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ACCURATE CALCULATIONS OF ENERGY LEVELS AND LIFETIMES OF HE-LIKE OXYGEN

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Abstract. Energy levels and lifetimes are calculated for all levels of $1s^2$ and 1snl ($n = 2-8$) configurations of He-like oxygen ion. Multiconfigurational-Dirac-Hartree-Fock (MCDHF) method is adopted for calculating these spectroscopic data. Comparisons are made with similar data obtained with FAC (Flexible Atomic Code) to assess the accuracy of the results. Comparisons were made with the available data in the literature and good agreement was found which confirms the reliability of our results.

1. INTRODUCTION

In the last few years, various theoretical and experimental research for providing atomic data for He-like ions have been carried out. Some data are available at the National Institute of Standards and Technology (NIST) database (see Kramida et al. 2019). In this work, we treat the case of the ion He-like oxygen. This work is a continuous work on the investigation of He-like ions (see Salhi et al., 2017ab, 2019ab).

For our calculations of energy levels and lifetimes, we have adopted the Multiconfigurational-Dirac-Hartree-Fock (MCDHF) method (see Jönsson et al. 2013). Further relativistic corrections arising from the Breit interaction and QED effects have also been included. Additionally, in order to make a rigorous accuracy assessment of our results, we have also performed calculations by the code Flexible Atomic Code (FAC) of Gu (2008). This is also a fully relativistic code which can provide a variety of atomic parameters.

2. RESULTS AND DISCUSSIONS

2. 1. ENERGY LEVELS

The calculated energy levels of $1s^2$, $1s2l$, $1s3l$, $1s4l$, $1s5l$, $1s6l$, $1s7l$ and $1s8l$ configurations for the He-like oxygen generate up to 127 levels. These calculations are performed by means of two codes GRASP2K and FAC. All the calculated energy levels have been compared with the results found in the NIST database (see Kramida et al. 2019). This agreement is shown in Fig. 1. The average difference between the MCDHF/RCI values generated by the code GRASP2K and the NIST values is 0.03% for the states listed in the NIST database while the average difference between

the calculated MBPT values generated by the code FAC and NIST database level energies is 0.04%. Another comparisons were made with a theoretical work (GRASP, FAC mentionned in the Fig. 1.) see Aggarwal et al. 2008, another one with the work see Delahaye et al. 2002 (SS in the Fig. 1.) and the last one with the work of Savukov see Savukov et al. 2003.

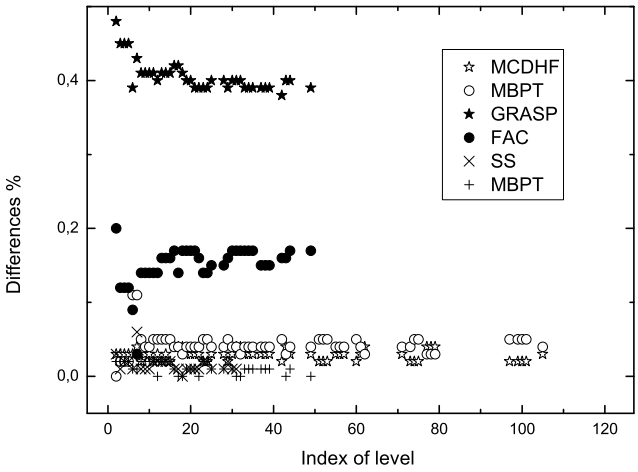

Figure 1: Comparison of our calculated energy levels MCDHF and MBPT data with data of other authors: GRASP and FAC (see Aggarwal et al. 2008), SS (see Delahaye et al. 2002) and MBPT (see Savukov et al. 2003).

Since some of energy levels are not available on NIST, our energy levels of $O\ VII$ from our both methods should be adopted in modelling applications. We may state that overall there is no discrepancy between our results and the other works.

2. 2. LIFETIMES

The lifetime τ for a level j is defined as follows

$$\tau_j = \frac{1}{\sum_i A_{ji}} \tag{1}$$

For brevity, we present in Table 1 the lifetimes of levels up to $n = 4$ calculated by the GRASP2K and FAC codes, which include the contributions from four types of transitions: $E1$, $E2$, $M1$ and $M2$. The two columns (MCDHF/RCI and MBPT) show our work of the calculation for the lifetimes. Just a large difference is found mainly in the level $1s\,3s\ ^3S_1$ with the value published in the NIST database ($(6.5 \pm 0.6)\ 10^{-11} s^{-1}$). However, for the others values the difference is minor.

Index	Configuration	MCDHF/RCI	MBPT	NIST
1	$1s^2\ ^1S_0$			
2	$1s\,2s\ ^3S_1$	1.000E-03		
3	$1s\,2p\ ^3P^o_0$	1.263E-08	1.205E-08	
4	$1s\,2p\ ^3P^o_1$	1.594E-09	1.928E-09	
5	$1s\,2p\ ^3P^o_2$	1.220E-08	1.164E-08	
6	$1s\,2s\ ^1S_0$	3.192E-01	2.231E-02	
7	$1s\,2p\ ^1P^o_1$	3.027E-13	2.926E-13	
8	$1s\,3s\ ^3S_1$	4.453E-11	4.640E-11	(6.5 ± 0.6)E-11
9	$1s\,3p\ ^3P^o_0$	1.888E-11	1.914E-11	(1.92 ± 0.2)E-11
10	$1s\,3p\ ^3P^o_1$	1.883E-11	1.909E-11	(1.92 ± 0.2)E-11
11	$1s\,3p\ ^3P^o_2$	1.892E-11	1.919E-11	(1.92 ± 0.2)E-11
12	$1s\,3s\ ^1S_0$	4.874E-11	4.820E-11	
13	$1s\,3d\ ^3D_1$	6.197E-12	6.180E-12	(7.0 ± 2.0)E-12
14	$1s\,3d\ ^3D_2$	6.203E-12	6.183E-12	(7.0 ± 2.0)E-12
15	$1s\,3d\ ^3D_3$	6.201E-12	6.183E-12	(7.0 ± 2.0)E-12
16	$1s\,3d\ ^1D_2$	6.554E-12	6.550E-12	(8.0 ± 1.5)E-12
17	$1s\,3p\ ^1P^o_1$	1.007E-12	9.561E-13	
18	$1s\,4s\ ^3S_1$	6.747E-11	7.411E-11	
19	$1s\,4p\ ^3P^o_0$	3.203E-11	3.325E-11	(3.12 ± 0.2)E-11
20	$1s\,4p\ ^3P^o_1$	3.197E-11	3.316E-11	(3.12 ± 0.2)E-11
21	$1s\,4p\ ^3P^o_2$	3.209E-11	3.331E-11	(3.12 ± 0.2)E-11
22	$1s\,4s\ ^1S_0$	6.939E-11	6.656E-11	
23	$1s\,4d\ ^3D_1$	1.433E-11	1.435E-11	(1.6 ± 0.15)E-11
24	$1s\,4d\ ^3D_2$	1.434E-11	1.436E-11	(1.6 ± 0.15)E-11
25	$1s\,4d\ ^3D_3$	1.434E-11	1.436E-11	(1.6 ± 0.15)E-11
26	$1s\,4f\ ^3F^o_3$	3.016E-11	3.015E-11	
27	$1s\,4f\ ^3F^o_2$	3.014E-11	3.013E-11	
28	$1s\,4d\ ^1D_2$	1.537E-11	1.528E-11	(1.62 ± 0.15)E-11
29	$1s\,4f\ ^3F^o_4$	3.015E-11	3.014E-11	
30	$1s\,4f\ ^1F^o_3$	3.018E-11	3.018E-11	
31	$1s\,4p\ ^1P^o_1$	2.346E-12	2.208E-12	

Table 1: Lifetimes (τ in s^{-1}) for the lowest 31 levels arising from the $1s^2$ and 1snl with $n = 2 - 4$ configurations of O VII. Two calculations are performed using GRASP2K and FAC codes and compared with other results from the NIST database.

We hope that the present extended results will be useful for future comparisons and may encourage experimentalists to measure their lifetimes.

3. CONCLUSION

In the present study, fine structure energy levels and lifetimes for He-like oxygen are presented. We calculate also the weighted oscillator strengths and transition probabilities but for brevity on the presentation of results, we restrict in this study the presentation of results for energy levels and lifetimes and the other data will be published elsewhere. The self-consistent field approximation and the Breit interaction

Hamiltonian as well as QED effects have been included in the calculations to improve the generated wave functions. The calculated energy levels and lifetimes show a good agreement with other published results from the literature. The present data sets are believed to be the most comprehensive and accurate ones to date for $O\ VII$. The accuracy of the present calculations is high enough to facilitate identification of many observed spectral lines. They are also useful for modeling and diagnosing a variety of plasmas including astronomical and fusion plasma.

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