Teorinė Si$^+$ ir Ti$^+$ jonų energijos spektro priklausomybė nuo smulkiosios struktūros konstantos

Theoretical Studies of Si$^+$ and Ti$^+$ Ions Energy Spectra Dependence on Fine-Structure Constant

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Contemporary atomic theory, using numerical methods, allows to calculate energy spectra, transition energies and probabilities, interactions with external fields, hyperfine interaction shifts, and other effects in multielectron atoms and ions. In some cases these methods and appropriate computational strategies allow to reach accuracies of 1% or better, compared to experimental results.

Paul Dirac was the first to mention a possible variability of fundamental constants in expanding universe [1]. Such a change may manifest itself in spectra of distant quasars, due to the dependence of atomic energy levels on the fine-structure constant α, which is responsible for the strength of electromagnetic interaction between electric charges. So far the researches on the time and space variability of α yield inconclusive results — there are indications of directional dependence [2], but no definite time variation of α has been confirmed yet. One of the methods relies on comparing the transitions frequencies in quasar spectra with present laboratory values.

In this work Si$^+$ and Ti$^+$ ions energy spectra and their α-dependence are calculated using Grasp2k [3] relativistic atomic structure package. In order to calculate energy spectra, multiconfiguration Dirac-Hartree-Fock (MCDHF) approach and relativistic configuration interaction (RCI) method, which includes Breit and quantum electrodynamic (QED) corrections (vacuum polarization (VP) and self-energy (SE)), are used [4]. Then, calculated energy spectra values are compared to values recommended by the National Institute of Standards and Technology. Subsequently, energy spectra are calculated using the same method with different α constant value. A particular transition frequency ω dependence on α constant may be approximately expressed by linear function:

$$\omega = \omega_0 + qx, \qquad (1)$$

where

$$x = \left[\left(\frac{\alpha_0}{\alpha} \right)^2 - 1 \right]. \qquad (2)$$

ω_0 is the laboratory value of the transition energy (i.e. with contemporary α value $\alpha = \alpha_0$).

The q coefficient, which is basically an inclination coefficient, represents the transition energy sensitivity to α variation. Calculations of q coefficients make it possible to compare laboratory spectra with quasar absorption spectra. This in turn yields an estimate of α variation. Also, calculations show the dependence of q coefficient on relativistic effects.

The first column of the Table 1 presents the calculated q coefficients for several energy levels of Si II and Ti II ions, together with Breit and QED corrections. Final q coefficients with all calculated corrections are presented in the last column.

Table 1. Si II and Ti II q parameter values including different corrections.

Energy levels	q_{MCDHF}	Δq_{Breit}	Δq_{VP}	Δq_{SE}	q
Si II					
$3s^2\,3p\,{}^2P^o_{1/2}$	0	0	0	0	0
$3s\,{}^2S\,3p^2({}^3_2P)\,{}^4P_{1/2}$	472	-1	0	-32	439
$3s\,{}^2S\,3p^2({}^3_2P)\,{}^4P_{3/2}$	588	-7	0	-32	549
$3s\,{}^2S\,3p^2({}^1_2D)\,{}^2D_{3/2}$	531	-17	1	-22	493
$3s^2\,4s\,{}^2S_{1/2}$	40	-21	0	5	24
Ti II					
$3d^2({}^3_2F)\,{}^3F\,4s\,{}^4F_{3/2}$	0	0	0	0	0
$3d^2({}^3_2F)\,{}^3F\,4p\,{}^4G^o_{5/2}$	400	5	1	-28	378
$3d^2({}^3_2F)\,{}^3F\,4p\,{}^4F^o_{3/2}$	592	-8	0	-29	555
$3d^2({}^3_2F)\,{}^3F\,4p\,{}^4F^o_{5/2}$	735	-23	0	-28	684
$3d^2({}^3_2F)\,{}^3F\,4p\,{}^4D^o_{1/2}$	770	-9	0	-28	733
$3d^2({}^3_2F)\,{}^3F\,4p\,{}^2D^o_{3/2}$	922	-37	0	-28	857

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