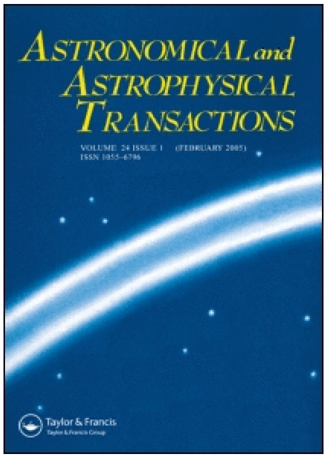

Astronomical & Astrophysical Transactions
The Journal of the Eurasian Astronomical Society
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713453505

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Online Publication Date: 01 January 1997
To cite this Article: Shabaev, V. M., Shabaeva, M. B. and Tupitsyn, I. I. (1997) 'Hyperfine structure of lithium-like ions', Astronomical & Astrophysical Transactions, 12:2, 243 - 246
To link to this article: DOI: 10.1080/10556799708232080
URL: http://dx.doi.org/10.1080/10556799708232080

Astronomical and Astrophysical Transactions, 1997,
Vol. 12, pp. 243–246
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HYPERFINE STRUCTURE OF LITHIUM-LIKE IONS

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(Received November 9, 1995)

The hyperfine splitting values of the ground state of lithium-like ions are calculated in the range $Z = 7$–28. The calculations are based on a combination of the $\frac{1}{Z}$ perturbation theory and the nonrelativistic configuration interaction Hartree–Fock (CI–HF) method. The relativistic corrections are calculated in the zeroth and first orders in $\frac{1}{Z}$. The nuclear charge and magnetization distribution corrections and the radiative corrections are taken into account. The uncertainty of the calculations is estimated to be in the range 0.06–0.15 percent.

KEY WORDS Atomic structure, hyperfine structure

1 INTRODUCTION

An astronomical search of the radio lines in the millimeter region, corresponding to the transitions between the hyperfine structure components of lithium-like ions, requires the prediction of wavelengths with an accuracy of ~ 0.1 percent (Sunyaev and Churazov, 1984; Morris, private communication). In this connection the hyperfine structure of lithium-like ions was calculated using various methods (Sunyaev and Churazov, 1984, Vainshtein *et al.*, 1986; Band *et al.*, 1985, Ivanov *et al.*, 1988; Shabaeva and Shabaev, 1992; 1996; Shabaev *et al.*, 1996). The required precision was first achieved in (Shabaeva and Shabaev, 1992; 1996) where the hyperfine structure of $^{57}Fe^{23+}$ was calculated using the $\frac{1}{Z}$ perturbation theory. In Shabaeva *et al.* (1996) this calculation was extended to the ions which are candidates for an astronomical search planned in IRAM (France) (D. Morris, private communication). For this method, based on a combination of the $\frac{1}{Z}$ perturbation theory and the configuration interaction Hartree-Fock (CI-HF) method, was used. In the present paper we extend the calculations of Shabaeva *et al.* (1996) to all lithium-like ions in the range $Z = 7$–28.

2 BASIC FORMULAE AND CALCULATIONS

The hyperfine splitting of the ground state of lithium-like ions is convently written in the form:

$$\begin{aligned} \Delta E_\mu &= \frac{1}{6}\alpha(\alpha Z)^3 \frac{m}{m_p} \frac{\mu}{\mu_N} \frac{2I+1}{2I} \frac{1}{(1+\frac{m}{M})^3} mc^2 \\ &\times \left[A(\alpha Z) + \frac{1}{Z}B(\alpha Z) + \frac{1}{Z^2}R(Z,\alpha Z)\right] \\ &\times (1-\delta)(1-\varepsilon)(1+\Delta_{\text{rad}}). \end{aligned} \tag{1}$$

Here α is the fine structure constant, Z is the nuclear charge, m is the electron mass, m_p is the proton mass, μ is the nuclear magnetic moment, μ_N is the nuclear magneton, I is the nuclear spin, and M is the nuclear mass. $A(\alpha Z)$ is the relativistic factor (Breit, 1930):

$$A(\alpha Z) = \frac{2[2(1+\gamma) + \sqrt{2(1+\gamma)}]}{(1+\gamma)^2\gamma(4\gamma^2-1)} = 1 + \frac{17}{8}(\alpha Z)^2 + \frac{449}{128}(\alpha Z)^4 + \dots \tag{2}$$

The term $\frac{1}{Z}B(\alpha Z)$ denotes the $\frac{1}{Z}$ interelectronic interaction contribution calculated in Shabaeva and Shabaev (1992, 1996). In the lowest orders in αZ the function $B(\alpha Z)$ is given by

$$B(\alpha Z) = -2.6557 - 6.2138(\alpha Z)^2. \tag{3}$$

The exact αZ values of $B(\alpha Z)$ are listed in Shabaeva and Shabaev (1995). The term $\frac{1}{Z^2}R(Z,\alpha Z)$ is the complete interelectronic interaction contribution with the $\frac{1}{Z}$ term subtracted. We evaluate this term in the non-relativistic approximation by subtracting the non-relativistic limit of the first two terms in the braces of equation (1) from the complete non-relativistic contribution calculated by the CI–HF method:

$$\frac{1}{Z^2}R(Z,0) = \{\dots\}_{nr} - (1 - \frac{2.6557)}{Z}. \tag{4}$$

The CI–HF calculation is discussed in detail in Shabaev *et al.* (1996). The nuclear charge distribution correction δ and the nuclear magnetization distribution correction ε (the Bohr–Weisskopf correction), considered within the single-particle model of the nucleus taking account of the angular asymmetry of the spin distribution, are calculated using analytical formulas and tables from Shabaev (1994). In the case of $^{14}N^{6+}$, where $I = 1$, we assume that the total nuclear moment is possesed by the odd neutron and the odd proton (Shabaev *et al.*, 1995).

The radiative correction, with relative error $\sim \alpha$, is determined by the single-electron contribution which in the lowest orders in αZ is equal (Zwanziger, 1960; Brodsky and Erickson, 1966; Sapirstein, 1983):

$$\Delta_{\text{rad}} = \frac{\alpha}{2\pi} + \left(\ln 2 - \frac{5}{2}\right)\alpha(\alpha Z) - \frac{8}{3\pi}\ln^2\left(\frac{1}{\alpha Z}\right)\alpha(\alpha Z)^2 +$$

Table 1. The wavelengths of the transitions between the hyperfine structure components of the ground state of lithium-like ions

Ion	I^π	$\frac{\mu}{\mu_N}$	$A(\alpha Z)$	$\frac{B(\alpha Z)}{Z}$	$\frac{R(Z,0)}{Z^2}$	δ	ε	Δ_{rad}	λ (*cm*)
$^{14}N^{4+}$	$1+$	0.40376	1.00557	-0.38171	0.01800	0.00067	-0.00004	0.00042	7.072
$^{15}N^{4+}$	$\frac{1}{2}+$	-0.28319	1.00557	-0.38171	0.01800	0.00067	0.0011	0.00042	7.571
$^{17}O^{5+}$	$\frac{5}{2}+$	-1.8938(1)	1.00728	-0.33462	0.01380	0.00082	0.00033	0.00032	1.1813
$^{19}F^{6+}$	$\frac{1}{2}+$	2.6289	1.00923	-0.29808	0.01090	0.00099	0.00036	0.00022	0.34102
$^{21}Ne^{7+}$	$\frac{3}{2}+$	-0.66180	1.01142	-0.26891	0.00877	0.00115	0.00059	0.00012	1.4243
$^{23}Na^{8+}$	$\frac{3}{2}+$	2.2176(1)[a]	1.01384	-0.24511	0.00711	0.00125	0.00035	0.00002	0.30924
$^{25}Mg^{9+}$	$\frac{5}{2}+$	-0.85545(8)	1.01650	-0.22533	0.00606	0.00142	0.00058	-0.00007	0.6680
$^{27}Al^{10+}$	$\frac{5}{2}+$	3.6415	1.01941	-0.20865	0.00524	0.00155	0.00048	-0.00016	0.12060
$^{29}Si^{11+}$	$\frac{1}{2}+$	-0.55529(3)	1.02257	-0.19441	0.00444	0.00172	0.00063	-0.00025	0.37250
$^{31}P^{12+}$	$\frac{1}{2}+$	1.1316	1.02597	-0.18212	0.00385	0.00192	0.00070	-0.00033	0.14602
$^{33}S^{13+}$	$\frac{3}{2}+$	0.64382	1.02963	-0.17141	0.00338	0.00210	0.0011	-0.00041	0.31230
$^{35}Cl^{14+}$	$\frac{3}{2}+$	0.82187	1.03355	-0.16200	0.00298	0.00232	-0.00026	-0.00049	0.20073
$^{37}Cl^{14+}$	$\frac{3}{2}+$	0.68412	1.03355	-0.16200	0.00298	0.00232	-0.00055	-0.00049	0.24107
$^{39}K^{16+}$	$\frac{3}{2}+$	0.39149(2)[a]	1.04219	-0.14628	0.00239	0.00271	-0.00021	-0.00064	0.29403
$^{43}Ca^{17+}$	$\frac{7}{2}-$	-1.3176	1.04691	-0.13966	0.00216	0.00295	0.0012	-0.00071	0.08647
$^{45}Sc^{18+}$	$\frac{7}{2}-$	4.7565	1.05191	-0.13371	0.00196	0.00320	0.00092	-0.00077	0.020450
$^{47}Ti^{19+}$	$\frac{5}{2}-$	-0.78848(1)	1.05719	-0.12834	0.00179	0.00346	0.0016	-0.00084	0.10114
$^{49}Ti^{19+}$	$\frac{7}{2}-$	-1.1042	1.05719	-0.12834	0.00179	0.00346	0.0014	-0.00084	0.07581
$^{51}V^{20+}$	$\frac{7}{2}-$	5.1487	1.06277	-0.12348	0.00163	0.00368	0.0011	-0.00090	0.14073
$^{53}Cr^{21+}$	$\frac{3}{2}-$	-0.47454(3)	1.06864	-0.11905	0.00150	0.00391	0.0015	-0.00096	0.11404
$^{55}Mn^{22+}$	$\frac{5}{2}-$	3.4687	1.07481	-0.11502	0.00138	0.00424	0.0011	-0.00101	0.015176
		3.4532(13)							0.015244
$^{57}Fe^{23+}$	$\frac{1}{2}-$	0.090623	1.08130	-0.11133	0.00128	0.00452	0.0028	-0.00106	0.3073
		0.0990764							0.3068
		0.09044(7)							0.3079
$^{59}Co^{24+}$	$\frac{7}{2}-$	4.627(9)	1.08811	-0.10795	0.00119	0.00483	0.0013	-0.00111	0.009296
$^{61}Ni^{25+}$	$\frac{3}{2}-$	-0.72002(4)	1.09524	-0.10485	0.00110	0.00510	0.0019	-0.00116	0.04367

[a] An average of the values given in Raghavan (1989).

$$
\begin{aligned}
&+ \quad \frac{2}{\pi}\left(-\frac{16}{3}\ln 2+\frac{37}{72}+\frac{4}{15}+\frac{7}{2}\right)\ln\left(\frac{1}{\alpha Z}\right)\alpha(\alpha Z)^2 \\
&+ \quad (3.12\pm 0.30)\alpha(\alpha Z)^2-\frac{1}{2\pi}\frac{17}{8}\alpha(\alpha Z)^2. \qquad (5)
\end{aligned}
$$

Here we add the last term to cancel the contribution arising from the relativistic correction $\frac{17}{8}(\alpha Z)^2$ multiplied by $\frac{\alpha}{2\pi}$.

The wavelengths of the transitions between the hyperfine structure components, calculated using equation (1) are presented in Table 1. The nuclear magnetic moments are taken from Raghavan (1989). Because there are discrepancies in the experimental values of μ for some ions we calculate λ for all μ given in Raghavan (1989). We estimate that, except $^{59}Co^{24+}$ for which the uncertainty of the nuclear magnetic moment is large enough, the uncertainty of the hyperfine splitting values given in the table is in the range 0.06–0.15 percent, increasing from low to high Z.

Acknowledgment

We wish to thank Dr. D. Morris for stimulating discussion.

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