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The α-dependence of transition frequencies

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Synopsis Using multiconfiguration Dirac-Hartree-Fock (MCDHF) method we calculated the dependence of the transition frequencies on fine-structure constant α. The energies and relativistic energy shifts are compared with results from Dzuba *et al* [1], Berengut *et al* [2] and King *et al* [3].

Certain unification theories suggest the possibility that fundamental constants of nature are time dependent. We present new results of the dependence of the transition frequencies on fine-structure constant α. The calculations were done with the MCDHF method.

Table 1. Comparison of the results

Ion	Upper state	Energy	q	Ref.
C IV	$1s^2 2p\ ^2P_{1/2}$	64484	108	[1]
		65200	104	[2]
		65094	104	Our
	$^2P_{3/2}$	64591	231	[1]
		65328	232	[2]
		65222	232	Our
Ti II	$3d^2 4p\ ^4G_{5/2}$	29544	396(50)	[3]
		29759	396	[2]
		27804	394	Our
	$^4F_{3/2}$	30836	541(50)	[3]
		30691	541	[2]
		28907	568	Our
	$^4F_{5/2}$	30959	673(50)	[3]
		30813	673	[2]
		29019	684	Our
	$^4D_{1/2}$	32532	677(50)	[3]
		32416	677	[2]
		30916	719	Our
	$^4D_{3/2}$	32603	791(50)	[3]
		32510	791	[2]
		30942	698	Our
Mn II	$3d^5 4p\ ^7P_2$	38366	918	[1]
		38366	869	[2]
		36144	826	Our
	$^7P_3$	38543	1110	[1]
		38585	1030	[2]
		36310	993	Our
	$^7P_4$	38807	1366	[1]
		38814	1276	[2]
		36546	1247	Our

In Table 1 we present the atomic energy levels which are calculated using GRASP2K program package [4]. The q values are computed with the formula:

$$w = w_0 + qx, \tag{1}$$

where $x = (\alpha^2/\alpha_0^2) - 1$, α_0 is the laboratory value of the fine structure constant, and q is the relativistic energy shift. Dzuba *et al* [1] presented the results of calculations of the dependence of the transition frequencies on α for many atoms and ions where data exist for quasar spectra. Berengut *et al* [2] used the relativistic Hartree-Fock method, many-body perturbation theory and configuration interaction method to calculate the dependence of atomic transition frequencies on the fine structure constant α.

In the case of C IV (ground state $1s^2 2s\ ^2S_{1/2}$), the agreement with other authors is quite good (mostly due to the fact that relativistic effects for the carbon and its ions are small). For the Ti II (ground state $3d^2 4s\ ^4F_{3/2}$) and Mn II spectra (ground state $3d^5 4s\ ^7S_3$) the calculated energies are all smaller in our approximation, and q values show larger deviations. All calculations were done in single-configuration Dirac-Hartree-Fock model. We will present the correlated calculations for several atoms and ions which are of interest for searches of α time variation.

References

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