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Screening Constant by Unit Nuclear Charge Calculations of Resonance Energies of the $_3(K, T, A)_n\ ^{1,3}L^\pi$ Rydberg Series of He-Like Ions

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Abstract: We report accurate energies of the $_3(2,0,+)_n\ ^1D^e$, $^1G^e$, $^3F°$, $_3(0, 2,+)_n\ ^1D^e$, $_3(1,1,+)_n\ ^3D^e$, $^3P^e$, $^3F^e$, $_3(-1,1,+)_n\ ^3P^e$, and $_3(1,1,+)_n\ ^1D°$, $^1F°$, series of He- like ions using the Screening constant by unit nuclear charge method. It is shown that the angular correlation quantum number *K* is effectively related to the cosinus of the angle between the position vectors of the two electrons.

Keywords: Resonance Energies, Rydberg Series, He-Like Ions, Classification Scheme

1. Introduction

Helium-like systems are very rich in structures attributed to doubly excited states with mixed configurations. Studies of autoionizing states in the helium isoelectronic sequence are very useful prototypes for the analysis of "many-particles" investigations. As the independent particles model is unappropriated for interpreting doubly excited states (DES) of He-like systems, most atomic spectra are treated on the classification scheme with the set of correlation quantum numbers *K*, *T* and *A*. For a given state of He-like systems, the classification scheme is labelled as $_N(K,T)_n^{A}\ ^{2S+1}L^\pi$ [1]. For the DES converging to the $N = 2$ hydrogenic threshold, the Screening constant by unit nuclear charge (SCUNC) has been used previously [2, 3] to report accurate results for He-like systems. Using the complex-coordinate rotation (CCR) method, Chung and Lin [4] studied over 540 doubly excited states of Li^+ resonances below the $N = 2$ and $N = 3$ thresholds and tabulated relativistic resonances parameters by grouping the DES into Rydberg series labelled in the (*K*, *T*, *A*) scheme classification. Using the Feshbach formalism, Bachau *et al.*, [5] reported a complete set of data belonging to the lowest resonances of $^{1,3}S^e$, $^{1,3}P°$, $^{1,3}D^e$, $^{1,3}F°$ and $^{1,3}G^e$ symmetries of He-like doubly excited states lying between the $N = 2$ and $N = 3$ thresholds with $Z = 2$-10. But, energy positions are missing for $Z > 10$ and in the NIST database, no data is quoted for the Rydberg series of the helium-isoelectronic series converging to the $N \geq 3$ hydrogenic thresholds. In addition, it is also challenging to succeed on interpreting quantitatively the physical meaning of the *K* correlation quantum number. In fact, if *T* is roughly speaking the projection of *L* onto the interelectronic axis and describes then the orientations between the orbitals of the two electrons, *K* is related to the cosinus of the interelectronic angle θ_{12} as $K \approx -\langle r_< \cos\theta_{12}\rangle$ where $r_<$ denotes the radius of the inner electron. Physically, the larger the positive value of *K*, the value of $-\cos\theta_{12}$ is closer to unity. In addition for states with positive *K*, r_{12} increases and $_N\langle r_{12}^{-1}\rangle_n$ decreases while for states with negative *K*, r_{12} decreases while $_N\langle r_{12}^{-1}\rangle_n$ increases as explained recently [6]. On the other hand, the set of new quantum models for interpreting atomic spectra must first be appropriated in the well description of electron-electron correlation and relativistic effects in two electron systems. So a complete description of all the Rydberg series belonging to the He-like systems is necessary.

The goal of the present study is to extend recent calculations of Sakho [6] on the $^{1,3}P°$ series to the $_3(2,0,+)_n$ $^1D^e$, $_3(0,2,+)_n$ $^1D^e$, $_3(1,1,+)_n$ $^3D^e$, $_3(1,1,+)_n$ $^3P^e$, $_3(-1,1,+)_n$ $^3P^e$, $_3(1,1,+)_n$ $^3F^e$, $_3(2,0,+)_n$ $^1G^e$, $_3(1,1,+)_n$ $^1D°$, $_3(1,1,+)_n$ $^1F°$, and $_3(2,0,+)_n$ $^3F°$ Rydberg series of Helium - like ions (Z =3-40) applying the Screening constant by unit nuclear charge (SCUNC) method. Quantitative interpretation of the *K*-angular correlation quantum number is also aimed in this work. In section 2 presents the theoretical procedure adopted in this work. The results obtained are discussed in section 3,

2. Theory

2.1. Brief Description of the SCUNC Formalism

In the framework of Screening constant by unit Nuclear charge formalism, total energy of $(N\ell, n\ell')\,^{2S+1}L^{\pi}$ excited states are expressed in the form

$$E(N\ell n\ell'\,;\,^{2S+1}L^{\pi}) = -Z^2\left(\frac{1}{N^2} + \frac{1}{n^2}\left[1 - \beta(N\ell n\ell'\,;\,^{2S+1}L^{\pi}\,;\,Z)\right]^2\right)\text{Ryd} \tag{1}$$

In this equation, the principal quantum numbers *N* and *n*, are respectively for the inner and the outer electron of He-isoelectronic series. In this equation, the β-parameters are screening constant by unit nuclear charge expanded in inverse powers of *Z* and given by

$$\beta(N\ell\, n\ell'\,;\,^{2S+1}L^{\pi}\,;\,Z) = \sum_{k=1}^{q} f_k\left(\frac{1}{Z}\right)^k \tag{2}$$

where $f_k = f_k(N\ell\, n\ell'\,;\,^{2S+1}L^{\pi})$ are parameters to be evaluated.

With respect to the new classification scheme, equation (1) takes the form [2, 3]

$$E\left[_N(K,T)_n^A\ ^{2S+1}L^{\pi}\right] = -Z^2\left\{\frac{1}{N^2} + \frac{1}{n^2}\left(1 - \beta\left[_N(K,T)_n^A;\ ^{2S+1}L^{\pi}\,;\,Z\right]\right)^2\right\}\text{Ryd} \tag{3}$$

Using equation (2), we get from (3)

$$E\left[_N(K,T)_n^A\ ^{2S+1}L^{\pi}\right] = -Z^2\left\{\frac{1}{N^2} + \frac{1}{n^2}\left[1 - \sum_{k=1}^{q} f_k\left(_N(K,T)_n^A;\ ^{2S+1}L^{\pi}\right)\times\left(\frac{1}{Z}\right)^k\right]^2\right\}\text{Ryd} \tag{4}$$

2.2. Expressions of the Resonance Energies

For all the Rydberg series investigated in the present work and lying to the *N* = 3 hydrogenic threshold, total energy is expressed as follows using Eq. (4)

$$E_n = -Z^2\left\{\frac{1}{9} + \frac{1}{n^2}\left(1 - \frac{f_1[(K,T,A)\ ^{2S+1}L^{\pi}]}{Z(n-1)} - \frac{f_2[(K,T,A)\ ^{2S+1}L^{\pi}]}{Z} + \frac{f_1[(K,T,A)\ ^{2S+1}L^{\pi}]\times(Z-Z_0)}{Z^3(n+3)}\right)^2\right\}\text{Ryd}\,. \tag{5}$$

The $f_1[(K,T,A)\ ^{2S+1}L^{\pi}]$-screening constants in Eq. (5) are evaluated from accurate relativistic data of Chung and Lin [4] on Li^+. To take into account the effect of the nucleus volume with increasing *Z*, a tiny correction of type we have introduced in Eq. (5)

$$\frac{f_1[(K,T,A)\ ^{2S+1}L^{\pi}]\times(Z-Z_0)}{Z^3(n+3)}$$

The $f_1[(K,T,A)\ ^{2S+1}L^{\pi}]$-screening constants in Eq. (5) are evaluated from accurate relativistic data of Chung and Lin [4] on Li^+ (Z_0 = 3). If we denote by $E\,[_3(T,K,A)_n\,^{2S+1}L^{\pi}]$ the energy positions measured with respect to the ground state E_0 of Li^+, total energy (5) is given by

$$E_n = E\,[_3(T,K,A)_n{}^{2S+1}L^{\pi}] - E_0. \tag{6}$$

For Li^+, E_0 = – 198.0977 eV and the reduced Rydberg is equal to 13.604635 eV [4].

The present study is limited to the Rydberg series starting with the lowest *n* = 3 resonance.

3. Results and Discussion

The results obtained in this work are listed in Tables 1-6.

The resonances are ordered so that total energy decreases along the series. For example, the total energies of the $_3(2,0)_n^+$ $^1D^e$ series are greater than those of the $_3(1,1)_n^+$ $^3P^e$ resonances. These states are then first listed in Table 1. The order of the other series are of similar. To clarify accuracy in the present calculations, some data are compared with the Feshbach formalism (FF) computations of Bachau *et al*., [5]. For Table 1 where total energies of the $_3(2,0)_n^+$ $^1D^e$, $_3(1,1)_n^+$ $^3P^e$, $_3(2,0)_n^+$ $^3F°$ and $_3(1,1)_n^+$ $^1D°$ (*n* = 3-4) (*n* = 3-4) Rydberg states of He-like ions (Z = 3-12) are listed, the agreements are seen to be very good. It should be underlined the lack of precision in the FF computations for the $_3(2,0)_3^+$ $^3F°$ and $_3(1,1)_3^+$ $^1D°$ levels mentioned with the same value of total energies at 10.4800 a. u. For these levels, the present SCUNC predictions are equal to 10.4871 a. u for the $_3(2,0)_3^+$ $^3F°$ level and 10.4726 a. u. for the $_3(1,1)_3^+$ $^1D°$ state. The SCUNC data at 10.4726 a. u. may then be preferable.

Table 1. *Total energy (–E, in a. u) for the* $_3(2,0)_n^+$ $^1D^e$*,* $_3(1,1)_n^+$ $^3P^e$*,* $_3(2,0)_n^+$ $^3F°$ *and* $_3(1,1)_n^+$ $^1D°$ *(n = 3-4) (n = 3-4) Rydberg series of Helium-like ions (Z = 3-12). The present screening constant by unit nuclear charge (SCUNC) calculations are compared with the Feshbach formalism (FF) results of Bachau et al., [5].*

	$_3(2,0)_n^+$ $^1D^e$				$_3(1,1)_n^+$ $^3P^e$			
n	3		4		3		4	
Z	SCUNC	FF	SCUNC	FF	SCUNC	FF	SCUNC	FF
3	0.8422	0.8447	0.6686	0.6697	0.8313	0.8331	0.6611	0.6618
4	1.5663	1.5670	1.2356	1.2360	1.5512	1.5510	1.2250	1.2250
5	2.5112	2.5110	1.9757	1.9760	2.4919	2.4910	1.9619	1.9620
6	3.6776	3.6770	2.8891	2.8890	3.6540	3.6530	2.8720	2.8720
7	5.0658	5.0650	3.9758	3.9750	5.0378	5.0370	3.9555	3.9560
8	6.6758	6.6750	5.2361	5.2360	6.6436	6.6440	5.2125	5.2140
9	8.5079	8.5080	6.6698	6.6700	8.4713	8.4720	6.6430	6.6450
10	10.5621	10.5600	8.2771	8.2770	10.5211	10.5220	8.2470	8.2500
11	12.8384		10.0579		12.7930		10.0246	
12	15.3368		12.0123		15.2870		11.9758	
	$_3(2,0)_n^+$ $^3F°$				$_3(1,1)_n^+$ $^1D°$			
n	3		4		3		4	
Z	SCUNC	FF	SCUNC	FF	SCUNC	FF	SCUNC	FF
3	0.8230	0.8244	0.6598	0.6602	0.8191	0.8201	0.6560	0.6563
4	1.5389	1.5380	1.2229	1.2220	1.5336	1.5333	1.2176	1.2170
5	2.4758	2.4730	1.9591	1.9580	2.4691	2.4680	1.9522	1.9520
6	3.6342	3.6300	2.8686	2.8680	3.6260	3.6260	2.8600	2.8600
7	5.0144	5.0100	3.9515	3.9500	5.0047	5.0050	3.9413	3.9410
8	6.6166	6.6110	5.2079	5.2070	6.6053	6.6070	5.1960	5.1960
9	8.4408	8.4350	6.6377	6.6370	8.4279	8.4310	6.6242	6.6250
10	10.4871	10.4800	8.2412	8.2400	10.4726	10.4800	8.2260	8.2270
11	12.7555		10.0182		12.7394		10.0013	
12	15.2460		11.9687		15.2284		11.9502	

Table 2 compares the present SCUNC charge results for excited $_3(0,2)_n^+$ 3D°, $_3(0,2)_n^+$ 1De (n = 3-4), $_3(1,1)_n^+$ 3Fe and $_3(2,0)_n^+$ 1Ge states of He-like ions with the FF predictions of Bachau *et al*., [5]. Here again, the agreements between the calculations are very good up to $Z = 10$.

Table 2. *Total energy (–E, in a. u) for the* $_3(0,2)_n^+$ $^3D°$*,* $_3(0,2)_n^+$ $^1D^e$ *(n = 3-4),* $_3(1,1)_n^+$ $^3F^e$ *and* $_3(2,0)_n^+$ $^1G^e$ *Rydberg series of He-like ions (Z = 3-12). The present screening constant by unit nuclear charge (SCUNC) calculations are compared with the Feshbach formalism (FF) results of Bachau et al., [5].*

	$_3(0,2)_n^+$ $^3D°$				$_3(0,2)_n^+$ $^1D^e$			
n	3		4		3		4	
Z	SCUNC	FF	SCUNC	FF	SCUNC	FF	SCUNC	FF
3	0.7973	0.7970	0.6436	0.6434	0.7964	0.7957	0.6430	0.6427
4	1.5027	1.5010	1.1995	1.1980	1.5014	1.4980	1.1987	1.1970
5	2.4291	2.4260	1.9285	1.9260	2.4274	2.4230	1.9274	1.9240
6	3.5768	3.5740	2.8307	2.8270	3.5748	3.5700	2.8293	2.8250
7	4.9464	4.9440	3.9063	3.9020	4.9439	4.9380	3.9047	3.8990
8	6.5378	6.5360	5.1554	5.1500	6.5349	6.5300	5.1535	5.1460
9	8.3512	8.3510	6.5780	6.5720	8.3480	8.3430	6.5758	6.5670
10	10.3867	10.3900	8.1741	8.1670	10.3831	10.3800	8.1716	8.1620
11	12.6443		9.9437		12.6403		9.9410	
12	15.1241		11.8870		15.1197		11.8840	

	$_3(1,1)_n^+$ $^3F^e$				$_3(2,0)_n^+$ $^1G^e$			
n	3		4		3		4	
Z	SCUNC	FF	SCUNC	FF	SCUNC	FF	SCUNC	FF
3	0.7883	0.7886	0.6465	0.6462	0.7759	0.7769	0.6412	0.6410
4	1.4884	1.4880	1.2032	1.2040	1.4703	1.4660	1.1952	1.1940
5	2.4099	2.4100	1.9331	1.9350	2.3862	2.3770	1.9225	1.9200
6	3.5532	3.5554	2.8363	2.8410	3.5238	3.5090	2.8233	2.8200
7	4.9183	4.9210	3.9131	3.9190	4.8834	4.8640	3.8975	3.8950
8	6.5054	6.5090	5.1633	5.1720	6.4650	6.4410	5.1452	5.1420
9	8.3147	8.3200	6.5871	6.5980	8.2687	8.2400	6.5665	6.5640
10	10.3460	10.3500	8.1845	8.1980	10.2945	10.2600	8.1613	8.1590
11	12.5995		9.9554		12.5425		9.9297	
12	15.0752		11.8999		15.0126		11.8717	

The very good agreements between the SCUNC and the FF [5] calculations are also obtained comparing the results quoted in Table 3 and 4 respectively for the $_3(1, 1)_n^+$ $^1F°$, $_3(-1, 1)_n^+$ $^3P^e$ and $_3(1, 1)_n^+$ $^3D^e$ (n = 3-4) states of He-like ions (Z = 3-10).

Table 3. *Total energy (–E, in a. u) for the* $_3(1, 1)_n^+$ $^1F°$ *and* $_3(-1, 1)_n^+$ $^3P^e$ *(n = 3-4) Rydberg series of He-like ions (Z = 3-12). The present screening constant by unit nuclear charge (SCUNC) calculations are compared with the Feshbach formalism (FF) results of Bachau et al., [5].*

	$_3(1, 1)_n^+$ $^1F°$				$_3(-1, 1)_n^+$ $^3P^e$			
n	**3**		**4**		**3**		**4**	
Z	**SCUNC**	**FF**	**SCUNC**	**FF**	**SCUNC**	**FF**	**SCUNC**	**FF**
3	0.7720	0.7710	0.6425	0.6420	0.7557	0.7560	0.6250	0.6251
4	1.4640	1.4580	1.1969	1.1970	1.4418	1.4430	1.1717	1.1700
5	2.3777	2.3660	1.9247	1.9260	2.3490	2.3510	1.8915	1.8890
6	3.5133	3.4960	2.8259	2.8290	3.4778	3.4820	2.7846	2.7820
7	4.8709	4.8480	3.9007	3.9060	4.8285	4.8360	3.8511	3.8480
8	6.4505	6.4220	5.1490	5.1560	6.4012	6.4110	5.0912	5.0870
9	8.2523	8.2190	6.5708	6.5790	8.1958	8.2090	6.5048	6.5010
10	10.2763	10.2400	8.1662	8.1770	10.2126	10.2300	8.0919	8.0880
11	12.5224		9.9352		12.4515		9.8526	
12	14.9907		11.8778		14.9125		11.7868	

Table 4. *Total energy (–E, in a. u) for the* $_3(1, 1)_n^+$ $^3D^e$ *(n = 3-4) Rydberg series of Helium-like ions (Z = 3-12). The present screening constant by unit nuclear charge (SCUNC) calculations are compared with the Feshbach formalism (FF) results of Bachau et al., [5].*

n	**3**		**4**	
Z	**SCUNC**	**FF**	**SCUNC**	**FF**
3	0.8131	0.8131	0.6530	0.6533
4	1.5251	1.5240	1.2131	1.2120
5	2.4580	2.4550	1.9463	1.9440
6	3.6125	3.6090	2.8528	2.8500
7	4.9887	4.9850	3.9327	3.9290
8	6.5868	6.5830	5.1861	5.1810
9	8.4069	8.4040	6.6129	6.6060
10	10.4491	10.4500	8.2133	8.2050
11	12.7134		9.9873	
12	15.1998		11.9348	

Table 5 presents calculations of excitation energies for doubly $^{1,3}L^e$ (L = P, D, F, G) and $^{1,3}L°$ (L = D, F) excited states of He-like (Z = 4-10) systems. Energies are calculated with respect to the ground state of the corresponding system. Comparison is done with some literature data such as those from Density functional theory (DFT) of Roy *et al.*, [11], Complex rotation method (CCR) of Ho and Bathia [12], time-dependent variation perturbation (TDVP) of Ray and Mukherjee [13] and those from Multiconfiguration (MC) of Lipsky *et al.*, [14]. It should be underlined that, in the DFT and TDVP models, the doubly excited states are labeled in the *Nlnl'* $^{2S+1}L^{\pi}$ notation disregarding the appropriated $_N(K, T, A)_n$ $^{2S+1}L^{\pi}$ classification scheme. Overall good agreement are obtained between the calculations.

Table 5. *Excitation energy for doubly* $^{1,3}L^e$ *and* $^{1,3}L°$ *excited states of He-like Be III (Z = 4) and B VI (Z = 5) ions. The results of Bachau et al., [5] have been calculated here by using the same ground state from NIST [15]. The other results published in a. u are taken from Roy et al., [11].*

		$_3(0,2)_3^+$ $^1D^e$	$_3(0,2)_4^+$ $^1D^e$	$_3(1,1)_3^+$ $^3D^e$	$_3(1,1)_3^+$ $^1F°$	$_3(1,1)_4^+$ $^1F°$
4	SCUNC	12.1552	12.4579	12.1315	12.1926	12.4597
	FF	12.1586	12.4596	12.1326	12.1986	12.4596

	CCR	12.1567				
	DFT	12.1454	12.4528	12.1272	12.2227	12.4590
	TDVP	12.1323	12.4394	12.1343	12.1999	12.4598
	MC				12.1988	12.4592
5	SCUNC	19.6074	20.1074	19.5767	12.6571	20.1101
	FF	19.6118	20.1108	19.5798	19.6688	20.1088
	CCR	19.6076		19.5766		
	DFT	19.5906	20.0975	19.5678	12.6877	20.1052
	TDVP	19.5992	20.0853		12.6628	20.1157
	MC			19.5812	12.6663	20.1055
		${}_3(1,1)_4^+\ {}^3D^e$	${}_3(1,1)_5^+\ {}^3D^e$	${}_3(2,0)_3^+\ {}^3F^o$	${}_3(2,0)_4^+\ {}^3F^o$	${}_3(2,0)_5^+\ {}^3F^o$
4	SCUNC	12.4435	12.5706	12.1177	12.4337	12.5637
	FF	12.4446		12.1186	12.4346	
	MC	12.4462	12.5678	12.1209	12.4365	12.5618
	DFT	12.4398	12.5616	12.1110	12.4431	
5	SCUNC	20.0884	20.3029	19.5590	20.0757	20.2938
	FF	20.0908		19.5618	20.0768	
	DFT	20.0798	20.2882	19.5479	20.0843	20.2901
	MC	20.0925	20.2992	19.5643	20.0794	20.2911

SCUNC, Screening constant by unit nuclear charge, present work
FF, Feshbach formalism, Bachau *et al*., [5].
DFT, Density functional theory, Roy et al., [11].
CCR, complex rotation method, Ho and Bathia [12].
TDVP, time-dependent variation perturbation, Ray and Mukherjee [13].
MC, Multiconfiguration, Lipsky *et al*. [14].

On the other hand, according to the physical meaning of the K correlation angular quantum number, for states with positive K, the two electrons tend to stay on the opposite sides of the nucleus while in states with negative K the two electrons tend to stay on the same side of the nucleus. In addition, the angular correlation quantum number K is related to the cosinus of the interelectronic angle θ12 as $K \approx -\langle r_< \cos\theta_{12}\rangle$ where $r_<$ denotes the radius of the inner electron. Physically, the larger the positive value of K, the value of $-\cos\theta_{12}$ is closer to unity. These statements can be verified quantitatively in the framework of the SCUNC method by evaluating the radial expectation values ${}_N\langle r_{12}^{-1}\rangle_n$ given by (in a.u) [6]

$$ {}_N\left\langle \frac{1}{r_{12}} \right\rangle_n = \frac{Z^2}{2N^2} + \frac{Z^2}{2n^2} - E\left[{}_N(K,T)_n^A\ {}^{2S+1}L^{\pi}\right]. \quad (7) $$

For the $N = 3$ threshold, we get

$$ {}_3\left\langle \frac{1}{r_{12}} \right\rangle_n = \frac{Z^2}{18} + \frac{Z^2}{2n^2} - E\left[{}_3(K,T)_n^A\ {}^{2S+1}L^{\pi}\right]. \quad (8) $$

Then

- The larger the positive value of K, the value of $-\cos\theta_{12}$ is closer to unity and $\theta_{12} \to \pi$. Subsequently, the interelectronic distance r_{12} increases and ${}_3\langle r_{12}^{-1}\rangle_n$ decreases.

- For states with positive K, the two electrons tend to stay on the opposite sides of the nucleus, as a results the interelectronic distance r_{12} increases and ${}_3\langle r_{12}^{-1}\rangle_n$ decreases.

-For states with negative K the two electrons tend to stay on the same side of the nucleus. The interelectronic distance r_{12} decreases while ${}_3\langle r_{12}^{-1}\rangle_n$ increases.

So, quantitatively, ${}_3\langle r_{12}^{-1}\rangle_n$ $(K > 0) <$ ${}_3\langle r_{12}^{-1}\rangle_n$ $(K < 0)$.

Table 6 lists radial expectation values ${}_3\langle r_{12}^{-1}\rangle_3$ for the ${}_3(0,2)_3^+$ 1De, ${}_3(2,0)_3^+\ {}^1D^e$, ${}_3(1,1)_3^+\ {}^3F^e$, ${}_3(2,0)_3^+\ {}^3F^o$, ${}_3(1,1)_3^+\ {}^3P^e$ and ${}_3(-1,1)_3^+\ {}^3P^e$ levels of some He-like ions (Z = 3-10). Comparison shows clearly that, for both ${}_3(0,2)_3^+\ {}^1D^e$, ${}_3(2,0)_3^+\ {}^1D^e$ ($K = 0$ and $K = 2$), ${}_3(1,1)_3^+\ {}^3F^e$, ${}_3(2,0)_3^+\ {}^3F^o$ ($K = 1$ and $K = 2$), the radial expectation values ${}_3\langle r_{12}^{-1}\rangle_3$ is lower for the greater value of K. As a result, r_{12} increases and $\theta_{12} \to \pi$ so $-\cos\theta_{12}$ tend to unity. This confirms quantitatively that the larger the positive value of K, the value of $-\cos\theta_{12}$ is closer to unity. Besides, for the ${}_3(1,1)_3^+\ {}^3P^e$ and ${}_3(-1,1)_3^+\ {}^3P^e$ levels where K takes the values 1 and – 1.

Table 6. *Present calculations of radial expectation values* ${}_3\langle r_{12}^{-1}\rangle_3$ *(in a. u) for quantitative interpretation of the correlation quantum number K.*

Z	${}_3(0,2)_3^+$ ${}^1D^e$	${}_3(2,0)_3^+$ ${}^1D^e$	${}_3(1,1)_3^+$ ${}^3F^e$	${}_3(2,0)_3^+$ ${}^3F^o$	${}_3(1,1)_3^+$ ${}^3P^e$	${}_3(-1,1)_3^+$ ${}^3P^e$
3	0.204	0.158	0.212	0.177	0.169	0.244
4	0.276	0.211	0.289	0.239	0.227	0.336
5	0.350	0.267	0.368	0.302	0.286	0.429
6	0.425	0.322	0.447	0.366	0.346	0.522
7	0.501	0.379	0.526	0.430	0.407	0.616
8	0.576	0.435	0.606	0.495	0.468	0.710
9	0.652	0.492	0.685	0.559	0.529	0.804
10	0.728	0.549	0.765	0.624	0.590	0.899

Table 6 shows clearly that, the radial expectation values $_3\langle r_{12}^{-1}\rangle_3$ is lower for $K = 1$. This important result indicates again that $_N\langle r_{12}^{-1}\rangle_n$ (K > 0) < $_N\langle r_{12}^{-1}\rangle_n$ (K < 0) as demonstrated in the recent work of Sakho [6].

4. Conclusion

In this paper, accurate resonance energies of the $_3(K, T, A)_n$ $^{1,3}L^{\pi}$ Rydberg series of the helium-like ions (Z = 3-12) are reported. Calculations are performing in the framework of the Screening constant by unit nuclear charge formalism. Good agreements are obtained with various literature data. In contrast with all the existing *ab initio* methods for which resonance energies cannot be calculated directed from analytical formula, it is demonstrated in this work the possibilities to report accurate resonance from a simple and single analytical formula. It should be underlined that, no resonance energies are listed in the NIST database for the $N > 2$ thresholds for many He-like systems. The present calculations may then be very useful for the NIST team as far as critical evaluation of atomic data relative to the doubly $_3(K, T, A)_n$ $^{1,3}L^{\pi}$ excited states in the Helium-like systems are concerned

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