PAPER • OPEN ACCESS

$K \alpha_{1,2} \alpha_3$ and $K^h \alpha_{1,2}$ satellite transition energies and rates for Ar and Ca

To cite this article: K Kozioł and J Rzadkiewicz 2020 J. Phys.: Conf. Ser. 1412 142002

View the article online for updates and enhancements.

You may also like

- <u>Theoretical study of the photoionization</u> process of Ne-like Ar, Fe, Kr and Xe ions L C Gao, D H Zhang, L Y Xie et al.
- <u>Combined experimental and theoretical</u> <u>description of direct current magnetron</u> <u>sputtering of Al by Ar and Ar/N₂ plasma</u> Jan Trieschmann, Stefan Ries, Nikita Bibinov et al.
- <u>The fabrication, characterization and</u> <u>functionalization in molecular electronics</u> Yi Zhao, Wenqing Liu, Jiaoyang Zhao et al.





DISCOVER how sustainability intersects with electrochemistry & solid state science research



This content was downloaded from IP address 18.220.82.93 on 12/05/2024 at 16:29

Journal of Physics: Conference Series

$K\alpha_{1,2}\alpha_3$ and $K^h\alpha_{1,2}$ satellite transition energies and rates for Ar and Ca

K Kozioł^{*} and J Rzadkiewicz[†]

National Centre for Nuclear Research (NCBJ), Andrzeja Sołtana 7, 05-400 Otwock-Świerk, Poland

The calculations of radiative energies and transition rates for $K\alpha_{1,2}\alpha_3$ and $K^h\alpha_{1,2}$ satellite $(M_1,$ Synopsis $M_{2,3}$, and N_1 spectator holes) lines for Ar and Ca have been carried out by using the GRASP2K and AMBIT codes. The influence of electron correlation on transition rates has been studied.

The radiative transitions in K-shell hollow (i.e., having empty K shell) atoms can occur via one-electron one-photon (OEOP: $1s^{-2} \rightarrow$ $1s^{-1}2p^{-1}$, named $K^h\alpha_{1,2}$) or via much less probable two-electron one-photon (TEOP: $1s^{-2} \rightarrow$ $2s^{-1}2p^{-1}$, named $K\alpha_{1,2}\alpha_3$) transitions. It has been found that TEOP transition rates are very sensitive to the electron correlations [1], while OEOP transition rates are only weakly sensitive.

Transition rates for $K^h \alpha_{1,2}$ and Table 1. $K^h \alpha_{1,2} M_1^{-1}$ lines of Ar, calculated in length (A_L) and velocity (A_V) gauge. 'CI' means extensive Configuration-Interaction calculations.

Code	Transition rate (s^{-1})	
	A_L	A_V
$K^h \alpha_2 \ (1s^{-2} \to 1s^{-1}2p_{1/2}^{-1})$		
grasp2k	2.66E + 14	$2.57E{+}14$
grasp2k (CI)	$2.69E{+}14$	$2.57E{+}14$
AMBIT	$2.56E{+}14$	$2.45E{+}14$
$K^h \alpha_1 \ (1s^{-2} \to 1s^{-1}2p_{3/2}^{-1})$		
grasp2k	3.85E + 12	3.44E + 12
grasp2k (CI)	$3.54E{+}12$	$3.39E{+}12$
AMBIT	$3.43E{+}12$	$3.29E{+}12$
$K^h \alpha_{1,2} M_1^{-1} \ (1s^{-2}3s^{-1} \to 1s^{-1}2p^{-1}3s^{-1})$		
grasp2k	$2.79E{+}14$	$2.68E{+}14$
grasp2k (CI)	2.64E + 14	$2.55E{+}14$
AMBIT	$2.58E{+}14$	$2.49E{+}14$

We reported recently that incorporation of $K\alpha_{1,2}\alpha_3$ and $K^h\alpha_{1,2}$ satellite transitions is crucial to proper estimate the OEOP-to-TEOP branching ratio and $K\alpha_{1,2}\alpha_3$ linewidth [1]. Then the calculations of radiative energies and transition rates for satellite $K\alpha_{1,2}\alpha_3$ and $K^h\alpha_{1,2}$ lines for Ar and Ca atoms have been carried out by means of the GRASP2K [2] and AMBIT [3]

*E-mail: Karol.Koziol@ncbj.gov.pl

codes, based on the Multi-Configuration Dirac-Hartree–Fock method. The influence of electron correlation on transition rates has been studied. The results of our studies set new theoretical limits for the TEOP transitions in the low-Z atomic range. We also hope that this work will guide future experiments with a high accuracy.



Figure 1. Convergence of calculations of $K\alpha_{1,2}\alpha_3$ and $K\alpha_{1,2}\alpha_3 M_1^{-1}$ transition rates for Ar for various configuration-interaction active spaces.

Acknowledgments: The work was supported by the Polish Ministry of Science and Higher Education within the framework of the National Centre for Nuclear Research Grant for Young Scientists and PhD Students 2018–2019.

References

- [1] Kozioł K and Rzadkiewicz J 2017 Phys. Rev. A **96** 031402
- [2] Jöönsson P, Gaigalas G, Bieroń J, Froese Fischer C and Grant I P 2013 Comput. Phys. Commun. **184** 2197
- [3] Kahl E V and Berengut J C 2018 Comput. Phys. Commun.In Press. DOI: 10.1016/j.cpc.2018.12.014



Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI. Published under licence by IOP Publishing Ltd

[†]E-mail: Jacek.Rzadkiewicz@ncbj.gov.pl