

Semi-empirical calculation of K to L_i sub-shell, K to L, and M shell vacancy transfer probability for elements in the atomic range $16 \leq Z \leq 92$

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Abstract:

This study introduces novel semi-empirical calculations to obtain vacancy transfer probabilities from the K shell for elements in the atomic range $16 \leq Z \leq 92$. These calculations are derived from experimental data extracted from the scientific literature and previously tabulated by the research team. The results are compared with theoretical, semi-empirical, and experimental values reported in the literature, demonstrating a good agreement between the obtained findings and those of previous works.

Keywords: Semi-empirical calculation, vacancy transfer probabilities, weighted average values.

1. Introduction

Utilizing both theoretical and experimental methods, along with fitting empirical and semi-empirical formulae to experimental data, is paramount in determining vacancy transfer probabilities, particularly with K-shell vacancies across various elements. This significance arises from their numerous applications in physics, chemistry, medical research, and nuclear science and technology. Their utility extends to fields such as X-ray spectroscopy, which is crucial for nuclear safeguards, safety, and security applications, as well as plasma physics, astrophysics, materials science, radiation dosimetry, plasma characterization, radiation protection, and industrial radiation processing. Vacancy transfer is intricately tied to the interaction of photons with matter, which can occur through various mechanisms largely dependent on the energy of the incident photons. Central to this interaction is photoionization, wherein a bound electron is ejected, leaving behind a vacancy that is subsequently occupied by an electron from a higher-energy shell. The nature of this transition, whether radiative or nonradiative, is governed by quantum mechanical principles known as selection rules (Turşucu et al. 2012). Numerous researchers have undertaken calculations to assess vacancy transfer probabilities from the K-shell to the X-shell/subshell ($X = L, M$). Experimental measurements of vacancy transfer probabilities from the K shell using various methods have been reported (Akman 2016a, 2016b; Alım et al. 2017a, 2017b; Anand et al. 2018, 2015, 2014, 2013, 2012; Apaydın and Tıraşoğlu 2012; Aylikci et al. 2015; Baydaş 2005; Bennal et al. 2010; Çalışkan et al. 2002; Cengiz et al. 2011, 2010, 2008; Demir and Şahin 2007; Durak et al. 2012; Durak and Özdemir 2000, 1998; Durdu et al. 2022; Ertuğral et al. 2010, 2006, 2005, 2003; Ertuğrul 2003, 2002a, 2002b, 2002c, 2002d; Ertuğrul et al. 1997a, 1997b; George et al. 2014; Gudennavar and Bubbly 2023; Han et al. 2007; Han and Demir 2010; Kaya et al. 2014; Mirji et al. 2015a, 2015b; Onder et al. 2013; Öz, 2006; S. Puri et al. 1993; Rao et al. 1972; Reyes-Herrera and Miranda 2009, 2008; Santra et al. 2005; Schönfeld and JanBen 1996; Şimşek et al. 2003; Söğüt 2009,

2006; Söğüt *et al.* 2009; Sreevidya *et al.* 2014; Turhan *et al.* 2020, 2017; Turhan and Akman 2023; Turşucu *et al.* 2013, 2012; Turşucu and Demir 2013; Uğurlu *et al.* 2020; Uğurlu and Demir 2020). These methods vary depending on experimental conditions such as the ionization process, target material, and detectors employed. Rao *et al.* (1972) specifically focused on determining the average number of primary L_i subshell vacancies resulting from transitions to the K-shell across elements with atomic numbers ranging from 20 to 96, while Bambynek *et al.* (1972) provided a comprehensive review. Puri *et al.* (1993) conducted calculations for the total K-to- L_1 , L_2 , and L_3 subshell probabilities (η_{KL_i}) for elements with atomic numbers ranging from 18 to 96, employing theoretical radiative transition rates from Scofield (1974), and radiationless transition rates tabulated by Chen *et al.* (1979). Schönfeld and JanBen (1996) compiled semi-empirical data in a table for K-to-L-shell (η_{KL}^T) total vacancy transfer probabilities, covering elements with atomic numbers from 10 to 100. Aylikci *et al.* (2015) calculated empirical and semi-empirical η_{KL}^T values for the elements with atomic numbers $21 \leq Z \leq 30$. Berkani *et al.* (2024) presented total empirical vacancy transfer probabilities η_{KL}^T for elements with $16 \leq Z \leq 92$, and radiative transfer probabilities η_{KL2}^R and η_{KL3}^R for $23 \leq Z \leq 92$, and η_{KM}^R for $24 \leq Z \leq 92$. These results were based on an existing compilation of experimental data fitted to an analytical function of the atomic number Z .

In this paper we present novel semi-empirical calculations for atomic parameters η_{KL}^T , η_{KL2}^R , η_{KL3}^R , and η_{KM}^R , pertinent to vacancy transfer probabilities. These calculations are based on meticulously tabulated experimental data collected from the scientific literature by the research group (Berkani *et al.* 2024). A total of 413 values for η_{KL}^T were compiled from 49 papers, covering studies conducted between April 1993 and June 2023 by several researchers (Akman 2016b, 2016a; Alım *et al.* 2017b, 2017a; Anand *et al.* 2018, 2015, 2014, 2013, 2012; Apaydın and Tıraşoğlu 2012; Aylikci *et al.* 2015; Baydaş 2005; Bennal *et al.* 2010; Cengiz *et al.* 2011, 2010, 2008; Durdu *et al.* 2022; Ertuğral *et al.* 2010, 2006, 2005, 2003; Ertuğrul 2003, 2002c,

2002b, 2002a; Ertuğrul *et al.* 1997b; George *et al.* 2014; Gudennavar and Bubbly, 2023; Han *et al.* 2007; Han and Demir 2010; Kaya *et al.* 2014; Mirji *et al.* 2015a, 2015b; Onder *et al.* 2013; Öz 2006; S. Puri *et al.* 1993; Santra *et al.* 2005; Şimşek *et al.* 2003; Söğüt 2009, 2006; Söğüt *et al.* 2009; Sreevidya *et al.* 2014; Turhan *et al.* 2020; Turhan and Akman 2023; Turşucu *et al.* 2013, 2012; Turşucu and Demir 2013; Uğurlu *et al.* 2020; Uğurlu and Demir 2020). For η_{KL2}^R and η_{KL3}^R , a total of 138 values for each parameter were compiled from 20 papers published between February 1997 and December 2017, from different works (Akman 2016b; Anand *et al.* 2014; Bennal and Badiger 2006; Çalışkan *et al.* 2002; Demir and Şahin 2007; Durak *et al.* 2012; Durak and Özdemir 2000, 1998; Ertuğrul 2003, 2002a, 2002b, 2002c, 2002d; Ertuğrul *et al.* 1997a; Reyes-Herrera and Miranda 2009, 2008; Söğüt 2009, 2006; Sreevidya *et al.* 2014; Turhan *et al.* 2017). Additionally, for η_{KM}^R , a total of 103 values were gathered from 10 papers published between February 1997 and July 2016, from works of (Akman 2016b; Anand *et al.* 2014; Çalışkan *et al.* 2002; Demir and Şahin 2007; Durak and Özdemir 2000, 1998; Ertuğrul 2002d; Ertuğrul *et al.* 1997a; Söğüt 2006; Sreevidya *et al.* 2014). These semi-empirical calculations cover a broad atomic range, with η_{KL}^T calculated for elements with $16 \leq Z \leq 92$, η_{KL2}^R and η_{KL3}^R for elements with $23 \leq Z \leq 92$, and η_{KM}^R for elements within the range $24 \leq Z \leq 92$. The calculations are carried out using an interpolation procedure, which involves fitting an analytical function, using the weighted average values calculated by Berkani *et al.* (2024) as a function of the atomic number Z , and then fitting the experimental to weighted average ratios. The semi-empirical values obtained for a wide range of elements are presented in tabular form, facilitating easy reference and comparison. Additionally, a comprehensive comparison is made with other theoretical, experimental, and semi-empirical values reported in the literature. Notably, a strong correlation is observed between the obtained semi-empirical results and those reported in previous studies, validating the approach efficacy and the accuracy of the semi-empirical calculations.

2. Semi-empirical calculation

Numerous efforts have been undertaken to compute vacancy transfer probabilities, whether through theoretical models or empirical and semi-empirical approaches involving the fitting of experimental data with various functional forms. The K-to- X -shell/subshell ($X = L, M$, etc.) vacancy transfer probabilities representing the average number of vacancies generated in the X -shell/subshell per vacancy originating in the K-shell, and are defined following (Berkani *et al.* 2025; Sampaio *et al.* 2016) as

$$\eta_{KX_i} = \frac{\Gamma_{KX_i}^R + 2\Gamma_{KX_i;X_i}^A + \sum_{j(Y_j \neq X_i)} \Gamma_{KX_i;Y_j}^A}{\Gamma_K^R + \Gamma_K^A}, \quad (1)$$

where $\Gamma_{KX_i}^R$ is the partial radiative transition rate of a vacancy in the K shell to a vacancy in a X_i subshell, and $\Gamma_{KX_i;Y_j}^A$ is the partial radiationless transition rate of a K-shell vacancy to a X_i subshell and another vacancy in a X_j subshell ($j \neq i$ if $X = Y$). The statistical weight 2 in the term $\Gamma_{KX_i;X_i}^A$ takes into account the possibility that radiationless transitions can create two vacancies in the same subshell X_i . Additionally, for $X = L, M$, etc.,

$$\eta_{KX}^T = \sum_i \eta_{KX_i} \quad (2)$$

Additionally, to empirically fit the experimental vacancy transfer probability data, an empirical formula of the form (Berkani *et al.* 2024)

$$\eta_{\text{emp}} = \sum_{i=0}^n A_i Z^i \quad (3)$$

is employed, where the coefficients $A_0, A_1 \dots A_n$, are determined from the experimental data and relate the vacancy transfer probability to the atomic number Z .

In this study, a method was employed to deduce the semi-empirical vacancy transfer probabilities as follows: initially, the quantity $\eta_W = \frac{1}{\sum_{i=1}^N \frac{1}{(\Delta(\eta)_{\text{exp}-i})^2}} \cdot \sum_{i=1}^N \frac{\eta_{\text{exp}-i}}{(\Delta(\eta)_{\text{exp}-i})^2}$, given in

the texts of Amari *et al.* 2024a, Daoudi *et al.* 2020, Hamidani *et al.* 2023, and Zidi *et al.* 2024, was plotted against Z , as shown in Fig. 1a (for η_{KL}^T), Fig. 2a (for η_{KL2}^R), Fig. 3a (for η_{KL3}^R), and Fig. 4a (for η_{KM}^R). This quantity was calculated and reported by Berkani *et al.* (2024). Here η_W represents the weighted average value, $\eta_{\text{exp}-i}$ denotes the i^{th} experimental value, $\Delta(\eta)_{\text{exp}-i}$ signifies the assigned uncertainty for the i^{th} experimental value, and N indicates the number of experimental data points for the element.

Subsequently, these values were fitted using a fourth-order polynomial:

$$\eta_W = A_0 + \sum_{i=1}^4 A_i Z^i = f(Z) \quad (4)$$

Following this, the ratio $S = \frac{\eta_{\text{exp}}}{\eta_W}$ was plotted against the atomic number Z and the data points were fitted using a second-degree polynomial, as seen in Fig. 1b (for η_{KL}^T), Fig. 2b (for η_{KL2}^R), Fig. 3b (for η_{KL3}^R), and Fig. 4b (for η_{KM}^R). (Meddough *et al.* 2024):

$$S = B_0 + \sum_{i=1}^2 B_i Z^i = g(Z) \quad (5)$$

The semi-empirical vacancy transfer probabilities can be expressed as follows:

$$\eta_{s-\text{emp}} = f(Z) \times g(Z) \quad (6)$$

Table 1 presents the fitting coefficients for both equations (4) and (5). The semi-empirical values, calculated using equation (6), are presented and organized for η_{KL}^T within the range $16 \leq Z \leq 92$, η_{KL2}^R and η_{KL3}^R within the range $23 \leq Z \leq 92$, and for η_{KM}^R within the range $24 \leq Z \leq 92$, in Tables 2 to 5.

The deviation between the calculated semi-empirical values $\eta_{s-\text{emp}}$ and their corresponding experimental values η_{exp} for vacancy transfer probabilities is quantified by the root-mean-square error (ϵ_{RMS}). This measure is computed using the formula (Kahoul *et al.* 2014, 2012, 2011; Sahnoune *et al.* 2020):

$$\epsilon_{\text{RMS}} = \left[\frac{1}{N} \sum_{j=1}^N \left(\frac{\eta_{j-\text{exp}} - \eta_{s-\text{emp}}}{\eta_{s-\text{emp}}} \right)^2 \right]^{1/2} \quad (7)$$

Here, N represents the total number of experimental data points for each element. The root-mean-square error (ϵ_{RMS}) is a frequently used quantity to check the quality and accuracy of the fit and measure the difference between observed (experimental) values and those predicted by a model (semi-empirical). For each element, (ϵ_{RMS}) serves as a crucial indicator of the reliability of the semi-empirical model in capturing the experimental data.

The root-mean-square error (ϵ_{RMS}) values of the semi-empirical results are shown for $\eta_{\text{KL}}^{\text{T}}$, $\eta_{\text{KL}2}^{\text{R}}$, $\eta_{\text{KL}3}^{\text{R}}$, and $\eta_{\text{KM}}^{\text{R}}$ parameters in Tables 2-5. It should also be noted that as the elements shown in bold in these tables have not yet had their experimental values reported, ϵ_{RMS} values for these elements have not been added

3. Results and discussion

This work presents a comprehensive assessment of semi-empirical vacancy transfer probabilities, including $\eta_{\text{KL}}^{\text{T}}$, $\eta_{\text{KL}2}^{\text{R}}$, $\eta_{\text{KL}3}^{\text{R}}$, and $\eta_{\text{KM}}^{\text{R}}$. Detailed comparisons are provided with theoretical values, fitted outcomes, and experimental data from various sources (Tables 2-5).

The root-mean-square error (ϵ_{RMS}) for the semi-empirical results is also included in these tables.

To facilitate a thorough evaluation, all vacancy transfer probability values are plotted against the atomic number Z in Fig. 5. The present semi-empirical calculations (derived from formula (6)) demonstrate good agreement with theoretical, fitted, and experimental values across the range $16 \leq Z \leq 92$ for $\eta_{\text{KL}}^{\text{T}}$, $23 \leq Z \leq 92$ for $\eta_{\text{KL}2}^{\text{R}}$, and $\eta_{\text{KL}3}^{\text{R}}$, and $24 \leq Z \leq 92$ for $\eta_{\text{KM}}^{\text{R}}$. Specifically, marginal discrepancies are observed (ranging from 0.04% to 5.51% and 0.22% to 5.25%) for $\eta_{\text{KL}}^{\text{T}}$. When compared to the average experimental values from Rao *et al.* (1972) and the theoretical results from Berkani *et al.* (2025) respectively. However, larger deviations are found for elements $_{88}\text{Ra}$, $_{90}\text{Th}$, and $_{92}\text{U}$ when compared with Rao *et al.* (1972) (9.08%, 14.19%, and

21.46%, respectively). These discrepancies are not entirely unexpected for heavy elements, as relativistic effects complicate theoretical predictions. Additionally, the inherent challenges and heterogeneity in experimental measurements for the high- Z elements contribute to these variations, suggesting that these deviations fall within acceptable margins given the complexities involved. Similarly, comparisons with the semi-empirical values of Schönfeld and JanBen (1996) and the empirical values of Berkani *et al.* (2024) reveal variations ranging from 0.01% to 7.54% and 0.1% to 6.31%, respectively. However, for the last five elements, deviations increase to a range of 9.49% to 21.61% compared to Schönfeld and JanBen (1996), while for the last three elements, deviations range from 8.30% to 13.59% when compared to Berkani *et al.* (2024). Encouragingly, the obtained semi-empirical results align closely with the experimental data from Ertuğral *et al.* 2006 (within 0.11% to 2.52%), Öz 2006 (within 0.13% to 0.87%), and Ertuğral *et al.* 2005 (within 0.13% to 1.98%), except for elements $_{90}\text{Th}$ and $_{92}\text{U}$, exhibiting deviations of 11.17% and 17.94%, respectively. These relative differences (RD%) were calculated using the formula $\text{RD}\% = \frac{|\eta - \eta_{s-\text{emp}}|}{\eta_{s-\text{emp}}} \times 100$ (Amari *et al.* 2024b; Zidi *et al.* 2024b). The semi-empirical results (Fig. 5) demonstrate strong alignment with the results of Rao *et al.* (1972), with relative differences ranging from 0.11% to 4.15% except for $_{17}\text{Cl}$ (which deviates 9.21%) for $\eta_{\text{KL}2}^{\text{R}}$, 0.02% to 1.83% for $\eta_{\text{KL}3}^{\text{R}}$, and 0.28% to 5.41% for $\eta_{\text{KM}}^{\text{R}}$, and of Berkani *et al.* (2025) with relative differences from 0.41% to 3.58% for $\eta_{\text{KL}2}^{\text{R}}$, and 0.08% to 1.15% for $\eta_{\text{KL}3}^{\text{R}}$, excluding elements $_{26}\text{Fe}$ and $_{30}\text{Zn}$, with deviations of 42.15% and 8.57%, respectively. Our comparison with experimental measurements also indicates a good agreement, showing deviations from 0.00% to 2.58%, 0.4% to 3.71%, and 0.12% to 2.04% for Ertuğrul (2002d), 0.32% to 2.28%, 0.09% to 2.45%, and 0.16% to 2.68% for Çalışkan *et al.* (2002), 0.11% to 0.93%, 0.19% to 1.21%, and 0.18% to 2.51% for Durak and Özdemir (1998), and 0.21% to 1.06%, 0.09% to 0.87%, and 0.19% to 1.44% for Ertuğrul *et al.* (1997a). These

deviation values correspond to η_{KL2}^R , η_{KL3}^R , and η_{KM}^R , respectively. Furthermore, excellent agreement is observed with the empirical values reported by Berkani *et al.* (2024)

Figure 6 further reinforces the validity of the approach by illustrating the ε_{RMS} between the semi-empirical calculations and experimental data for η_{KL}^T , η_{KL2}^R , η_{KL3}^R , and η_{KM}^R , across various elements. The ε_{RMS} values for most elements reside within a narrow range of 0% to 5%, indicating strong agreement between calculated results and experimental data. However, exceptions exist for certain elements: ^{38}Sr , ^{41}Nb , ^{44}Ru , ^{45}Rh , ^{46}Pd , ^{77}Ir , ^{83}Bi , ^{90}Th , and ^{92}U for η_{KL}^T , ^{23}V , ^{24}Cr , ^{27}Co , and ^{28}Ni for η_{KL2}^R and η_{KL3}^R , and ^{24}Cr , ^{28}Ni , ^{56}Ba , and ^{66}Dy for η_{KM}^R . As mentioned in a previous paper, these deviations likely stem from data heterogeneity, as values were sourced from diverse references with varying experimental conditions (Berkani *et al.* 2024). Despite these exceptions, the overall consistency of the ε_{RMS} values for most elements support the credibility of the semi-empirical results. Furthermore, the findings exhibit consistency with various theoretical, experimental, empirical, and semi-empirical studies, strengthening their validity.

4. Conclusion

This work presents a novel set of semi-empirical vacancy transfer probabilities η_{KL}^T , η_{KL2}^R , η_{KL3}^R , and η_{KM}^R , along with their corresponding fitting coefficients. These probabilities were determined using simple methods for a wide range of elements, covering atomic numbers $16 \leq Z \leq 92$ for η_{KL}^T , $24 \leq Z \leq 92$ for η_{KL2}^R and η_{KL3}^R , and $23 \leq Z \leq 92$ for η_{KM}^R . Notably, the results demonstrate relatively good agreement with data from other research groups across the entire atomic range, underscoring the effectiveness of the chosen methodology.

Beyond complementing existing data, the newly obtained semi-empirical vacancy transfer probabilities offer a valuable resource for the scientific and technical community. Their inclusion in atomic databases will provide researchers and professionals with a comprehensive

and up-to-date reference for various applications. Furthermore, this methodology contributes to theoretical atomic physics by refining vacancy transfer parameters, which are essential for improving electron interaction models. The enhanced dataset serves as a reliable benchmark for adjusting theoretical calculations of Auger and radiative transition rates, facilitating more accurate modeling of electron correlation and relativistic effects in heavy elements. These improvements are particularly significant for high- Z elements, where relativistic effects play a dominant role.

Figures captions:

Fig. 1. (a): Distribution of weighted values $(\eta_{KL}^T)_W$, The curve is the fitting according to the Eq. (4); (b): distribution of $\frac{(\eta_{KL}^T)_{\text{exp}}}{(\eta_{KL}^T)_W}$, the curve is the fitting according to Eq. (5), within the range $16 \leq Z \leq 92$ as a function of the atomic number Z .

Fig. 2. (a): Distribution of weighted values $(\eta_{KL2}^R)_W$, The curve is the fitting according to the Eq. (4); (b): distribution of $\frac{(\eta_{KL2}^R)_{\text{exp}}}{(\eta_{KL2}^R)_W}$, the curve is the fitting according to Eq. (5), within the range $24 \leq Z \leq 92$ as a function of the atomic number Z .

Fig. 3. (a): Distribution of weighted values $(\eta_{KL3}^R)_W$, , the curve is the fitting according to the Eq. (4); (b): distribution of $\frac{(\eta_{KL3}^R)_{\text{exp}}}{(\eta_{KL3}^R)_W}$, the curve is the fitting according to Eq. (5), within the range $24 \leq Z \leq 92$ as a function of the atomic number Z .

Fig. 4. (a): Distribution of weighted values $(\eta_{KM}^R)_W$, , the curve is the fitting according to Eq. (4), (b): distribution of $\frac{(\eta_{KM}^R)_{\text{exp}}}{(\eta_{KM}^R)_W}$, the curve is the fitting according to Eq. (5) (Fig. 1b), within the range $23 \leq Z \leq 92$ as a function of the atomic number Z .

Fig. 5. Comparison of current semi-empirical vacancy transfer probabilities with theoretical, fitted, and experimental values for η_{KL}^T , η_{KL2}^R , η_{KL3}^R , and η_{KM}^R as a function of atomic number Z .

Fig. 6. Root-mean-square error (ϵ_{RMS}) for η_{KL}^T , η_{KL2}^R , η_{KL3}^R , and η_{KM}^R as a function of atomic number Z .

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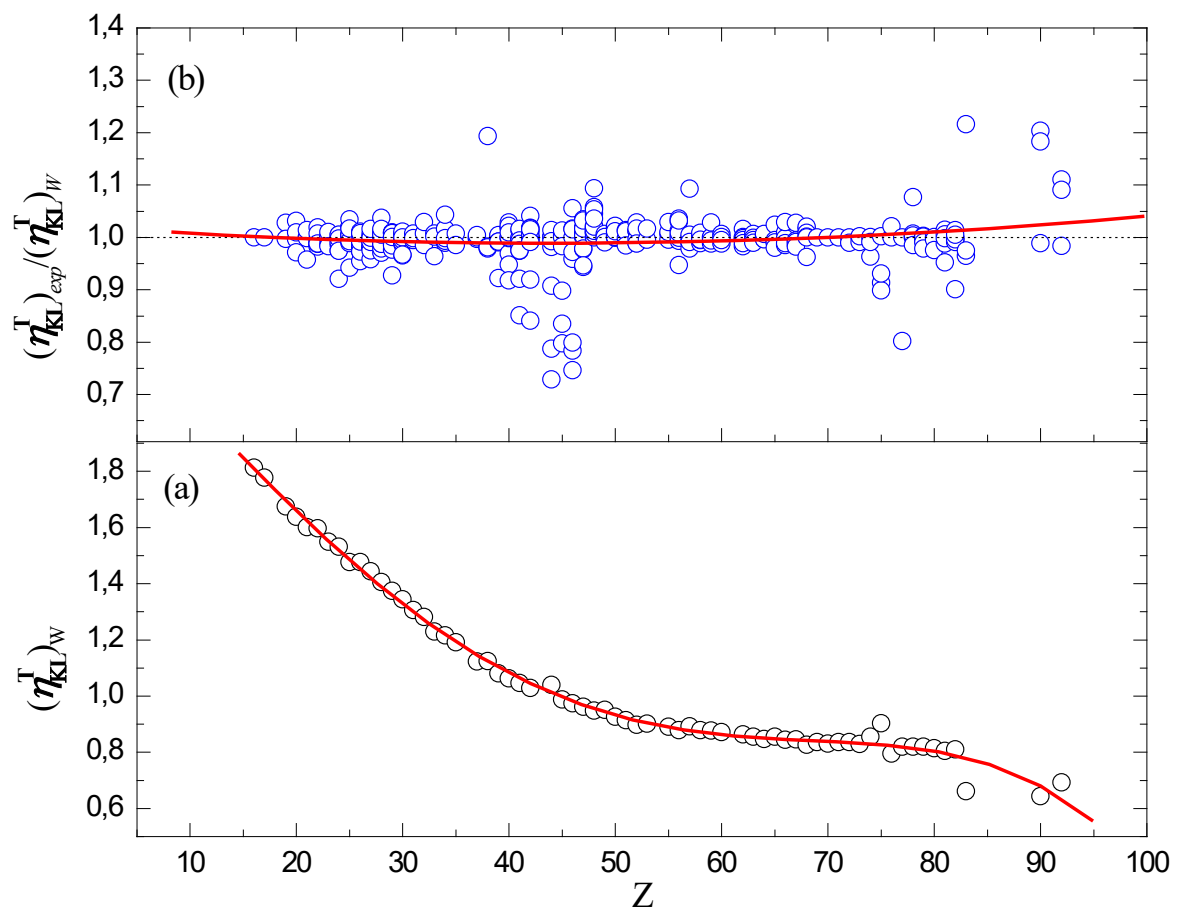


Fig. 1

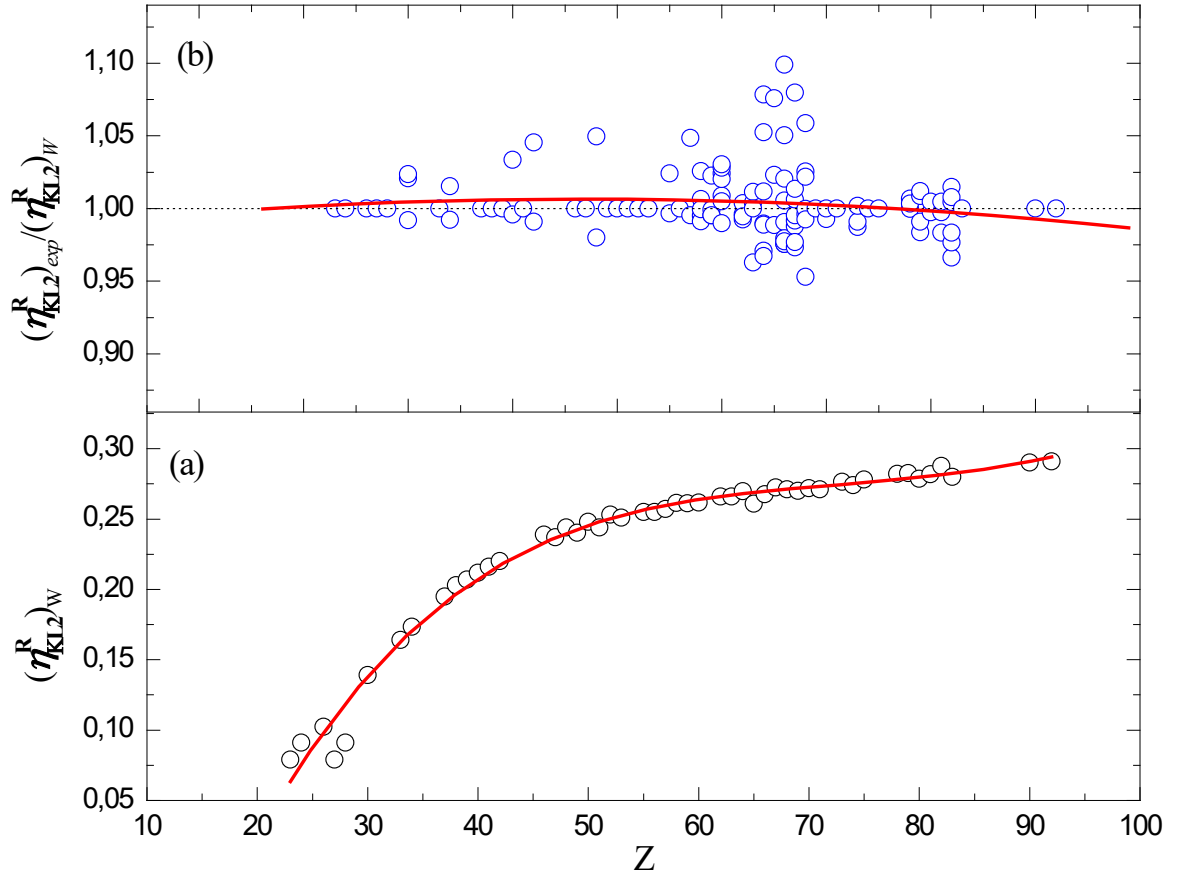


Fig. 2

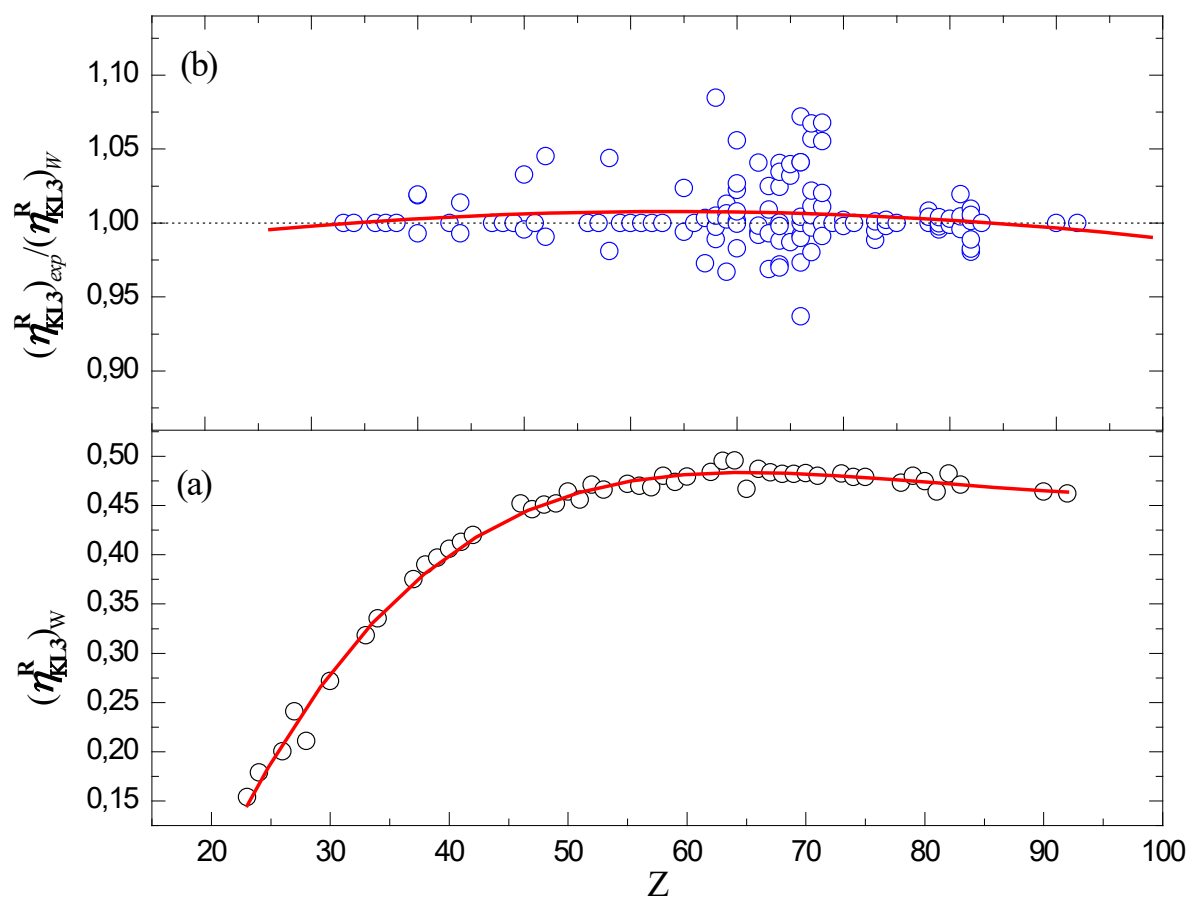


Fig. 3

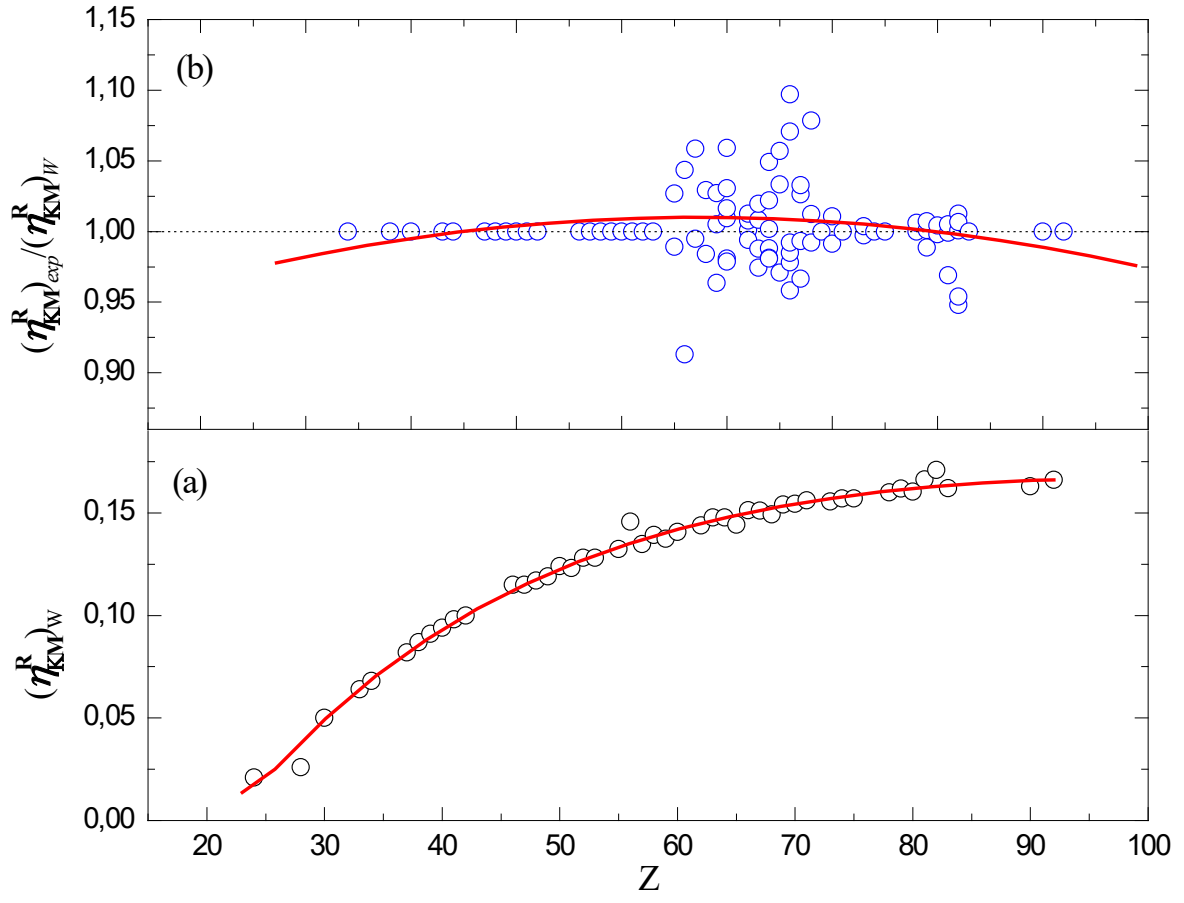


Fig. 4

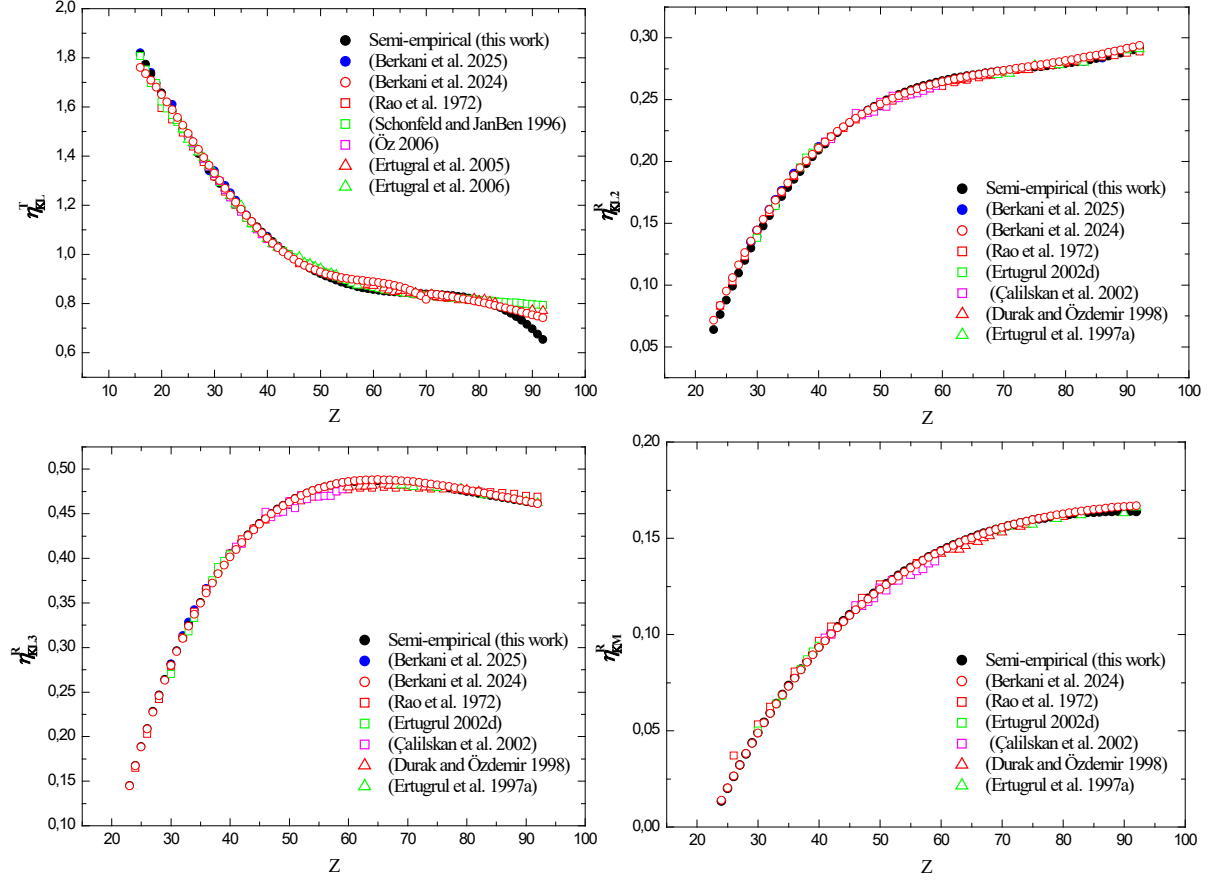


Fig. 5

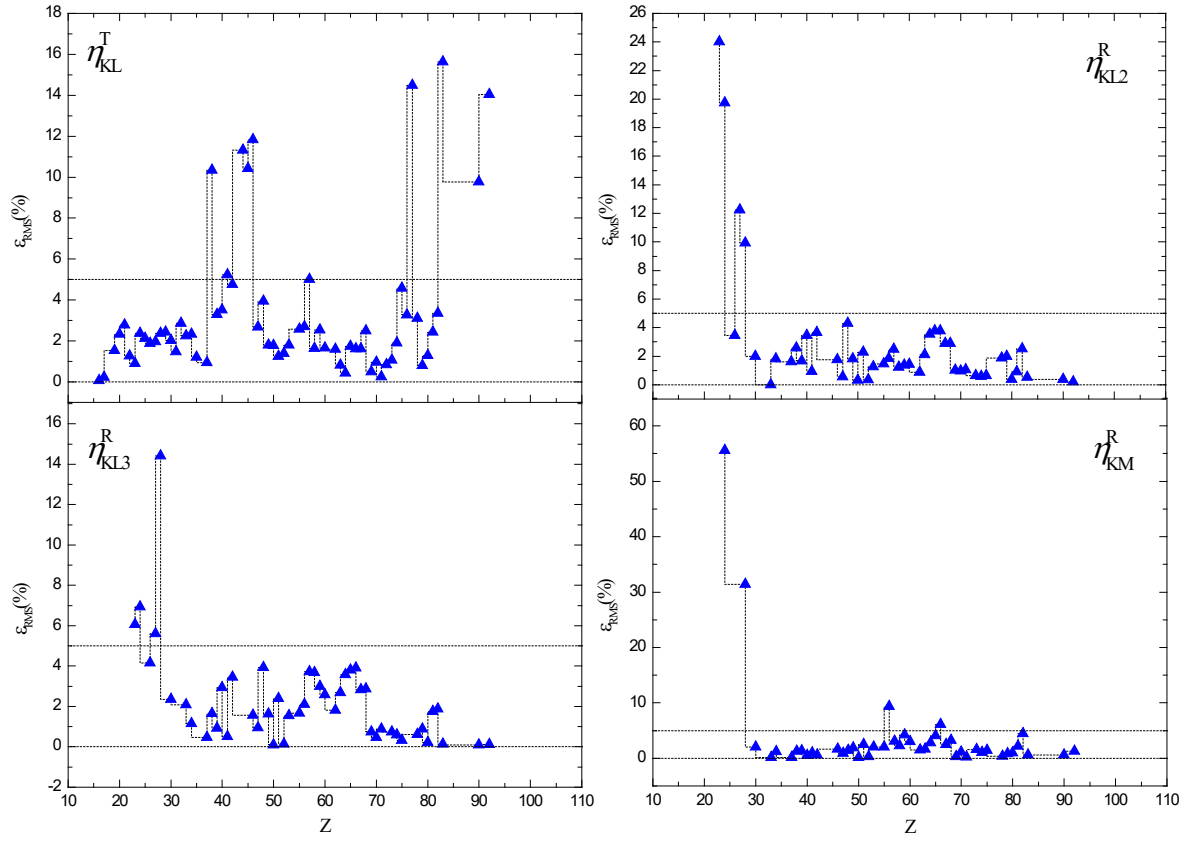


Fig. 6

Table 1. Summary of fitting coefficients and coefficients of determination (R^2) for calculating the semi-empirical values of vacancy transfer probabilities.

η	Z-group	The fitting coefficients according to eq (4)		The fitting coefficients according to eq (5)	
η_{KL}^T	16 to 92	A_0	2.43883	B_0	1.02081
		A_1	- 0.03711	B_1	- 0.00145
		A_2	3.40392×10^{-4}	B_2	1.64692×10^{-5}
		A_3	1.41458×10^{-5}		
		A_4	-9.10523×10^{-8}		
		R^2	0.99376		
η_{KL2}^R	23 to 92	A_0	- 0.40867	B_0	0.99074
		A_1	0.03019	B_1	6.75661×10^{-4}
		A_2	$- 4.96051 \times 10^{-4}$	B_2	$- 7.23948 \times 10^{-6}$
		A_3	3.49776×10^{-6}		
		A_4	$- 8.37308 \times 10^{-9}$		
		R^2	0.98460		
η_{KL3}^R	23 to 92	A_0	- 0.73512	B_0	0.98309
		A_1	0.05717	B_1	9.17699×10^{-4}
		A_2	$- 9.77319 \times 10^{-4}$	B_2	$- 8.52124 \times 10^{-6}$
		A_3	7.22962×10^{-6}		
		A_4	$- 1.98005 \times 10^{-8}$		
		R^2	0.99193		
η_{KM}^R	24 to 92	A_0	- 0.22884	B_0	0.94422
		A_1	0.01438	B_1	0.0023
		A_2	$- 2.12253 \times 10^{-4}$	B_2	-1.99925×10^{-5}
		A_3	1.53033×10^{-6}		
		A_4	$- 4.51053 \times 10^{-9}$		
		R^2	0.99221		

Table 2. Semi-empirical (this work), theoretical, fitted and experimental (other works) of total vacancy transfer probabilities $\eta_{\text{KL}}^{\text{T}}$ from $_{16}\text{S}$ to $_{92}\text{U}$.

Z, Symbol	This work		Other works			
	Semi-Empirical	$\varepsilon_{\text{RMS}}(\%)$	Theoretical (Berkani <i>et al.</i> 2025)	Empirical (Berkani <i>et al.</i> 2024)	Fitted (Schönfeld and JanBen 1996)	Experimental (Rao <i>et al.</i> 1972) (Ertuğral <i>et al.</i> 2006)
Z=16, S	1.8132	0.07	1.82	1.7596	1.807	
Z=17, Cl	1.7731	0.22		1.7348	1.751	
Z=18, Ar	1.7336		1.74	1.7082	1.697	
Z=19, K	1.6947	1.53		1.6801	1.697	
Z=20, Ca	1.6564	2.33		1.6507	1.621	1.595
Z=21, Sc	1.6188	2.77		1.6202	1.594	
Z=22, Ti	1.5820	1.26	1.61	1.5888	1.566	1.548
Z=23, V	1.5459	0.89		1.5569	1.539	
Z=24, Cr	1.5106	2.38		1.5244	1.508	1.495
Z=25, Mn	1.4762	2.13		1.4917	1.478	1.483 ^a
Z=26, Fe	1.4425	1.88		1.4589	1.447	1.451 ^a
Z=27, Co	1.4098	1.96		1.4262	1.418	1.418 ^a
Z=28, Ni	1.3779	2.38		1.3938	1.388	1.375
Z=29, Cu	1.3469	2.44	1.34	1.3617	1.357	1.357 ^a
Z=30, Zn	1.3169	2.03	1.34	1.3301	1.326	1.316
Z=31, Ga	1.2878	1.48		1.2992	1.294	1.298 ^a
Z=32, Ge	1.2597	2.87	1.28	1.2690	1.263	1.255
Z=33, As	1.2326	2.25	1.25	1.2397	1.232	1.231 ^a
Z=34, Se	1.2064	2.32	1.22	1.2113	1.202	1.200
Z=35, Br	1.1812	1.21		1.1840	1.174	1.174 ^a
Z=36, Kr	1.1570		1.16	1.1579	1.149	1.149
Z=37, Rb	1.1339	0.95		1.1329	1.125	1.128 ^a
Z=38, Sr	1.1117	10.34		1.1091	1.102	1.104
Z=39, Y	1.0905	3.29		1.0866	1.081	1.081 ^a
Z=40, Zr	1.0703	3.52	1.0727	1.0655	1.062	1.064
Z=41, Nb	1.0511	5.24		1.0457	1.045	1.044 ^a
Z=42, Mo	1.0329	4.76		1.0273	1.029	1.030
Z=43, Tc	1.0157			1.0103	1.014	
Z=44, Ru	0.9995	11.31		0.9946	1.000	1.000
Z=45, Rh	0.9842	10.42		0.9803	0.987	
Z=46, Pd	0.9699	11.84		0.9673	0.975	0.963
Z=47, Ag	0.9565	2.67		0.9556	0.964	
Z=48, Cd	0.9440	3.95	0.957	0.9451	0.953	0.952
Z=49, In	0.9324	1.8		0.9359	0.944	
Z=50, Sn	0.9217	1.77	0.936	0.9278	0.934	0.932
Z=51, Sb	0.9118	1.24		0.9208	0.925	
Z=52, Te	0.9028	1.39	0.92	0.9147	0.917	0.914
Z=53, I	0.8945	1.8		0.9095	0.909	
Z=54, Xe	0.8871			0.9051	0.902	0.899
Z=55, Cs	0.8803	2.58		0.9014	0.895	
Z=56, Ba	0.8743	2.69		0.8982	0.888	0.887
Z=57, La	0.8689	5.01		0.8954	0.882	
Z=58, Ce	0.8641	1.64		0.8929	0.876	0.876
Z=59, Pr	0.8600	2.54		0.8905	0.871	0.874 ^b
Z=60, Nd	0.8563	1.66		0.8880	0.866	0.877 ^b
Z=61, Pm	0.8532			0.8853	0.861	0.872 ^b
Z=62, Sm	0.8505	1.59		0.8822	0.857	0.857
Z=63, Eu	0.8482	0.82		0.8785	0.853	0.862 ^b
Z=64, Gd	0.8463	0.44		0.8740	0.85	0.853 ^b
Z=65, Tb	0.8447	1.74		0.8685	0.847	0.846 ^b
Z=66, Dy	0.8433	1.62		0.8617	0.843	0.851 ^b
Z=67, Ho	0.8421	1.62		0.8535	0.841	0.852 ^b
						0.841 ^b

Z=68, Er	0.8411	2.49		0.8435	0.838	0.836	0.843 ^b
Z=69, Tm	0.8401	0.49		0.8315	0.835		0.836 ^b
Z=70, Yb	0.8391	0.97		0.8173	0.833	0.831	0.831 ^b
Z=71, Lu	0.8380	0.24		0.8388	0.831		0.836 ^b
Z=72, Hf	0.8368	0.83		0.8359	0.829	0.826	0.827 ^b
Z=73, Ta	0.8354	1.07		0.8327	0.827		0.822 ^b
Z=74, W	0.8336	1.9		0.8294	0.825	0.821	0.823 ^b
Z=75, Re	0.8316	4.57		0.8260	0.823		0.824 ^b
Z=76, Os	0.8291	3.26		0.8224	0.821	0.816	
Z=77, Ir	0.8260	14.48		0.8186	0.819		0.819 ^b
Z=78, Pt	0.8224	3.1		0.8146	0.818	0.813	
Z=79, Au	0.8180	0.79		0.8105	0.816		0.820 ^b
Z=80, Hg	0.8129	1.29	0.811	0.8062	0.813	0.809	0.811 ^b
Z=81, Tl	0.8069	2.43		0.8017	0.812		0.816 ^b
Z=82, Pb	0.7999	3.36		0.7971	0.811	0.806	0.809 ^b
Z=83, Bi	0.7918	15.63	0.805	0.7923	0.809		0.803 ^b
Z=84, Po	0.7826			0.7873	0.807	0.805	
Z=85, At	0.7720			0.7822	0.805		
Z=86, Rn	0.7601		0.8	0.7769	0.804	0.802	
Z=87, Fr	0.7467			0.7714	0.803		
Z=88, Ra	0.7316			0.7658	0.801	0.798	
Z=89, Ac	0.7149			0.7600	0.799		
Z=90, Th	0.6962	9.77		0.7540	0.797	0.795	0.774 ^b
Z=91, Pa	0.6756			0.7479	0.795		
Z=92, U	0.6529	14.04		0.7416	0.794	0.793	0.770 ^b

^a(Öz 2006)

^b(Ertuğral *et al.* 2005)

Table 3. Semi-empirical (this work), theoretical, and experimental (other works) of radiative vacancy transfer probabilities η_{KL2}^R from ${}_{23}\text{V}$ to ${}_{92}\text{U}$.

Z, Symbol	This work		Other works		
	Semi-Empirical	$\varepsilon_{RMS}(\%)$	Theoretical (Berkani <i>et al.</i> 2025)	Experimental (Rao <i>et al.</i> 1972)	Empirical (Berkani <i>et al.</i> 2024)
Z=23, V	0.0637	24.02			0.0715
Z=24, Cr	0.0760	19.74		0.083	0.0835
Z=25, Mn	0.0877				0.0950
Z=26, Fe	0.0989	3.44		0.103	0.1059
Z=27, Co	0.1096	12.23			0.1163
Z=28, Ni	0.1199	9.92		0.123	0.1261
Z=29, Cu	0.1296		0.1348		0.1355
Z=30, Zn	0.1389	1.98	0.144	0.142	0.1444
Z=31, Ga	0.1477				0.1529
Z=32, Ge	0.1561		0.161	0.159	0.1608
Z=33, As	0.1640	0.00	0.169		0.1684
Z=34, Se	0.1716	1.82	0.176	0.175	0.1756
Z=35, Br	0.1787				0.1823
Z=36, Kr	0.1855		0.19	0.188	0.1887
Z=37, Rb	0.1919	1.62			0.1947
Z=38, Sr	0.1979	2.58		0.2	0.2004
Z=39, Y	0.2036	1.67			0.2057
Z=40, Zr	0.2090	3.45	0.2115	0.211	0.2108
Z=41, Nb	0.2140	0.93			0.2155
Z=42, Mo	0.2187	3.66		0.220	0.2199
Z=43, Tc	0.2232				0.2241
Z=44, Ru	0.2274			0.227	0.2280
Z=45, Rh	0.2313				0.2316
Z=46, Pd	0.2349	1.75		0.234	0.2350
Z=47, Ag	0.2383	0.55			0.2382
Z=48, Cd	0.2415	4.31	0.241	0.240	0.2411
Z=49, In	0.2444	1.80			0.2439
Z=50, Sn	0.2472	0.32	0.245	0.245	0.2465
Z=51, Sb	0.2497	2.28			0.2489
Z=52, Te	0.2521	0.36	0.25	0.249	0.2511
Z=53, I	0.2542	1.26			0.2532
Z=54, Xe	0.2562			0.253	0.2551
Z=55, Cs	0.2581	1.45			0.2569
Z=56, Ba	0.2598	1.85		0.256	0.2586
Z=57, La	0.2614	2.49			0.2602
Z=58, Ce	0.2628	1.23		0.259	0.2616
Z=59, Pr	0.2641	1.37			0.2630
Z=60, Nd	0.2653	1.44		0.261	0.2642
Z=61, Pm	0.2664				0.2654
Z=62, Sm	0.2675	0.88		0.264	0.2665
Z=63, Eu	0.2684	2.11			0.2676
Z=64, Gd	0.2693	3.55		0.266	0.2686
Z=65, Tb	0.2701	3.78			0.2695
Z=66, Dy	0.2708	3.77		0.268	0.2704
Z=67, Ho	0.2715	2.89			0.2712
Z=68, Er	0.2722	2.89		0.27	0.2721
Z=69, Tm	0.2728	1.03			0.2729
Z=70, Yb	0.2734	0.95		0.272	0.2737
Z=71, Lu	0.2739	1.06			0.2744
Z=72, Hf	0.2745			0.274	0.2752
Z=73, Ta	0.2751	0.64			0.2759
Z=74, W	0.2756	0.58		0.275	0.2767

Z=75, Re	0.2762	0.65			0.278 ^d	0.2775
Z=76, Os	0.2767			0.277		0.2782
Z=77, Ir	0.2773					0.2790
Z=78, Pt	0.2779	1.86		0.278		0.2798
Z=79, Au	0.2786	1.98			0.278 ^d	0.2806
Z=80, Hg	0.2793	0.37	0.28	0.28	0.280 ^c	0.2815
Z=81, Tl	0.2800	0.90				0.2823
Z=82, Pb	0.2807	2.50		0.281	0.281 ^c	0.2832
Z=83, Bi	0.2815	0.53	0.281		0.280 ^d	0.2841
Z=84, Po	0.2824			0.284		0.2851
Z=85, At	0.2833					0.2860
Z=86, Rn	0.2843		0.284	0.285		0.2870
Z=87, Fr	0.2853					0.2881
Z=88, Ra	0.2864			0.286		0.2891
Z=89, Ac	0.2876					0.2902
Z=90, Th	0.2889	0.38		0.288	0.290 ^d	0.2914
Z=91, Pa	0.2902					0.2925
Z=92, U	0.2916	0.21		0.289	0.291 ^d	0.2937

^a(Ertuğrul 2002d)

^b(Çalilskan *et al.* 2002)

^c(Durak and Özdemir 1998)

^d(Ertuğrul *et al.* 1997a)

Table 4. Semi-empirical (this work), theoretical, and experimental (other works) of radiative vacancy transfer probabilities η_{KL3}^R from ${}_{23}\text{V}$ to ${}_{92}\text{U}$.

Z, Symbol	This work		Other works		
	Semi-Empirical	$\varepsilon_{RMS}(\%)$	Theoretical (Berkani <i>et al.</i> 2025)	Experimental (Rao <i>et al.</i> 1972)	Empirical (Berkani <i>et al.</i> 2024)
Z=23, V	0.1452	6.06			0.1447
Z=24, Cr	0.1674	6.93		0.165	0.1669
Z=25, Mn	0.1887				0.1881
Z=26, Fe	0.2089	4.16		0.203	0.2083
Z=27, Co	0.2282	5.61			0.2275
Z=28, Ni	0.2465	14.40		0.242	0.2458
Z=29, Cu	0.2639		0.2637		0.2631
Z=30, Zn	0.2804	2.35	0.2815	0.279	0.2795
Z=31, Ga	0.2960				0.2951
Z=32, Ge	0.3108		0.3133	0.311	0.3099
Z=33, As	0.3248	2.09	0.3283		0.3239
Z=34, Se	0.3381	1.14	0.342	0.340	0.3370
Z=35, Br	0.3505				0.3495
Z=36, Kr	0.3623		0.3661	0.365	0.3612
Z=37, Rb	0.3733	0.46			0.3722
Z=38, Sr	0.3837	1.64		0.387	0.3826
Z=39, Y	0.3934	0.92			0.3923
Z=40, Zr	0.4024	2.93	0.405	0.405	0.4014
Z=41, Nb	0.4109	0.51			0.4098
Z=42, Mo	0.4188	3.45		0.421	0.4177
Z=43, Tc	0.4261				0.4251
Z=44, Ru	0.4329			0.433	0.4319
Z=45, Rh	0.4392				0.4383
Z=46, Pd	0.4450	1.57		0.443	0.4441
Z=47, Ag	0.4503	0.95			0.4495
Z=48, Cd	0.4551	3.92	0.4536	0.452	0.4544
Z=49, In	0.4595	1.63			0.4589
Z=50, Sn	0.4636	0.09	0.46	0.460	0.4630
Z=51, Sb	0.4672	2.40			0.4667
Z=52, Te	0.4704	0.13	0.4659	0.465	0.4701
Z=53, I	0.4733	1.54			0.4731
Z=54, Xe	0.4759			0.469	0.4758
Z=55, Cs	0.4782	1.67			0.4781
Z=56, Ba	0.4801	2.10		0.473	0.4802
Z=57, La	0.4818	3.71			0.4820
Z=58, Ce	0.4832	3.67		0.475	0.4835
Z=59, Pr	0.4844	3.00			0.4848
Z=60, Nd	0.4853	2.58		0.477	0.4859
Z=61, Pm	0.4860				0.4867
Z=62, Sm	0.4865	1.81		0.479	0.4873
Z=63, Eu	0.4869	2.68			0.4877
Z=64, Gd	0.4870	3.58		0.479	0.4880
Z=65, Tb	0.4870	3.81			0.4881
Z=66, Dy	0.4868	3.90		0.480	0.4880
Z=67, Ho	0.4865	2.83			0.4878
Z=68, Er	0.4861	2.87		0.479	0.4875
Z=69, Tm	0.4856	0.74			0.4870
Z=70, Yb	0.4850	0.46		0.480	0.4865
Z=71, Lu	0.4842	0.87			0.4858
Z=72, Hf	0.4834			0.479	0.4851
Z=73, Ta	0.4825	0.73			0.4842
Z=74, W	0.4816	0.58		0.478	0.4833

Z=75, Re	0.4806	0.33			0.479 ^d	0.4824
Z=76, Os	0.4796			0.478		0.4813
Z=77, Ir	0.4785					0.4803
Z=78, Pt	0.4774	0.61		0.477		0.4791
Z=79, Au	0.4763	0.89			0.478 ^d	0.4780
Z=80, Hg	0.4751	0.21	0.4755	0.476	0.476 ^c	0.4768
Z=81, Tl	0.4739	1.74				0.4755
Z=82, Pb	0.4728	1.88		0.475	0.474 ^c	0.4743
Z=83, Bi	0.4716	0.13	0.4732		0.471 ^d	0.4730
Z=84, Po	0.4704			0.474		0.4717
Z=85, At	0.4693					0.4704
Z=86, Rn	0.4681		0.4695	0.473		0.4691
Z=87, Fr	0.4670					0.4678
Z=88, Ra	0.4658			0.472		0.4665
Z=89, Ac	0.4647					0.4652
Z=90, Th	0.4636	0.09		0.470	0.464 ^d	0.4638
Z=91, Pa	0.4625					0.4625
Z=92, U	0.4615	0.11		0.469	0.462 ^d	0.4611

^a(Ertuğrul 2002d)

^b(Çalilskan *et al.* 2002)

^c(Durak and Özdemir 1998)

^d(Ertuğrul *et al.* 1997a)

Table 5. Semi-empirical (this work), theoretical, and experimental (other works) of radiative vacancy transfer probabilities $\eta_{\text{KM}}^{\text{R}}$ from ^{24}Cr to ^{92}U .

Z, Symbol	This work		Other works		
	Semi-Empirical	$\varepsilon_{\text{rms}}(\%)$	Experimental		Empirical
			(Rao <i>et al.</i> , 1972)		(Berkani <i>et al.</i> 2024)
Z=24, Cr	0.0135	55.56			0.0139
Z=25, Mn	0.0199				0.0202
Z=26, Fe	0.0261		0.0371		0.0263
Z=27, Co	0.0321				0.0322
Z=28, Ni	0.0379	31.40			0.0380
Z=29, Cu	0.0436				0.0435
Z=30, Zn	0.0490	2.04	0.0532	0.050 ^a	0.0488
Z=31, Ga	0.0542				0.0540
Z=32, Ge	0.0592		0.0624		0.0590
Z=33, As	0.0641	0.16		0.064 ^a	0.0638
Z=34, Se	0.0688	1.16		0.068 ^a	0.0685
Z=35, Br	0.0733				0.0730
Z=36, Kr	0.0777		0.0806		0.0773
Z=37, Rb	0.0819	0.12		0.082 ^a	0.0815
Z=38, Sr	0.0859	1.28		0.087 ^a	0.0855
Z=39, Y	0.0898	1.34		0.091 ^a	0.0894
Z=40, Zr	0.0935	0.53	0.0967	0.094 ^a	0.0931
Z=41, Nb	0.0971	0.93		0.098 ^b	0.0967
Z=42, Mo	0.1006	0.60	0.104	0.10 ^b	0.1002
Z=43, Tc	0.1039				0.1035
Z=44, Ru	0.1071				0.1067
Z=45, Rh	0.1102				0.1098
Z=46, Pd	0.1131	1.68		0.115 ^b	0.1127
Z=47, Ag	0.1160	0.86	0.119	0.115 ^b	0.1156
Z=48, Cd	0.1187	1.43		0.117 ^b	0.1183
Z=49, In	0.1213	1.90		0.119 ^b	0.1209
Z=50, Sn	0.1238	0.16	0.126	0.124 ^b	0.1234
Z=51, Sb	0.1261	2.46		0.123 ^b	0.1258
Z=52, Te	0.1284	0.31		0.128 ^b	0.1281
Z=53, I	0.1306	1.99		0.128 ^b	0.1303
Z=54, Xe	0.1327				0.1324
Z=55, Cs	0.1347	2.06		0.131 ^b	0.1344
Z=56, Ba	0.1366	9.33	0.137	0.133 ^b	0.1363
Z=57, La	0.1384	3.11		0.134 ^b	0.1382
Z=58, Ce	0.1402	2.25		0.137 ^b	0.1399
Z=59, Pr	0.1418	4.18		0.138 ^b	0.1416
Z=60, Nd	0.1434	2.99	0.143	0.142 ^c	0.1432
Z=61, Pm	0.1449				0.1447
Z=62, Sm	0.1463	1.46		0.144 ^c	0.1462
Z=63, Eu	0.1477	1.63		0.144 ^c	0.1476
Z=64, Gd	0.1490	2.76		0.146 ^c	0.1489
Z=65, Tb	0.1502	4.04	0.149		0.1501
Z=66, Dy	0.1514	6.11		0.148 ^c	0.1513
Z=67, Ho	0.1525	2.48		0.150 ^c	0.1524
Z=68, Er	0.1535	3.21		0.151 ^c	0.1535
Z=69, Tm	0.1545	0.32		0.154 ^d	0.1545
Z=70, Yb	0.1554	1.13	0.154	0.153 ^c	0.1555
Z=71, Lu	0.1563	0.19		0.156 ^d	0.1564
Z=72, Hf	0.1571				0.1573
Z=73, Ta	0.1579	1.55		0.156 ^c	0.1581
Z=74, W	0.1586	1.01		0.157 ^c	0.1588
Z=75, Re	0.1593	1.44		0.157 ^d	0.1596

Z=76, Os	0.1599			0.1603
Z=77, Ir	0.1605			0.1609
Z=78, Pt	0.1610	0.36		0.1615
Z=79, Au	0.1615	0.82	0.160 ^d	0.1621
Z=80, Hg	0.1620	0.98	0.161 ^c	0.1626
Z=81, Tl	0.1624	2.14		0.1631
Z=82, Pb	0.1627	4.45	0.163 ^c	0.1636
Z=83, Bi	0.1630	0.61	0.162 ^d	0.1641
Z=84, Po	0.1633			0.1645
Z=85, At	0.1635			0.1649
Z=86, Rn	0.1637			0.1652
Z=87, Fr	0.1638			0.1656
Z=88, Ra	0.1639			0.1659
Z=89, Ac	0.1640			0.1662
Z=90, Th	0.1640	0.61	0.163 ^d	0.1664
Z=91, Pa	0.1640			0.1667
Z=92, U	0.1639	1.28	0.166 ^d	0.1669

^a(Ertuğrul 2002d)

^b(Çalilskan *et al.* 2002)

^c(Durak and Özdemir 1998)

^d(Ertuğrul *et al.* 1997a)