Approximation and replenishment of data on ion ionization potentials of superheavy elements

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There are a data gap in tables [1] on ion ionization potentials for elements Z > 103 with the number of electrons in the range $47 \leq N_e \leq 68$. The authors of tables [1] considered the results [2] doubtful in this case and for $85 \leq Z \leq 103$ employed also other values [3], although for most of the rest ions the source [2] is used, in which the total electron energies for the Lithium to the Dubnium isoelectronic series of the elements $Z \leq 118$ are calculated by the Dirac-Fock method. The reason is a violation of the correct order of filling electronic states used in [2] in this range of electron numbers. In this paper, the quasi-classical semi-empirical method is used to approximate analytically the table ionization potentials and to fill in the gap found in the data. This method is based on the fact that with the correct filling of the electron shells, the ionization potential of the ion of the element Z with the number of electrons N_e may be interpolated and extrapolated in the form

$$I_{N_e}(Z) = Z^{4/3} 10^{\lg e_{N_e}(\sigma)} E_h, \quad \lg e_{N_e}(\sigma) = \sum_{i=0}^{1} \sum_{k=0}^{2} b_{ik} N_e^k \sigma^i, \quad (1)$$

where $E_h = 27.211386 \, eV$, $\sigma = \pi Z^{-1/3}$, moreover, the estimated error does not exceed 1%.

[1] Kramida A, Ralchenko Y and Reader J Nist atomic spectra database (ver. 5.10)

URL https://physics.nist.gov/asd [2022, December 26]

- [2] Rodrigues G C, Indelicato P, Santos J P, Patte P and Parente F 2004 At. Data Nucl. Data Tables 86 117–233
- [3] Carlson T A, Nestor C W, Wasserman N and McDowell J D 1970 At. Data Nucl. Data Tables 2 63–69