$7.50(3)\times10^2$	$1.3262(11)\times10^{-3}$	$1.3261(11)\times10^{-3}$	$1.3260(11)\times10^{-3}$
$10\,^2P \to 13\,^2S$	$1.779(5)\times10^2$	$1.779(5)\times10^2$	$1.778(5)\times10^2$	$6.397(10)\times10^{-4}$	$6.396(10)\times10^{-4}$	$6.393(10)\times10^{-4}$
$11\,^2S \to 11\,^2P$	$4.738(16)\times10^4$	$4.738(16)\times10^4$	$4.738(16)\times10^4$	$3.763(15)\times10^{-3}$	$3.763(15)\times10^{-3}$	$3.764(15)\times10^{-3}$
$11\,^2S \to 12\,^2P$	$7.5(6)\times10^1$	$7.5(6)\times10^1$	$7.6(6)\times10^1$	$6.9(2)\times10^{-5}$	$6.9(2)\times10^{-5}$	$6.9(2)\times10^{-5}$
$11\,^2S \to 13\,^2P$	4.07(10)	4.06(10)	4.02(10)	$9.07(6)\times10^{-6}$	$9.06(6)\times10^{-6}$	$9.01(6)\times10^{-6}$
$11\,^2P \to 12\,^2S$	$2.230(3)\times10^4$	$2.230(3)\times10^4$	$2.229(3)\times10^4$	$4.5611(19)\times10^{-3}$	$4.5612(19)\times10^{-3}$	$4.5620(19)\times10^{-3}$
$11\,^2P \to 13\,^2S$	$1.085(3)\times10^3$	$1.085(3)\times10^3$	$1.085(3)\times10^3$	$1.1239(19)\times10^{-3}$	$1.1238(19)\times10^{-3}$	$1.1232(19)\times10^{-3}$
$12\,^2S \to 12\,^2P$	$6.742(10)\times10^4$	$6.742(10)\times10^4$	$6.742(10)\times10^4$	$3.136(6)\times10^{-3}$	$3.136(6)\times10^{-3}$	$3.136(6)\times10^{-3}$
$12\,^2S \to 13\,^2P$	$1.1394(4)\times10^2$	$1.1382(4)\times10^2$	$1.1394(4)\times10^2$	$6.169(4)\times10^{-5}$	$6.166(4)\times10^{-5}$	$6.145(4)\times10^{-5}$
$12\,^2P \to 13\,^2S$	$3.156(9)\times10^4$	$3.156(9)\times10^4$	$3.156(9)\times10^4$	$3.8855(17)\times10^{-3}$	$3.8855(17)\times10^{-3}$	$3.8856(17)\times10^{-3}$
$13\,^2S \to 13\,^2P$	$9.340(5)\times10^4$	$9.340(5)\times10^4$	$9.340(5)\times10^4$	$2.6470(20)\times10^{-3}$	$2.6469(20)\times10^{-3}$	$2.6463(20)\times10^{-3}$

Table 12
Nonrelativistic oscillator strengths obtained using the length (f_{if}^L) and velocity (f_{if}^V) formalisms for the transitions involving ^2S and ^2P states of Li atom. The oscillator strength uncertainties (numbers in parentheses) are calculated as the root mean squares of the uncertainties of $|\mu_{if}|^2$ and ΔE, where ΔE is the difference between the non-relativistic energies of the initial (i) and final (f) states.

Transition	$f_{if}^V(^6\mathrm{Li})$	$f_{if}^L(^6\mathrm{Li})$	$f_{if}^V(^7\mathrm{Li})$	$f_{if}^L(^7\mathrm{Li})$	$f_{if}^V(^\infty\mathrm{Li})$	$f_{if}^L(^\infty\mathrm{Li})$
$2\,^2S \to 2\,^2P$	$7.4675827(2)\times10^{-1}$	$7.467582622(4)\times10^{-1}$	$7.4678659(2)\times10^{-1}$	$7.467865893(4)\times10^{-1}$	$7.4695679(2)\times10^{-1}$	$7.469568098(4)\times10^{-1}$
$2\,^2S \to 2\,^2P$ Ref. [47]				$7.467871(10)\times10^{-1}$	$7.469571(54)\times10^{-1}$	$7.469572(10)\times10^{-1}$
$2\,^2S \to 2\,^2P$ Ref. [108]				$7.46786698(97)\times10^{-1}$	$7.469597(50)\times10^{-1}$	$7.469569396(98)\times10^{-1}$
$2\,^2S \to 2\,^2P$ Ref. [127][a]		$7.467579(4)\times10^{-1}$		$7.467862(4)\times10^{-1}$		$7.469563(5)\times10^{-1}$
$2\,^2S \to 3\,^2P$	$4.736485(5)\times10^{-3}$	$4.7364865(14)\times10^{-3}$	$4.735577(5)\times10^{-3}$	$4.7355776(14)\times10^{-3}$	$4.730128(5)\times10^{-3}$	$4.7301186(14)\times10^{-3}$
$2\,^2S \to 3\,^2P$ Ref. [46]						$4.711\ \times10^{-3}$

(*continued on next page*)

Table 12 (*continued*).

Transition	f_{if}^{V}(^{6}Li)	f_{if}^{L}(^{6}Li)	f_{if}^{V}(^{7}Li)	f_{if}^{L}(^{7}Li)	f_{if}^{V}($^{\infty}$Li)	f_{if}^{L}($^{\infty}$Li)
$2\,^2S \to 4\,^2P$	$4.27128(2)\times10^{-3}$	$4.271283(2)\times10^{-3}$	$4.27086(2)\times10^{-3}$	$4.270855(2)\times10^{-3}$	$4.26831(2)\times10^{-3}$	$4.268281(2)\times10^{-3}$
$2\,^2S \to 4\,^2P$ Ref. [42]						$4.218\ \times10^{-3}$
$2\,^2S \to 5\,^2P$	$2.55668(2)\times10^{-3}$	$2.55668(2)\times10^{-3}$	$2.55647(2)\times10^{-3}$	$2.55647(2)\times10^{-3}$	$2.55524(2)\times10^{-3}$	$2.55522(2)\times10^{-3}$
$2\,^2S \to 5\,^2P$ Ref. [128]						$2.619\ \times10^{-3}$
$2\,^2S \to 6\,^2P$	$1.569476(6)\times10^{-3}$	$1.569483(6)\times10^{-3}$	$1.569363(6)\times10^{-3}$	$1.569368(6)\times10^{-3}$	$1.568688(6)\times10^{-3}$	$1.568673(6)\times10^{-3}$
$2\,^2S \to 6\,^2P$ Ref. [128]					$1.5796\ \times10^{-3}$	$1.58060\ \times10^{-3}$
$2\,^2S \to 7\,^2P$	$1.017053(6)\times10^{-3}$	$1.017061(6)\times10^{-3}$	$1.016986(6)\times10^{-3}$	$1.016990(6)\times10^{-3}$	$1.016585(6)\times10^{-3}$	$1.016566(6)\times10^{-3}$
$2\,^2S \to 7\,^2P$ Ref. [128]					$1.0114\ \times10^{-3}$	$1.0121\ \times10^{-3}$
$2\,^2S \to 8\,^2P$	$6.92337(10)\times10^{-4}$	$6.92341(8)\times10^{-4}$	$6.92293(10)\times10^{-4}$	$6.92295(8)\times10^{-4}$	$6.92028(10)\times10^{-4}$	$6.92016(8)\times10^{-4}$
$2\,^2S \to 8\,^2P$ Ref. [128]					$6.880\ \times10^{-4}$	$6.872\ \times10^{-4}$
$2\,^2S \to 9\,^2P$	$4.91042(18)\times10^{-4}$	$4.91046(8)\times10^{-4}$	$4.91012(18)\times10^{-4}$	$4.91013(8)\times10^{-4}$	$4.90827(18)\times10^{-4}$	$4.90817(8)\times10^{-4}$
$2\,^2S \to 9\,^2P$ Ref. [128]					$4.439\ \times10^{-4}$	$4.452\ \times10^{-4}$
$2\,^2S \to 10\,^2P$	$3.60276(7)\times10^{-4}$	$3.60276(8)\times10^{-4}$	$3.60250(7)\times10^{-4}$	$3.60250(8)\times10^{-4}$	$3.60097(7)\times10^{-4}$	$3.60097(8)\times10^{-4}$
$2\,^2S \to 11\,^2P$	$2.71886(10)\times10^{-4}$	$2.71882(6)\times10^{-4}$	$2.71861(10)\times10^{-4}$	$2.71858(6)\times10^{-4}$	$2.71713(10)\times10^{-4}$	$2.71714(6)\times10^{-4}$
$2\,^2S \to 12\,^2P$	$2.1011(3)\times10^{-4}$	$2.10089(7)\times10^{-4}$	$2.1009(3)\times10^{-4}$	$2.10070(7)\times10^{-4}$	$2.0996(3)\times10^{-4}$	$2.09953(7)\times10^{-4}$
$2\,^2S \to 13\,^2P$	$1.6584(8)\times10^{-4}$	$1.658898(3)\times10^{-4}$	$1.6580(8)\times10^{-4}$	$1.658498(3)\times10^{-4}$	$1.6555(8)\times10^{-4}$	$1.656101(3)\times10^{-4}$
$2\,^2P \to 3\,^2S$	$1.1052523(2)\times10^{-1}$	$1.10525238(10)\times10^{-1}$	$1.1053013(2)\times10^{-1}$	$1.10530139(10)\times10^{-1}$	$1.1055958(2)\times10^{-1}$	$1.105595845(10)\times10^{-1}$
$2\,^2P \to 3\,^2S$ Ref. [46]						$1.1050\ \times10^{-1}$
$2\,^2P \to 4\,^2S$	$1.2830331(6)\times10^{-2}$	$1.2830328(15)\times10^{-2}$	$1.2830739(6)\times10^{-2}$	$1.2830736(15)\times10^{-2}$	$1.2833188(6)\times10^{-2}$	$1.2833185(15)\times10^{-2}$
$2\,^2P \to 4\,^2S$ Ref. [46]						$1.283\ \times10^{-2}$
$2\,^2P \to 5\,^2S$	$4.315785(4)\times10^{-3}$	$4.315788(13)\times10^{-3}$	$4.315911(4)\times10^{-3}$	$4.315914(13)\times10^{-3}$	$4.316669(4)\times10^{-3}$	$4.316674(13)\times10^{-3}$
$2\,^2P \to 5\,^2S$ Ref. [129]						$4.34\ \times10^{-3}$
$2\,^2P \to 6\,^2S$	$2.034174(2)\times10^{-3}$	$2.034167(5)\times10^{-3}$	$2.034231(2)\times10^{-3}$	$2.034224(5)\times10^{-3}$	$2.034575(2)\times10^{-3}$	$2.034569(5)\times10^{-3}$
$2\,^2P \to 6\,^2S$ Ref. [129]						$2.05\ \times10^{-3}$
$2\,^2P \to 7\,^2S$	$1.136791(2)\times10^{-3}$	$1.136789(2)\times10^{-3}$	$1.136822(2)\times10^{-3}$	$1.136821(2)\times10^{-3}$	$1.137010(2)\times10^{-3}$	$1.137009(2)\times10^{-3}$
$2\,^2P \to 7\,^2S$ Ref. [129]						$1.15\ \times10^{-3}$
$2\,^2P \to 8\,^2S$	$7.05071(2)\times10^{-4}$	$7.05071(7)\times10^{-4}$	$7.05090(2)\times10^{-4}$	$7.05090(7)\times10^{-4}$	$7.05202(2)\times10^{-4}$	$7.05204(7)\times10^{-4}$
$2\,^2P \to 8\,^2S$ Ref. [129]						$7.11\ \times10^{-4}$
$2\,^2P \to 9\,^2S$	$4.69482(6)\times10^{-4}$	$4.69483(4)\times10^{-4}$	$4.69493(6)\times10^{-4}$	$4.69494(4)\times10^{-4}$	$4.69558(6)\times10^{-4}$	$4.69561(4)\times10^{-4}$
$2\,^2P \to 10\,^2S$	$3.29234(6)\times10^{-4}$	$3.29234(11)\times10^{-4}$	$3.29237(6)\times10^{-4}$	$3.29238(11)\times10^{-4}$	$3.29258(6)\times10^{-4}$	$3.29261(11)\times10^{-4}$
$2\,^2P \to 11\,^2S$	$2.403(3)\times10^{-4}$	$2.403(3)\times10^{-4}$	$2.402(3)\times10^{-4}$	$2.402(3)\times10^{-4}$	$2.402(3)\times10^{-4}$	$2.402(3)\times10^{-4}$
$2\,^2P \to 12\,^2S$	$1.8097(10)\times10^{-4}$	$1.811(4)\times10^{-4}$	$1.8095(10)\times10^{-4}$	$1.811(4)\times10^{-4}$	$1.8088(10)\times10^{-4}$	$1.811(4)\times10^{-4}$
$2\,^2P \to 13\,^2S$	$1.400(2)\times10^{-4}$	$1.400(2)\times10^{-4}$	$1.400(2)\times10^{-4}$	$1.400(2)\times10^{-4}$	$1.398(2)\times10^{-4}$	$1.399(2)\times10^{-4}$
$3\,^2S \to 3\,^2P$	1.2146322(5)	1.214632127(2)	1.2146754(5)	1.214675371(2)	1.2149346(5)	1.214935226(2)
$3\,^2S \to 3\,^2P$ Ref. [46]						1.215
$3\,^2S \to 4\,^2P$	$4.4237(12)\times10^{-5}$	$4.42388(2)\times10^{-5}$	$4.4127(12)\times10^{-5}$	$4.41269(2)\times10^{-5}$	$4.3468(12)\times10^{-5}$	$4.34578(2)\times10^{-5}$
$3\,^2S \to 4\,^2P$ Ref. [42]						$3.6\ \times10^{-5}$
$3\,^2S \to 5\,^2P$	$1.28831(6)\times10^{-3}$	$1.288319(4)\times10^{-3}$	$1.28801(6)\times10^{-3}$	$1.288006(4)\times10^{-3}$	$1.28618(6)\times10^{-3}$	$1.286124(4)\times10^{-3}$
$3\,^2S \to 5\,^2P$ Ref. [129]						$1.3\ \times10^{-3}$
$3\,^2S \to 6\,^2P$	$1.125387(11)\times10^{-3}$	$1.12540(2)\times10^{-3}$	$1.125207(11)\times10^{-3}$	$1.12521(2)\times10^{-3}$	$1.124124(11)\times10^{-3}$	$1.12407(2)\times10^{-3}$
$3\,^2S \to 6\,^2P$ Ref. [129]						$1.13\ \times10^{-3}$
$3\,^2S \to 7\,^2P$	$8.1982(5)\times10^{-4}$	$8.1982(6)\times10^{-4}$	$8.1972(5)\times10^{-4}$	$8.1970(6)\times10^{-4}$	$8.1906(5)\times10^{-4}$	$8.1900(6)\times10^{-4}$
$3\,^2S \to 7\,^2P$ Ref. [129]						$8.26\ \times10^{-4}$
$3\,^2S \to 8\,^2P$	$5.8887(3)\times10^{-4}$	$5.8885(5)\times10^{-4}$	$5.8880(3)\times10^{-4}$	$5.8877(5)\times10^{-4}$	$5.8837(3)\times10^{-4}$	$5.8831(5)\times10^{-4}$
$3\,^2S \to 8\,^2P$ Ref. [129]						$5.92\ \times10^{-4}$
$3\,^2S \to 9\,^2P$	$4.3006(4)\times10^{-4}$	$4.3008(4)\times10^{-4}$	$4.3001(4)\times10^{-4}$	$4.3002(4)\times10^{-4}$	$4.2972(4)\times10^{-4}$	$4.2971(4)\times10^{-4}$
$3\,^2S \to 10\,^2P$	$3.2122(4)\times10^{-4}$	$3.2123(4)\times10^{-4}$	$3.2118(4)\times10^{-4}$	$3.2119(4)\times10^{-4}$	$3.2095(4)\times10^{-4}$	$3.2095(4)\times10^{-4}$
$3\,^2S \to 11\,^2P$	$2.4525(3)\times10^{-4}$	$2.4527(2)\times10^{-4}$	$2.4522(3)\times10^{-4}$	$2.4524(2)\times10^{-4}$	$2.4504(3)\times10^{-4}$	$2.4504(2)\times10^{-4}$
$3\,^2S \to 12\,^2P$	$1.9098(6)\times10^{-4}$	$1.9107(3)\times10^{-4}$	$1.9096(6)\times10^{-4}$	$1.9105(3)\times10^{-4}$	$1.9082(6)\times10^{-4}$	$1.9088(3)\times10^{-4}$
$3\,^2S \to 13\,^2P$	$1.51547(7)\times10^{-4}$	$1.51735(2)\times10^{-4}$	$1.51504(7)\times10^{-4}$	$1.51692(2)\times10^{-4}$	$1.51250(7)\times10^{-4}$	$1.51434(2)\times10^{-4}$
$3\,^2P \to 4\,^2S$	$2.231340(3)\times10^{-1}$	$2.231339450(13)\times10^{-1}$	$2.231432(3)\times10^{-1}$	$2.231432595(13)\times10^{-1}$	$2.231989(3)\times10^{-1}$	$2.231992310(13)\times10^{-1}$
$3\,^2P \to 4\,^2S$ Ref. [46]						$2.230\ \times10^{-1}$
$3\,^2P \to 5\,^2S$	$2.592359(2)\times10^{-2}$	$2.5923581(14)\times10^{-2}$	$2.592430(2)\times10^{-2}$	$2.5924296(14)\times10^{-2}$	$2.592860(2)\times10^{-2}$	$2.5928593(14)\times10^{-2}$
$3\,^2P \to 5\,^2S$ Ref. [129]						$2.60\ \times10^{-2}$
$3\,^2P \to 6\,^2S$	$8.85810(3)\times10^{-3}$	$8.85810(3)\times10^{-3}$	$8.85832(3)\times10^{-3}$	$8.85832(3)\times10^{-3}$	$8.85965(3)\times10^{-3}$	$8.85964(3)\times10^{-3}$
$3\,^2P \to 6\,^2S$ Ref. [129]						$8.88\ \times10^{-3}$
$3\,^2P \to 7\,^2S$	$4.257124(10)\times10^{-3}$	$4.257123(13)\times10^{-3}$	$4.257224(10)\times10^{-3}$	$4.257222(13)\times10^{-3}$	$4.257826(10)\times10^{-3}$	$4.257813(13)\times10^{-3}$
$3\,^2P \to 7\,^2S$ Ref. [129]						$4.27\ \times10^{-3}$
$3\,^2P \to 8\,^2S$	$2.425125(7)\times10^{-3}$	$2.42513(2)\times10^{-3}$	$2.425179(7)\times10^{-3}$	$2.42518(2)\times10^{-3}$	$2.425503(7)\times10^{-3}$	$2.42550(2)\times10^{-3}$
$3\,^2P \to 8\,^2S$ Ref. [129]						$2.44\ \times10^{-3}$
$3\,^2P \to 9\,^2S$	$1.53097(1)\times10^{-3}$	$1.530978(13)\times10^{-3}$	$1.53100(1)\times10^{-3}$	$1.531006(13)\times10^{-3}$	$1.53117(1)\times10^{-3}$	$1.531178(13)\times10^{-3}$
$3\,^2P \to 10\,^2S$	$1.03581(3)\times10^{-3}$	$1.03581(4)\times10^{-3}$	$1.03581(3)\times10^{-3}$	$1.03582(4)\times10^{-3}$	$1.03585(3)\times10^{-3}$	$1.03586(4)\times10^{-3}$
$3\,^2P \to 11\,^2S$	$7.369(8)\times10^{-4}$	$7.369(9)\times10^{-4}$	$7.369(8)\times10^{-4}$	$7.369(9)\times10^{-4}$	$7.367(8)\times10^{-4}$	$7.367(9)\times10^{-4}$

(*continued on next page*)

experimental data. Some of the Rydberg states we considered were investigated for the first time at this level of accuracy. The transition energies and the corresponding oscillator strengths were calculated for the $S \to P$ and $P \to S$ transitions of the two stable lithium isotopes (^{6}Li and ^{7}Li), as well as for $^{\infty}$Li. We found that the calculated transition energies are in very good agreement with the latest accurate experimental and theoretical studies. The calculated oscillator strengths show an certain pattern, in which. they have the largest value for the $n\,^2S \to n\,^2P$ and $n\,^2P \to (n+1)\,^2S$ transitions. One could envision preparing a lithium atom in a particular excited Rydberg state using a cascade of excitations, e.g. $2\,^2S \to 2\,^2P$, $2\,^2P \to 3\,^2S$, $3\,^2S \to 3\,^2P, \ldots$. The data obtained in this work may be employed in modeling of light emission and absorption events involving lithium atoms in the

Table 12 (*continued*).

Transition	$f_{if}^{V}(^{6}\mathrm{Li})$	$f_{if}^{L}(^{6}\mathrm{Li})$	$f_{if}^{V}(^{7}\mathrm{Li})$	$f_{if}^{L}(^{7}\mathrm{Li})$	$f_{if}^{V}(^{\infty}\mathrm{Li})$	$f_{if}^{L}(^{\infty}\mathrm{Li})$
$3\,^2P \to 12\,^2S$	$5.448(3)\times10^{-4}$	$5.43(4)\times10^{-4}$	$5.447(3)\times10^{-4}$	$5.43(4)\times10^{-4}$	$5.445(3)\times10^{-4}$	$5.43(4)\times10^{-4}$
$3\,^2P \to 13\,^2S$	$4.155(9)\times10^{-4}$	$4.155(8)\times10^{-4}$	$4.155(9)\times10^{-4}$	$4.155(8)\times10^{-4}$	$4.151(9)\times10^{-4}$	$4.152(8)\times10^{-4}$
$4\,^2S \to 4\,^2P$	1.640384(5)	1.64038365(2)	1.640441(5)	1.64044053(2)	1.640779(5)	1.64078232(2)
$4\,^2S \to 4\,^2P$ Ref. [42]						1.643
$4\,^2S \to 5\,^2P$	$9.7937(10)\times10^{-4}$	$9.79347(2)\times10^{-4}$	$9.7996(10)\times10^{-4}$	$9.79957(2)\times10^{-4}$	$9.8353(10)\times10^{-4}$	$9.83624(2)\times10^{-4}$
$4\,^2S \to 5\,^2P$ Ref. [129]						$9.52\ \times10^{-4}$
$4\,^2S \to 6\,^2P$	$2.81780(13)\times10^{-4}$	$2.81790(5)\times10^{-4}$	$2.81615(13)\times10^{-4}$	$2.81617(5)\times10^{-4}$	$2.80630(13)\times10^{-4}$	$2.80579(5)\times10^{-4}$
$4\,^2S \to 6\,^2P$ Ref. [129]						$2.91\ \times10^{-4}$
$4\,^2S \to 7\,^2P$	$4.78180(4)\times10^{-4}$	$4.7820(5)\times10^{-4}$	$4.78044(4)\times10^{-4}$	$4.7805(5)\times10^{-4}$	$4.77224(4)\times10^{-4}$	$4.7717(5)\times10^{-4}$
$4\,^2S \to 7\,^2P$ Ref. [129]						$4.85\ \times10^{-4}$
$4\,^2S \to 8\,^2P$	$4.3051(4)\times10^{-4}$	$4.3046(10)\times10^{-4}$	$4.3042(4)\times10^{-4}$	$4.3035(10)\times10^{-4}$	$4.2985(4)\times10^{-4}$	$4.2975(10)\times10^{-4}$
$4\,^2S \to 8\,^2P$ Ref. [129]						$4.36\ \times10^{-4}$
$4\,^2S \to 9\,^2P$	$3.459(2)\times10^{-4}$	$3.45893(18)\times10^{-4}$	$3.458(2)\times10^{-4}$	$3.45821(18)\times10^{-4}$	$3.454(2)\times10^{-4}$	$3.45386(18)\times10^{-4}$
$4\,^2S \to 10\,^2P$	$2.7143(4)\times10^{-4}$	$2.71504(10)\times10^{-4}$	$2.7138(4)\times10^{-4}$	$2.71450(10)\times10^{-4}$	$2.7109(4)\times10^{-4}$	$2.71126(10)\times10^{-4}$
$4\,^2S \to 11\,^2P$	$2.1332(8)\times10^{-4}$	$2.1343(2)\times10^{-4}$	$2.1329(8)\times10^{-4}$	$2.1338(2)\times10^{-4}$	$2.1308(8)\times10^{-4}$	$2.1312(2)\times10^{-4}$
$4\,^2S \to 12\,^2P$	$1.6921(4)\times10^{-4}$	$1.6938(2)\times10^{-4}$	$1.6918(4)\times10^{-4}$	$1.6935(2)\times10^{-4}$	$1.6903(4)\times10^{-4}$	$1.6914(2)\times10^{-4}$
$4\,^2S \to 13\,^2P$	$1.3600(3)\times10^{-4}$	$1.3617(4)\times10^{-4}$	$1.3596(3)\times10^{-4}$	$1.3613(4)\times10^{-4}$	$1.3569(3)\times10^{-4}$	$1.3585(4)\times10^{-4}$
$4\,^2P \to 5\,^2S$	$3.357429(14)\times10^{-1}$	$3.3574320(2)\times10^{-1}$	$3.357568(14)\times10^{-1}$	$3.3575682(2)\times10^{-1}$	$3.358401(14)\times10^{-1}$	$3.3583861(2)\times10^{-1}$
$4\,^2P \to 5\,^2S$ Ref. [129]						$3.35\ \times10^{-1}$
$4\,^2P \to 6\,^2S$	$3.86087(3)\times10^{-2}$	$3.860876(2)\times10^{-2}$	$3.86098(3)\times10^{-2}$	$3.860974(2)\times10^{-2}$	$3.86160(3)\times10^{-2}$	$3.861567(2)\times10^{-2}$
$4\,^2P \to 6\,^2S$ Ref. [129]						$3.87\ \times10^{-2}$
$4\,^2P \to 7\,^2S$	$1.323341(11)\times10^{-2}$	$1.32334(1)\times10^{-2}$	$1.323371(11)\times10^{-2}$	$1.32337(1)\times10^{-2}$	$1.323555(11)\times10^{-2}$	$1.32355(1)\times10^{-2}$
$4\,^2P \to 7\,^2S$ Ref. [129]						$1.33\ \times10^{-2}$
$4\,^2P \to 8\,^2S$	$6.40992(5)\times10^{-3}$	$6.4099(3)\times10^{-3}$	$6.41005(5)\times10^{-3}$	$6.4100(3)\times10^{-3}$	$6.41087(5)\times10^{-3}$	$6.4108(3)\times10^{-3}$
$4\,^2P \to 8\,^2S$ Ref. [129]						$6.42\ \times10^{-3}$
$4\,^2P \to 9\,^2S$	$3.68604(3)\times10^{-3}$	$3.6860(3)\times10^{-3}$	$3.68611(3)\times10^{-3}$	$3.6861(3)\times10^{-3}$	$3.68650(3)\times10^{-3}$	$3.6864(3)\times10^{-3}$
$4\,^2P \to 10\,^2S$	$2.34967(7)\times10^{-3}$	$2.3498(1)\times10^{-3}$	$2.34968(7)\times10^{-3}$	$2.3498(1)\times10^{-3}$	$2.34975(7)\times10^{-3}$	$2.3499(1)\times10^{-3}$
$4\,^2P \to 11\,^2S$	$1.605(2)\times10^{-3}$	$1.605(2)\times10^{-3}$	$1.605(2)\times10^{-3}$	$1.605(2)\times10^{-3}$	$1.604(2)\times10^{-3}$	$1.605(2)\times10^{-3}$
$4\,^2P \to 12\,^2S$	$1.1523(7)\times10^{-3}$	$1.158(14)\times10^{-3}$	$1.1522(7)\times10^{-3}$	$1.157(14)\times10^{-3}$	$1.1516(7)\times10^{-3}$	$1.159(14)\times10^{-3}$
$4\,^2P \to 13\,^2S$	$8.60(2)\times10^{-4}$	$8.601(16)\times10^{-4}$	$8.60(2)\times10^{-4}$	$8.600(16)\times10^{-4}$	$8.59(2)\times10^{-4}$	$8.593(16)\times10^{-4}$
$5\,^2S \to 5\,^2P$	2.052149(4)	2.05214715(12)	2.052218(4)	2.05221721(12)	2.052631(4)	2.05263818(12)
$5\,^2S \to 5\,^2P$ Ref. [129]						2.05
$5\,^2S \to 6\,^2P$	$3.47224(11)\times10^{-3}$	$3.47216(7)\times10^{-3}$	$3.47347(11)\times10^{-3}$	$3.47344(7)\times10^{-3}$	$3.48083(11)\times10^{-3}$	$3.48111(7)\times10^{-3}$
$5\,^2S \to 6\,^2P$ Ref. [129]						$3.42\ \times10^{-3}$
$5\,^2S \to 7\,^2P$	$7.2986(8)\times10^{-6}$	$7.3030(12)\times10^{-6}$	$7.2695(8)\times10^{-6}$	$7.2716(12)\times10^{-6}$	$7.0960(8)\times10^{-6}$	$7.0846(12)\times10^{-6}$
$5\,^2S \to 8\,^2P$	$1.6947(6)\times10^{-4}$	$1.6951(12)\times10^{-4}$	$1.6938(6)\times10^{-4}$	$1.6941(12)\times10^{-4}$	$1.6884(6)\times10^{-4}$	$1.6881(12)\times10^{-4}$
$5\,^2S \to 8\,^2P$ Ref. [129]						$1.75\ \times10^{-4}$
$5\,^2S \to 9\,^2P$	$2.1354(15)\times10^{-4}$	$2.1376(14)\times10^{-4}$	$2.1347(15)\times10^{-4}$	$2.1367(14)\times10^{-4}$	$2.1307(15)\times10^{-4}$	$2.1318(14)\times10^{-4}$
$5\,^2S \to 10\,^2P$	$1.9828(2)\times10^{-4}$	$1.985(11)\times10^{-4}$	$1.9823(2)\times10^{-4}$	$1.984(11)\times10^{-4}$	$1.9792(2)\times10^{-4}$	$1.980(11)\times10^{-4}$
$5\,^2S \to 11\,^2P$	$1.6925(3)\times10^{-4}$	$1.689(5)\times10^{-4}$	$1.6921(3)\times10^{-4}$	$1.689(5)\times10^{-4}$	$1.6897(3)\times10^{-4}$	$1.686(5)\times10^{-4}$
$5\,^2S \to 12\,^2P$	$1.4071(5)\times10^{-4}$	$1.4050(2)\times10^{-4}$	$1.4068(5)\times10^{-4}$	$1.405(2)\times10^{-4}$	$1.4050(5)\times10^{-4}$	$1.402(2)\times10^{-4}$
$5\,^2S \to 13\,^2P$	$1.1642(7)\times10^{-4}$	$1.163(3)\times10^{-4}$	$1.1637(7)\times10^{-4}$	$1.163(3)\times10^{-4}$	$1.1610(7)\times10^{-4}$	$1.160(3)\times10^{-4}$
$5\,^2P \to 6\,^2S$	$4.482040(11)\times10^{-1}$	$4.4820438(13)\times10^{-1}$	$4.482222(11)\times10^{-1}$	$4.4822223(13)\times10^{-1}$	$4.483316(11)\times10^{-1}$	$4.4832949(13)\times10^{-1}$
$5\,^2P \to 6\,^2S$ Ref. [129]						$4.49\ \times10^{-1}$
$5\,^2P \to 7\,^2S$	$5.09768(3)\times10^{-2}$	$5.097687(6)\times10^{-2}$	$5.09781(3)\times10^{-2}$	$5.097811(6)\times10^{-2}$	$5.09858(3)\times10^{-2}$	$5.098555(6)\times10^{-2}$
$5\,^2P \to 7\,^2S$ Ref. [129]						$5.11\ \times10^{-2}$
$5\,^2P \to 8\,^2S$	$1.745417(8)\times10^{-2}$	$1.74542(4)\times10^{-2}$	$1.745454(8)\times10^{-2}$	$1.74546(4)\times10^{-2}$	$1.745677(8)\times10^{-2}$	$1.74566(4)\times10^{-2}$
$5\,^2P \to 8\,^2S$ Ref. [129]						$1.75\ \times10^{-2}$
$5\,^2P \to 9\,^2S$	$8.47962(10)\times10^{-3}$	$8.47978(11)\times10^{-3}$	$8.47976(10)\times10^{-3}$	$8.47993(11)\times10^{-3}$	$8.48061(10)\times10^{-3}$	$8.48087(11)\times10^{-3}$
$5\,^2P \to 10\,^2S$	$4.89967(11)\times10^{-3}$	$4.8996(13)\times10^{-3}$	$4.89969(11)\times10^{-3}$	$4.8996(13)\times10^{-3}$	$4.89980(11)\times10^{-3}$	$4.8998(13)\times10^{-3}$
$5\,^2P \to 11\,^2S$	$3.141(4)\times10^{-3}$	$3.141(4)\times10^{-3}$	$3.141(4)\times10^{-3}$	$3.141(4)\times10^{-3}$	$3.140(4)\times10^{-3}$	$3.140(4)\times10^{-3}$
$5\,^2P \to 12\,^2S$	$2.1589(7)\times10^{-3}$	$2.15(3)\times10^{-3}$	$2.1587(7)\times10^{-3}$	$2.15(3)\times10^{-3}$	$2.1577(7)\times10^{-3}$	$2.14(3)\times10^{-3}$
$5\,^2P \to 13\,^2S$	$1.561(3)\times10^{-3}$	$1.561(4)\times10^{-3}$	$1.561(3)\times10^{-3}$	$1.561(4)\times10^{-3}$	$1.559(3)\times10^{-3}$	$1.560(4)\times10^{-3}$
$6\,^2S \to 6\,^2P$	2.457447(13)	2.4574403(9)	2.457526(13)	2.4575233(9)	2.458004(13)	2.4580223(9)
$6\,^2S \to 6\,^2P$ Ref. [129]						2.46
$6\,^2S \to 7\,^2P$	$6.5544(2)\times10^{-3}$	$6.5540(2)\times10^{-3}$	$6.5562(2)\times10^{-3}$	$6.5560(2)\times10^{-3}$	$6.5668(2)\times10^{-3}$	$6.5675(2)\times10^{-3}$
$6\,^2S \to 7\,^2P$ Ref. [129]						$6.46\ \times10^{-3}$
$6\,^2S \to 8\,^2P$	$7.173(5)\times10^{-5}$	$7.171(2)\times10^{-5}$	$7.183(5)\times10^{-5}$	$7.182(2)\times10^{-5}$	$7.241(5)\times10^{-5}$	$7.247(2)\times10^{-5}$
$6\,^2S \to 9\,^2P$	$3.490(7)\times10^{-5}$	$3.493(8)\times10^{-5}$	$3.486(7)\times10^{-5}$	$3.489(8)\times10^{-5}$	$3.463(7)\times10^{-5}$	$3.460(8)\times10^{-5}$
$6\,^2S \to 10\,^2P$	$9.235(4)\times10^{-5}$	$9.25(7)\times10^{-5}$	$9.230(4)\times10^{-5}$	$9.25(7)\times10^{-5}$	$9.201(4)\times10^{-5}$	$9.21(7)\times10^{-5}$
$6\,^2S \to 11\,^2P$	$1.0696(5)\times10^{-4}$	$1.075(3)\times10^{-4}$	$1.0691(5)\times10^{-4}$	$1.074(3)\times10^{-4}$	$1.0666(5)\times10^{-4}$	$1.071(3)\times10^{-4}$
$6\,^2S \to 12\,^2P$	$1.0198(3)\times10^{-4}$	$1.023(5)\times10^{-4}$	$1.0194(3)\times10^{-4}$	$1.022(5)\times10^{-4}$	$1.0174(3)\times10^{-4}$	$1.020(5)\times10^{-4}$
$6\,^2S \to 13\,^2P$	$9.084(8)\times10^{-5}$	$9.09(5)\times10^{-5}$	$9.080(8)\times10^{-5}$	$9.08(5)\times10^{-5}$	$9.053(8)\times10^{-5}$	$9.06(5)\times10^{-5}$
$6\,^2P \to 7\,^2S$	$5.60538(5)\times10^{-1}$	$5.60537(3)\times10^{-1}$	$5.60560(5)\times10^{-1}$	$5.60560(3)\times10^{-1}$	$5.60691(5)\times10^{-1}$	$5.60692(3)\times10^{-1}$
$6\,^2P \to 7\,^2S$ Ref. [129]						$5.61\ \times10^{-1}$
$6\,^2P \to 8\,^2S$	$6.31279(3)\times10^{-2}$	$6.312800(18)\times10^{-2}$	$6.31293(3)\times10^{-2}$	$6.312943(18)\times10^{-2}$	$6.31381(3)\times10^{-2}$	$6.313807(18)\times10^{-2}$
$6\,^2P \to 8\,^2S$ Ref. [129]						$6.32\ \times10^{-2}$
$6\,^2P \to 9\,^2S$	$2.15614(2)\times10^{-2}$	$2.15612(5)\times10^{-2}$	$2.15617(2)\times10^{-2}$	$2.15616(5)\times10^{-2}$	$2.15638(2)\times10^{-2}$	$2.15641(5)\times10^{-2}$
$6\,^2P \to 10\,^2S$	$1.04830(11)\times10^{-2}$	$1.0483(2)\times10^{-2}$	$1.04830(11)\times10^{-2}$	$1.0483(2)\times10^{-2}$	$1.04832(11)\times10^{-2}$	$1.0484(2)\times10^{-2}$
$6\,^2P \to 11\,^2S$	$6.073(7)\times10^{-3}$	$6.075(6)\times10^{-3}$	$6.072(7)\times10^{-3}$	$6.074(6)\times10^{-3}$	$6.071(7)\times10^{-3}$	$6.073(6)\times10^{-3}$

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Table 12 (*continued*).

Transition	$f_{if}^{V}(^{6}\mathrm{Li})$	$f_{if}^{L}(^{6}\mathrm{Li})$	$f_{if}^{V}(^{7}\mathrm{Li})$	$f_{if}^{L}(^{7}\mathrm{Li})$	$f_{if}^{V}(^{\infty}\mathrm{Li})$	$f_{if}^{L}(^{\infty}\mathrm{Li})$
$6\,^2P \to 12\,^2S$	$3.906(2)\times10^{-3}$	$3.93(7)\times10^{-3}$	$3.906(2)\times10^{-3}$	$3.93(7)\times10^{-3}$	$3.904(2)\times10^{-3}$	$3.94(7)\times10^{-3}$
$6\,^2P \to 13\,^2S$	$2.698(5)\times10^{-3}$	$2.6972(5)\times10^{-3}$	$2.697(5)\times10^{-3}$	$2.6969(5)\times10^{-3}$	$2.695(5)\times10^{-3}$	$2.6949(5)\times10^{-3}$
$7\,^2S \to 7\,^2P$	2.85922(7)	2.859194(19)	2.85931(7)	2.859290(19)	2.85983(7)	2.859867(19)
$7\,^2S \to 7\,^2P$ Ref. [129]						2.86
$7\,^2S \to 8\,^2P$	$9.9030(3)\times10^{-3}$	$9.9015(6)\times10^{-3}$	$9.9051(3)\times10^{-3}$	$9.9041(6)\times10^{-3}$	$9.9179(3)\times10^{-3}$	$9.9195(6)\times10^{-3}$
$7\,^2S \to 8\,^2P$ Ref. [129]						$9.80\ \times10^{-3}$
$7\,^2S \to 9\,^2P$	$3.158(2)\times10^{-4}$	$3.1547(11)\times10^{-4}$	$3.160(2)\times10^{-4}$	$3.1571(11)\times10^{-4}$	$3.171(2)\times10^{-4}$	$3.1721(11)\times10^{-4}$
$7\,^2S \to 10\,^2P$	$1(6)\times10^{-9}$	$1(9)\times10^{-9}$	$1(6)\times10^{-9}$	$2(9)\times10^{-9}$	$3(6)\times10^{-9}$	$3(9)\times10^{-9}$
$7\,^2S \to 11\,^2P$	$2.90(2)\times10^{-5}$	$2.95(16)\times10^{-5}$	$2.90(2)\times10^{-5}$	$2.94(16)\times10^{-5}$	$2.88(2)\times10^{-5}$	$2.93(16)\times10^{-5}$
$7\,^2S \to 12\,^2P$	$5.12(2)\times10^{-5}$	$5.18(16)\times10^{-5}$	$5.12(2)\times10^{-5}$	$5.17(16)\times10^{-5}$	$5.10(2)\times10^{-5}$	$5.15(16)\times10^{-5}$
$7\,^2S \to 13\,^2P$	$5.763(12)\times10^{-5}$	$5.76(8)\times10^{-5}$	$5.759(12)\times10^{-5}$	$5.76(8)\times10^{-5}$	$5.735(12)\times10^{-5}$	$5.73(8)\times10^{-5}$
$7\,^2P \to 8\,^2S$	$6.72775(4)\times10^{-1}$	$6.72774(6)\times10^{-1}$	$6.72800(4)\times10^{-1}$	$6.72800(6)\times10^{-1}$	$6.72954(4)\times10^{-1}$	$6.72958(6)\times10^{-1}$
$7\,^2P \to 8\,^2S$ Ref. [129]						$6.74\ \times10^{-1}$
$7\,^2P \to 9\,^2S$	$7.51295(12)\times10^{-2}$	$7.51299(17)\times10^{-2}$	$7.51309(12)\times10^{-2}$	$7.51316(17)\times10^{-2}$	$7.51393(12)\times10^{-2}$	$7.51412(17)\times10^{-2}$
$7\,^2P \to 10\,^2S$	$2.55870(5)\times10^{-2}$	$2.5587(3)\times10^{-2}$	$2.55871(5)\times10^{-2}$	$2.5588(3)\times10^{-2}$	$2.55876(5)\times10^{-2}$	$2.5589(3)\times10^{-2}$
$7\,^2P \to 11\,^2S$	$1.2438(14)\times10^{-2}$	$1.244(2)\times10^{-2}$	$1.2438(14)\times10^{-2}$	$1.244(2)\times10^{-2}$	$1.2434(14)\times10^{-2}$	$1.244(2)\times10^{-2}$
$7\,^2P \to 12\,^2S$	$7.216(4)\times10^{-3}$	$7.18(11)\times10^{-3}$	$7.215(4)\times10^{-3}$	$7.18(11)\times10^{-3}$	$7.212(4)\times10^{-3}$	$7.16(11)\times10^{-3}$
$7\,^2P \to 13\,^2S$	$4.655(7)\times10^{-3}$	$4.6564(36)\times10^{-3}$	$4.655(7)\times10^{-3}$	$4.6558(36)\times10^{-3}$	$4.651(7)\times10^{-3}$	$4.6527(36)\times10^{-3}$
$8\,^2S \to 8\,^2P$	3.258873(12)	3.258796(14)	3.258963(12)	3.258906(14)	3.259505(12)	3.259564(14)
$8\,^2S \to 8\,^2P$ Ref. [129]						3.26
$8\,^2S \to 9\,^2P$	$1.339(2)\times10^{-2}$	$1.33833(19)\times10^{-2}$	$1.339(2)\times10^{-2}$	$1.33865(19)\times10^{-2}$	$1.340(2)\times10^{-2}$	$1.34059(19)\times10^{-2}$
$8\,^2S \to 10\,^2P$	$6.6399(5)\times10^{-4}$	$6.634(5)\times10^{-4}$	$6.6426(5)\times10^{-4}$	$6.637(5)\times10^{-4}$	$6.6593(5)\times10^{-4}$	$6.659(5)\times10^{-4}$
$8\,^2S \to 11\,^2P$	$2.649(5)\times10^{-5}$	$2.63(7)\times10^{-5}$	$2.653(5)\times10^{-5}$	$2.63(7)\times10^{-5}$	$2.678(5)\times10^{-5}$	$2.65(7)\times10^{-5}$
$8\,^2S \to 12\,^2P$	$3.01(3)\times10^{-6}$	$3.21(9)\times10^{-6}$	$3.00(3)\times10^{-6}$	$3.20(9)\times10^{-6}$	$2.94(3)\times10^{-6}$	$3.15(9)\times10^{-6}$
$8\,^2S \to 13\,^2P$	$1.91(2)\times10^{-5}$	$1.90(5)\times10^{-5}$	$1.90(2)\times10^{-5}$	$1.90(5)\times10^{-5}$	$1.89(2)\times10^{-5}$	$1.88(5)\times10^{-5}$
$8\,^2P \to 9\,^2S$	$7.84941(13)\times10^{-1}$	$7.84939(8)\times10^{-1}$	$7.84969(13)\times10^{-1}$	$7.84969(8)\times10^{-1}$	$7.85136(13)\times10^{-1}$	$7.85150(8)\times10^{-1}$
$8\,^2P \to 10\,^2S$	$8.7026(9)\times10^{-2}$	$8.7028(4)\times10^{-2}$	$8.7026(9)\times10^{-2}$	$8.7029(4)\times10^{-2}$	$8.7031(9)\times10^{-2}$	$8.7038(4)\times10^{-2}$
$8\,^2P \to 11\,^2S$	$2.956(3)\times10^{-2}$	$2.956(4)\times10^{-2}$	$2.956(3)\times10^{-2}$	$2.956(4)\times10^{-2}$	$2.955(3)\times10^{-2}$	$2.956(4)\times10^{-2}$
$8\,^2P \to 12\,^2S$	$1.4359(9)\times10^{-2}$	$1.442(18)\times10^{-2}$	$1.4358(9)\times10^{-2}$	$1.442(18)\times10^{-2}$	$1.4351(9)\times10^{-2}$	$1.444(18)\times10^{-2}$
$8\,^2P \to 13\,^2S$	$8.341(13)\times10^{-3}$	$8.342(5)\times10^{-3}$	$8.340(13)\times10^{-3}$	$8.341(5)\times10^{-3}$	$8.334(13)\times10^{-3}$	$8.335(5)\times10^{-3}$
$9\,^2S \to 9\,^2P$	3.65721(8)	3.65700(5)	3.65729(8)	3.65713(5)	3.65772(8)	3.65789(5)
$9\,^2S \to 10\,^2P$	$1.6944(3)\times10^{-2}$	$1.6937(2)\times10^{-2}$	$1.6946(3)\times10^{-2}$	$1.6941(2)\times10^{-2}$	$1.6959(3)\times10^{-2}$	$1.6966(2)\times10^{-2}$
$9\,^2S \to 11\,^2P$	$1.0776(12)\times10^{-3}$	$1.076(2)\times10^{-3}$	$1.0778(12)\times10^{-3}$	$1.076(2)\times10^{-3}$	$1.0794(12)\times10^{-3}$	$1.077(2)\times10^{-3}$
$9\,^2S \to 12\,^2P$	$9.33(2)\times10^{-5}$	$9.25(10)\times10^{-5}$	$9.33(2)\times10^{-5}$	$9.24(10)\times10^{-5}$	$9.37(2)\times10^{-5}$	$9.20(10)\times10^{-5}$
$9\,^2S \to 13\,^2P$	$2.32(8)\times10^{-6}$	$2.06(16)\times10^{-6}$	$2.33(8)\times10^{-6}$	$2.06(16)\times10^{-6}$	$2.40(8)\times10^{-6}$	$2.05(16)\times10^{-6}$
$9\,^2P \to 10\,^2S$	$8.9704(3)\times10^{-1}$	$8.9705(3)\times10^{-1}$	$8.9707(3)\times10^{-1}$	$8.9708(3)\times10^{-1}$	$8.9722(3)\times10^{-1}$	$8.9728(3)\times10^{-1}$
$9\,^2P \to 11\,^2S$	$9.886(10)\times10^{-2}$	$9.888(13)\times10^{-2}$	$9.886(10)\times10^{-2}$	$9.889(13)\times10^{-2}$	$9.884(10)\times10^{-2}$	$9.889(13)\times10^{-2}$
$9\,^2P \to 12\,^2S$	$3.350(2)\times10^{-2}$	$3.34(3)\times10^{-2}$	$3.349(2)\times10^{-2}$	$3.34(3)\times10^{-2}$	$3.348(2)\times10^{-2}$	$3.34(3)\times10^{-2}$
$9\,^2P \to 13\,^2S$	$1.627(3)\times10^{-2}$	$1.628(2)\times10^{-2}$	$1.627(3)\times10^{-2}$	$1.628(2)\times10^{-2}$	$1.626(3)\times10^{-2}$	$1.627(2)\times10^{-2}$
$10\,^2S \to 10\,^2P$	4.0545(2)	4.0542(2)	4.0545(2)	4.0544(2)	4.0548(2)	4.0553(2)
$10\,^2S \to 11\,^2P$	$2.054(3)\times10^{-2}$	$2.052(2)\times10^{-2}$	$2.055(3)\times10^{-2}$	$2.053(2)\times10^{-2}$	$2.055(3)\times10^{-2}$	$2.056(2)\times10^{-2}$
$10\,^2S \to 12\,^2P$	$1.54(2)\times10^{-3}$	$1.526(9)\times10^{-3}$	$1.54(2)\times10^{-3}$	$1.526(9)\times10^{-3}$	$1.53(2)\times10^{-3}$	$1.525(9)\times10^{-3}$
$10\,^2S \to 13\,^2P$	$1.90(2)\times10^{-4}$	$1.906(6)\times10^{-4}$	$1.90(2)\times10^{-4}$	$1.899(6)\times10^{-4}$	$1.90(2)\times10^{-4}$	$1.857(6)\times10^{-4}$
$10\,^2P \to 11\,^2S$	1.0089(9)	1.009(2)	1.0089(9)	1.009(2)	1.0089(9)	1.009(2)
$10\,^2P \to 12\,^2S$	$1.1067(9)\times10^{-1}$	$1.109(4)\times10^{-1}$	$1.1066(9)\times10^{-1}$	$1.109(4)\times10^{-1}$	$1.1061(9)\times10^{-1}$	$1.110(4)\times10^{-1}$
$10\,^2P \to 13\,^2S$	$3.74(6)\times10^{-2}$	$3.753(11)\times10^{-2}$	$3.74(6)\times10^{-2}$	$3.752(11)\times10^{-1}$	$3.74(6)\times10^{-2}$	$3.752(11)\times10^{-2}$
$11\,^2S \to 11\,^2P$	4.452(19)	4.450(17)	4.451(19)	4.450(17)	4.450(19)	4.452(17)
$11\,^2S \to 12\,^2P$	$2.41(8)\times10^{-2}$	$2.4(2)\times10^{-2}$	$2.41(8)\times10^{-2}$	$2.4(2)\times10^{-2}$	$2.41(8)\times10^{-2}$	$2.4(2)\times10^{-2}$
$11\,^2S \to 13\,^2P$	$2.06(1)\times10^{-3}$	$1.99(5)\times10^{-3}$	$2.05(1)\times10^{-3}$	$1.99(5)\times10^{-3}$	$2.04(1)\times10^{-3}$	$1.97(5)\times10^{-3}$
$11\,^2P \to 12\,^2S$	1.1206(7)	1.120(2)	1.1205(7)	1.121(2)	1.1203(7)	1.121(2)
$11\,^2P \to 13\,^2S$	$1.225(2)\times10^{-1}$	$1.229(4)\times10^{-1}$	$1.225(2)\times10^{-1}$	$1.229(4)\times10^{-1}$	$1.224(2)\times10^{-1}$	$1.230(4)\times10^{-1}$
$12\,^2S \to 12\,^2P$	4.845(10)	4.848(9)	4.846(10)	4.848(9)	4.845(10)	4.848(9)
$12\,^2S \to 13\,^2P$	$2.794(2)\times10^{-2}$	$2.7949(9)\times10^{-2}$	$2.793(2)\times10^{-2}$	$2.7922(9)\times10^{-2}$	$2.783(2)\times10^{-2}$	$2.7957(9)\times10^{-2}$
$12\,^2P \to 13\,^2S$	1.2288(15)	1.232(4)	1.2288(15)	1.232(4)	1.2285(15)	1.232(4)
$13\,^2S \to 13\,^2P$	5.225(4)	5.257(3)	5.224(4)	5.258(3)	5.221(4)	5.260(3)

[a]In that work definition of the oscillator strength differs by a constant factor $1+(3/m_0)$ (see first paragraph of section E.).

interstellar media. Such models usually require accurate values of the transition energies and the oscillator strengths.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Sergiy Bubin reports financial support was provided by Nazarbayev University. Ludwik Adamowicz reports financial support was provided by National Science Foundation.

Data availability

Data will be made available on request.

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