Precision calculation of the spectra of Mg-like ions

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Many calculations performed within the method which combines the configuration-interaction (CI) with the many-body perturbation theory showed its advantage in comparison with other methods. In this work the low-lying states of Mg-like ions (Mg I, Al II, Si III, P IV, S V, Cl VI) are calculated within the CI method, the CI plus many-body perturbation theory (CI+MBPT) method, and the CI plus all-order (CI+AO) method [1, 2]. The effect of the Breit corrections and QED-corrections are considered. These corrections grow with the nuclear charge Z and improve agreement with experimental data [3] for the most heavy ions, QED corrections being more important than Breit corrections.

The accuracy of each of these methods grows with the Z, while the difference between the results of CI+MBPT and CI+AO methods decreases. The final precision of our calculation is about 0.1%.

In the Table 1 the energies of some low-lying states are presented.

Element	State	Energies (cm^{-1})				
		Exper.	CI	CI+MBPT	CI+AO	Breit and QED contribution
Mg I	$^1S_0$	182939	179554	182685	182875	14
	$^3P_0$	21850	20919	21792	21851	7
	$^3P_1$	21871	20939	21814	21872	7
	$^3P_2$	21911	20980	21857	21916	7
	$^1P_1$	35051	34471	35030	35052	7
Cl VI	$^1S_0$	1702996	1695325	1702847	1703001	187
	$^3P_0$	98062	97047	98064	98115	91
	$^3P_1$	98621	97624	98647	98701	91
	$^3P_2$	99782	98813	99854	99916	91
	$^1P_1$	148947	150326	149154	149102	94

Table 1: *Examples of some calculated energies for atom Mg I and ion Cl VI.*

References

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[3] `http://www.physics.nist.gov`