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THEORETICAL INVESTIGATION OF ENERGY LEVELS FOR BA VI

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This ion was selected for the investigation as it is of great importance to Astrophysics. It is evident that the lines can be observed in hot white dwarf stars [1]. In this work energy levels for Ba VI will be presented. The calculations for Ba VI are performed using general-purpose atomic structure package GRASP2018, based on multiconfiguration Dirac-Hartree-Fock and relativistic configuration interaction (RCI) methods.

As this ion is of Sb isoelectronic sequence, it was calculated using the same principle like in [2]. Active space (AS) method was used to compute radial wave functions layer by layer for four sets of virtual orbitals (AS_{1-4}). Single and double substitutions were done from multi reference set of orbitals up to 11s, 11p, 10d, 8f, 8g, 8h. Substitutions from [Kr]$4d^{10}$ core shells were forbidden. After calculating AS_4, RCI method was used to further increase the accuracy of Ba VI energy level calculations. In total, 231 energy levels belonging to the configurations $5s^25p4f^2$, $5s^25p^24f$, $5s5p^34f$, $5p^5$, $5s^25p^2\{5d,6p,6s\}$, $5s^25p^3$, $5s^25p5d^2$, $5s5p^35d$, $5s5p^36s$ and $5s5p^4$ were computed.

50 levels were selected based on the data availability at National Institute of Standards and Technology Atomic Spectra database (NIST) [3] for comparison. The relative difference to NIST data is displayed in Figure 1. The biggest disagreement is observed in $5s^25p^25d$ and $5s5p^4$ configuration levels, as the energies appear to be reversed in our calculations. The average relative difference compared to NIST [3] for AS_4 is 1.2%. In order to increase the accuracy of energy levels, core, core-valence, core-core correlations need to be investigated. During the conference further data from the calculations will be presented.

Conf.	^{M}L	J	E_{NIST} cm^{-1}	AS$_3$%	AS$_4$%	Conf.	^{M}L	J	E_{NIST} cm^{-1}	AS$_3$%	AS$_4$%
$5s^25p^3$	^4S	3/2	0.0	0.0	0.0	$5s^25p^2(^1D)5d$	^2G	7/2	212208.6	2.6	2.6
$5s^25p^3$	^2D	3/2	17260.6	1.2	1.1	$5s^25p^2(^1D)5d$	^2G	9/2	222540	-0.3	-0.3
$5s^25p^3$	^2D	5/2	23547.2	1.0	0.9	$5s^25p^2(^3P)5d$	^4P	5/2	214870.8	2.3	2.3
$5s^25p^3$	^2P	1/2	36155.7	2.2	2.1	$5s^25p^2(^3P)5d$	^4P	3/2	217346.5	2.2	2.2
$5s^25p^3$	^2P	3/2	49621	0.4	0.4	$5s^25p^2(^3P)5d$	^4P	1/2	218693.8	2.2	2.2
$5s5p^4(^3P)$	^4P	5/2	128436.3	-2.2	-2.1	$5s^25p^2(^3P)5d$	^2D	3/2	224093.2	0.9	0.8
$5s5p^4(^3P)$	^4P	3/2	139920.1	-2.1	-2.1	$5s^25p^2(^3P)5d$	^2D	5/2	228330.9	2.1	2.2
$5s5p^4(^3P)$	^4P	1/2	142851.9	-2.0	-2.0	$5s^25p^2(^1D)5d$	^2P	1/2	234313.6	0.4	0.4
$5s5p^4(^1D)$	^2D	3/2	158158.4	-0.7	-0.7	$5s^25p^2(^1D)5d$	^2P	3/2	246496.2	2.1	2.1
$5s5p^4(^1D)$	^2D	5/2	163566.3	-0.8	-0.8	$5s^25p^2(^1D)5d$	^2D	3/2	235818.7	2.3	2.3
$5s^25p^2(^3P)5d$	^2P	3/2	176498	-0.3	-0.3	$5s^25p^2(^1D)5d$	^2D	5/2	236640.5	3.1	3.0
$5s^25p^2(^3P)5d$	^2P	1/2	229293.1	-0.6	0.6	$5s^25p^2(^3P)5d$	^2F	7/2	242157.2	2.3	2.3
$5s5p^4(^3P)$	^2P	1/2	179076.6	4.8	4.8	$5s^25p^2(^3P)5d$	^2F	5/2	257298.9	2.2	2.1
$5s5p^4(^3P)$	^2P	3/2	213042.9	3.4	3.4	$5s^25p^2(^1S)5d$	^2D	5/2	243103.4	-0.5	-0.5
$5s^25p^2(^3P)5d$	^4F	3/2	180293.1	-0.2	-0.2	$5s^25p^2(^1S)5d$	^2D	3/2	256774.8	1.8	1.8
$5s^25p^2(^3P)5d$	^4F	5/2	183552.2	-0.5	-0.5	$5s^25p^2(^3P)6s$	^4P	1/2	247725.6	-0.1	-0.1
$5s^25p^2(^3P)5d$	^4F	7/2	192561.2	-0.6	-0.6	$5s^25p^2(^3P)6s$	^4P	3/2	261563.8	-0.3	-0.3
$5s^25p^2(^3P)5d$	^4F	9/2	199080	-0.6	-0.6	$5s^25p^2(^3P)6s$	^4P	5/2	267649.7	-0.2	-0.2
$5s^25p^2(^1D)5d$	^2F	5/2	191382.2	-0.6	-0.6	$5s^25p^2(^1D)5d$	^2S	1/2	251008.8	2.6	2.6
$5s^25p^2(^3P)5d$	^4D	1/2	193882.1	-0.4	-0.4	$5s^25p^2(^3P)6s$	^2P	1/2	265653.5	-0.2	-0.2
$5s^25p^2(^3P)5d$	^4D	7/2	196130.2	-0.5	-0.5	$5s^25p^2(^3P)6s$	^2P	3/2	271083.2	-0.1	-0.1
$5s^25p^2(^3P)5d$	^4D	3/2	197255.4	-0.2	-0.2	$5s^25p^2(^1D)6s$	^2D	5/2	288565.1	-0.2	-0.2
$5s^25p^2(^3P)5d$	^4D	5/2	201857	-0.3	-0.3	$5s^25p^2(^1D)6s$	^2D	3/2	290903.6	-0.2	-0.2
$5s5p^4(^1S)$	^2S	1/2	200937.6	0.0	0.0	$5s^25p^2(^1S)6s$	^2S	1/2	307387	0.1	0.1

Fig. 1. Comparison of energy levels computed in active spaces AS_3 and AS_4 with NIST [3] ASD recommended values for Ba VI.

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