

Few-body model approach to the bound states of helium-like exotic three-body systems

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Abstract. In this paper, calculated energies of the lowest bound S-state of Coulomb three-body systems containing an electron (e^-), a negatively charged muon (μ^-) and a nucleus (N^{Z+}) of charge number Z are reported. The 3-body relative wave function in the resulting Schrödinger equation is expanded in the complete set of hyperspherical harmonics (HH). Use of the orthonormality of HH leads to an infinite set of coupled differential equations (CDE) which are solved numerically to get the energy E .

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1. Introduction

Atoms and ions containing exotic particles like muon, kaon, taon, baryon and their antimatters are of immense have become an interesting research topic in many branches of physics including atomic, nuclear and elementary particle physics, plasma and astrophysics, experimental physics [1, 2]. Apart from being the simplest exotic atom formed by replacing an orbital electron of neutral helium, the muonic helium atom (${}^4\text{He}^{2+}\mu^-e^-$) is an important topic of investigation since its first formation and detection by Souder et al [3]. Muon being about 207 times heavier than an electron, the size of the muonic helium atom is smaller by a factor of about 1/400 of the ordinary electronic helium atom. Muonic helium atoms are the unusual pure atomic three body systems without any restriction due to Pauli exclusion principle for electron and muon being non-identical fermions. These are formed as by-products of the process of muon catalyzed fusion, hence are useful to understand the fusion reactions properly [4, 5]. The electromagnetic interaction between the electron and negatively charged muon can be better understood by this simplest muonic system by precise measurements of hyperfine structure [6, 7].

As exotic particles are mostly unstable, their parent atoms (or ions) are also very short lived. These exotic short-lived atoms or ions can be formed by trapping the accelerated exotic particles inside matter and replacing one or more electron(s) in an ordinary atom by exotic particle(s). The absorbed exotic particle revolves round the



nucleus of the target atom in orbit of radius equal to that of the electron before its ejection from the atom, which subsequently cascades down the ladder of resulting exotic atomic states by the emission of X-rays and Auger transitions before being lost on its way to the nucleus. If the absorbed exotic particle is a negatively charged muon, it passes through various intermediate atmospheres before being trapped in the vicinity of the atomic nucleus [8]. In the course of its journey inside the matter, it scatters from atom to atom as free electron and gradually loses its energy until it is captured into an atomic orbit. In the lowest energy level (1S), it experiences only Coulomb interaction with nuclear protons while it experiences weak interaction with the rest of the nucleons. As discussed above, exotic muonic atoms (or ions) are produced by replacing one or more electron(s) of neutral atoms by one or more exotic particle(s) like muon, pion, kaon, anti-proton having an electric charge equal to that of the electron [9]. The most studied exotic few-body Coulomb system are the muonic atoms (or muonic ions) which are formed by removing one or more orbital electron(s) by one or more negatively charged muon(s). However the present communication we shall consider only those atoms or ions in which the positively charged nucleus is being orbited by one electron and one negatively charged muon.

These atoms have been under theoretical scanner of several authors [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26] for being investigated. In this communication, we adopt hyperspherical harmonics expansion (HHE) approach for a systematic study of the ground state of atoms/ ions containing an orbital electron plus a negatively charged muon revolving round the positively charged nucleus forming a three-body system. In our model, we assume that the electromagnetic interaction of the valence particles with the nucleus is sufficiently weak to influence the internal structure of the nucleus. Again, the fact that the muon is much lighter than the nucleus allows us to regard the nucleus to remain a static source of electrostatic interaction. However, a hydrogen-like two-body model, consisting a quasi-nucleus ($\mu^- N^{(Z-2)+}$, formed by the muon and the nucleus) plus an orbital electron can also be tested due to much smaller size of muonic orbital than that for an electronic orbital.

In HHE formalism for a general three-body system of three unequal mass particles the choice of Jacobi coordinates correspond to three different partitions and in the i^{th} partition, particle labeled by 'i' remains as a spectator while the remaining two particles labeled 'j' and 'k' form the interaction pair. So the total potential contains three binary interaction terms (i.e. $V = V_{jk}(r_{jk}) + V_{ki}(r_{ki}) + V_{ij}(r_{ij})$) and for computation of matrix element of $V(r_{ij})$, potential of the (ij) pair, the chosen HH is expanded in the set of HH corresponding to the partition in which \vec{r}_{ij} is proportional to the first Jacobi vector [27] by the use of Raynal-Revai coefficients (RRC) [28]. The energies obtained for the lowest bound S-state is compared with the ones of the literature.

In Section II, we briefly introduce the hyperspherical coordinates and the scheme of the transformation of HH belonging to two different partitions. Results of calculation and discussions will be presented in Section III and finally we shall draw our conclusion in section IV.

2. HHE Method

The choice of Jacobi coordinates for systems of three particles of mass m_i, m_j, m_k is shown in Fig.1.

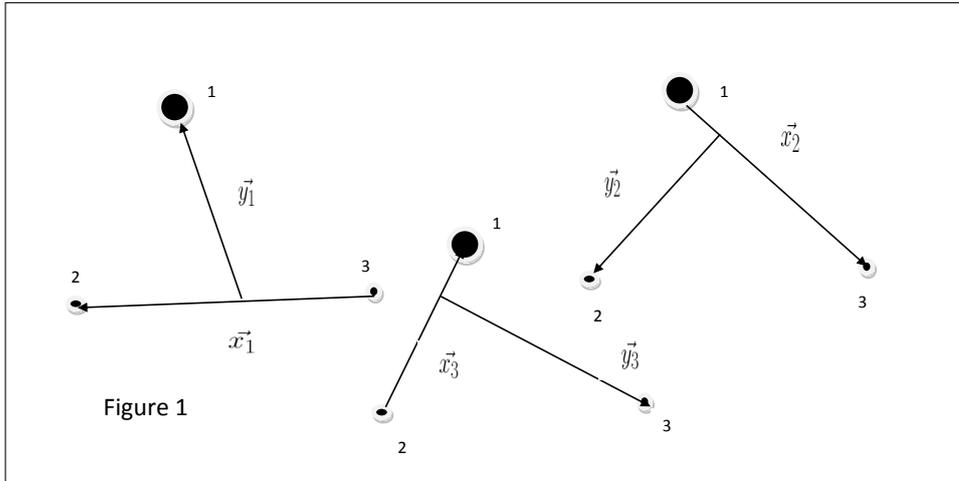


Figure 1. Jacobi coordinates in different partitions of a three-body system.

The Jacobi coordinates [29] in the i^{th} partition can be defined as:

$$\left. \begin{aligned} \vec{x}_i &= \left[\frac{m_j m_k M}{m_i (m_j + m_k)^2} \right]^{\frac{1}{4}} (\vec{r}_j - \vec{r}_k) \\ \vec{y}_i &= \left[\frac{m_i (m_j + m_k)^2}{m_j m_k M} \right]^{\frac{1}{4}} \left(\vec{r}_i - \frac{m_j \vec{r}_j + m_k \vec{r}_k}{m_j + m_k} \right) \\ \vec{R} &= (m_i \vec{r}_i + m_j \vec{r}_j + m_k \vec{r}_k) / M \end{aligned} \right\} \quad (1)$$

where $M = m_i + m_j + m_k$ and the sign of \vec{x}_i is determined by the condition that (i, j, k) should form a cyclic permutation of $(1, 2, 3)$.

The Jacobi coordinates are connected to the hyperspherical coordinates [30] as

$$\left. \begin{aligned} x_i &= \rho \cos \phi_i & ; & & y_i &= \rho \sin \phi_i \\ \rho &= \sqrt{x_i^2 + y_i^2} & ; & & \phi_i &= \tan^{-1}(y_i/x_i) \end{aligned} \right\} \quad (2)$$

The relative three-body Schrödinger's equation in hyperspherical coordinates can be written as

$$\left[-\frac{\hbar^2}{2\mu} \left\{ \frac{\partial^2}{\partial \rho^2} + \frac{5}{\rho} \frac{\partial}{\partial \rho} + \frac{\hat{K}^2(\Omega_i)}{\rho^2} \right\} + V(\rho, \Omega_i) - E \right] \Psi(\rho, \Omega_i) = 0 \quad (3)$$

where $\Omega_i \rightarrow \{\phi_i, \theta_{x_i}, \phi_{x_i}, \theta_{y_i}, \phi_{y_i}\}$, effective mass $\mu = \left[\frac{m_i m_j m_k}{M} \right]^{\frac{1}{2}}$, potential $V(\rho, \Omega_i) = V_{jk} + V_{ki} + V_{ij}$. The square of hyper angular momentum operator $\hat{K}^2(\Omega_i)$ satisfies the eigenvalue equation [30]

$$\hat{K}^2(\Omega_i) \mathcal{Y}_{K\alpha_i}(\Omega_i) = K(K+4) \mathcal{Y}_{K\alpha_i}(\Omega_i) \quad (4)$$

where the eigen function $\mathcal{Y}_{K\alpha_i}(\Omega_i)$ is the hyperspherical harmonics (HH). An explicit expression for the HH with specified grand orbital angular momentum $L (= |l_{x_i} + l_{y_i}|)$ and its projection M is given by

$$\begin{aligned} \mathcal{Y}_{K\alpha_i}(\Omega_i) &\equiv \mathcal{Y}_{K l_{x_i} l_{y_i} L M}(\phi_i, \theta_{x_i}, \phi_{x_i}, \theta_{y_i}, \phi_{y_i}) \\ &\equiv {}^{(2)}P_K^{l_{x_i} l_{y_i}}(\phi_i) \left[Y_{l_{x_i}}^{m_{x_i}}(\theta_{x_i}, \phi_{x_i}) Y_{l_{y_i}}^{m_{y_i}}(\theta_{y_i}, \phi_{y_i}) \right]_{LM} \end{aligned} \quad (5)$$

with $\alpha_i \equiv \{l_{x_i}, l_{y_i}, L, M\}$ and $[\]_{LM}$ denoting angular momentum coupling. The hyper-angular momentum quantum number $K (= 2n_i + l_{x_i} + l_{y_i}; n_i \rightarrow \text{a non-negative integer})$

is not a conserved quantity for the three-body system. In a given partition (say partition “ i ”), the wave-function $\Psi(\rho, \Omega_i)$ is expanded in the complete set of HH

$$\Psi(\rho, \Omega_i) = \sum_{K\alpha_i} \rho^{-5/2} U_{K\alpha_i}(\rho) \mathcal{Y}_{K\alpha_i}(\Omega_i) \quad (6)$$

Substitution of Eq. (6) in Eq. (3) and use of ortho-normality of HH, leads to a set of coupled differential equations (CDE) in ρ

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{d\rho^2} + \frac{(K+3/2)(K+5/2)\hbar^2}{2\mu\rho^2} - E \right] U_{K\alpha_i}(\rho) + \sum_{K'\alpha'_i < K\alpha_i} \langle K'\alpha'_i | V(\rho, \Omega_i) | K\alpha_i \rangle U_{K'\alpha'_i}(\rho) = 0. \quad (7)$$

where

$$\langle K'\alpha'_i | V(\rho, \Omega_i) | K\alpha_i \rangle = \int \mathcal{Y}_{K\alpha_i}^*(\Omega_i) V(\rho, \Omega_i) \mathcal{Y}_{K'\alpha'_i}(\Omega_i) d\Omega_i \quad (8)$$

3. Results and discussions

For the present calculation, we assign the label ‘ i ’ to the nucleus of mass $m_i = m_N$ (and charge $+Ze$), the label ‘ j ’ to the negatively charged muon of mass $m_j = m_\mu$ (and charge $-e$) and the label ‘ k ’ to the electron of mass $m_k = m_e$ (and charge $-e$). Hence, for this particular choice of masses, Jacobi coordinates of Eq. (1) in the partition “ j ” become

$$\left. \begin{aligned} \vec{x}_i &= \left[\frac{m_\mu m_e (m_N + m_\mu + m_e)}{m_N (m_\mu + m_e)^2} \right]^{\frac{1}{4}} (\vec{r}_j - \vec{r}_k) \\ \vec{y}_i &= \left[\frac{m_\mu m_e (m_N + m_\mu + m_e)}{m_N (m_\mu + m_e)^2} \right]^{-\frac{1}{4}} \left(\vec{r}_i - \frac{m_\mu \vec{r}_j + m_e \vec{r}_k}{m_\mu + m_e} \right) \end{aligned} \right\} \quad (9)$$

and the corresponding Schrödinger equation (Eq. (7)) is

$$\left[-\frac{\hbar^2}{2\mu} \left\{ \frac{d^2}{d\rho^2} - \frac{(K+3/2)(K+5/2)}{\rho^2} \right\} - E \right] U_{K\alpha_i}(\rho) + \sum_{K'\alpha'_i < K\alpha_i} \left[\frac{\beta_i}{\rho \cos\phi_i} - \frac{Z}{\rho |\beta_i \sin\phi_i \hat{y}_i - \frac{1}{2\beta_i} \cos\phi_i \hat{x}_i|} \right] U_{K'\alpha'_i}(\rho) - \frac{Z}{\rho |\beta_i \sin\phi_i \hat{y}_i + \frac{1}{2\beta_i} \cos\phi_i \hat{x}_i|} U_{K'\alpha'_i}(\rho) = 0 \quad (10)$$

where $\beta_i = \left[\frac{m_\mu m_e (m_N + m_\mu + m_e)}{m_N (m_\mu + m_e)^2} \right]^{\frac{1}{4}}$ and $\mu = \left(\frac{m_N m_\mu m_e}{m_N + m_\mu + m_e} \right)^{\frac{1}{2}}$ is the effective mass of the system. In atomic units we take $\hbar^2 = m_e = m = e^2 = 1$. Masses of the particles involved in this work are partly taken from [30, 31, 32, 33].

In the ground state of electron-muon three-body system, the total orbital angular momentum, $L=0$ and there is no restriction (on l_{x_i}) due to Pauli exclusion principle as electron and muon are non-identical fermions. Since $L = 0$, $l_{x_i} = l_{y_i}$, and the set of quantum numbers represented by α_i is $\{l_{x_i}, l_{x_i}, 0, 0\}$. Hence, the quantum numbers $\{K\alpha_i\}$ can be represented by $\{Kl_{x_i}\}$ only. Eq. (10) is solved following the method described in our previous work [30] to get the ground state energy E .

One of the major drawbacks of HH expansion method is its slow rate of convergence for Coulomb-type long range interaction potentials, unlike for the Yukawa-type short-range potentials for which the convergence is reasonably fast [29, 34]. Hence, to achieve the desired degree of convergence, sufficiently large K_m value has to be included in the calculation. But, if all K values up to a maximum of K_m are

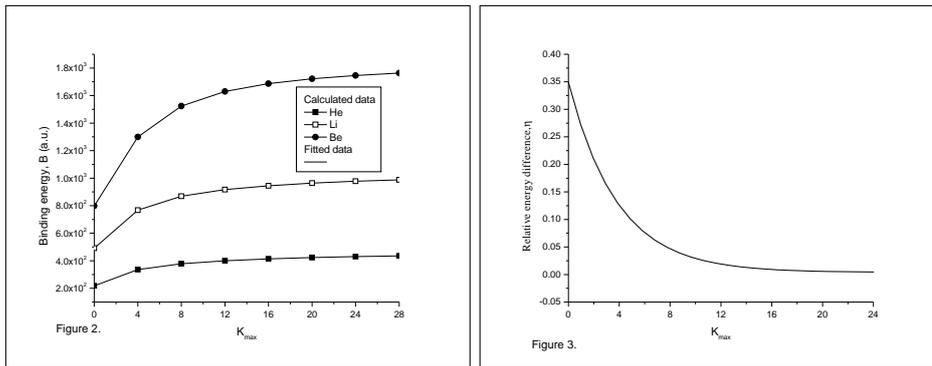


Figure 2. Pattern of dependence of the ground-state energy (B) of muonic atom/ions on the increase in K_{max} .

Figure 3. Pattern dependence of the ground-state relative energy difference $\eta = \frac{B_{K_m+4} - B_{K_m}}{B_{K_m+4}}$ of muonic helium (${}^\infty\text{He}^{2+}\mu^-e^-$) on the increase in K_{max} .

included in the HH expansion then the number of the basis states can be determined by relation

$$N_{K_m} = \frac{(K_m + 2)(K_m + 4)}{8} \quad (11)$$

It follows from Eq. (11) that number of basis states and hence the size of coupled differential equations (CDE) (Eq. (7)) increases rapidly with increase in K_m . For the available computer facilities, we are allowed to solve up to $K_m = 28$ reliably. The calculated ground state energies (B_{K_m}) with increasing K_m for muonic helium (${}^\infty\text{He}^{2+}\mu^-e^-$), muonic lithium (${}^\infty\text{Li}^{3+}\mu^-e^-$) and muonic beryllium (${}^\infty\text{Be}^{4+}\mu^-e^-$) are presented in columns 2, 4 and 6 of Table 1. Energies for a number of muonic atom/ions of different atomic number (Z) at $K_m = 28$ are presented in column 4 of Table 2. The pattern of convergence of the energy of the lowest bound S-state with respect to increasing K_m can be checked by gradually increasing K_m values in suitable steps (dK) and comparing the relative energy difference $\eta = \frac{B_{K+dK} - B_K}{B_{K+dK}}$ with that found in the previous step. From Table 1, it can be seen that at $K_m = 28$, the energy of the lowest bound S-state of $e^-\mu^-{}^\infty\text{He}^{2+}$ converges up to 3rd decimal places and similar convergence trends are observed in the remaining cases. The pattern of increase in binding energy (B) with respect to increasing K_{max} is shown in Figure 3 for few representative cases. In Figure 4 the relative energy difference η is plotted against K_{max} to demonstrate the relative convergence trend in energy. The calculated ground state energies muonic three-body systems of different nuclear charge Z (and of infinite nuclear mass), have been plotted against Z as shown in Figure 4 to study the dependence of the bound state energies on the strength of the nuclear charge using data from Table 2. The curve of Figure 4 shows a gradual increase in energy with the increase in the strength nuclear charge Z approximately following the empirical equation

$$B(Z) = -154.64851 + 4.47088Z + 131.84786Z^2 - 2.79311Z^3 + 0.02174Z^4 \quad (12)$$

Eq. (12) may be used to estimate the ground state energy of muonic atom/ions of given Z assuming infinite nuclear core. Finally, in Table 2, energies of the lowest bound

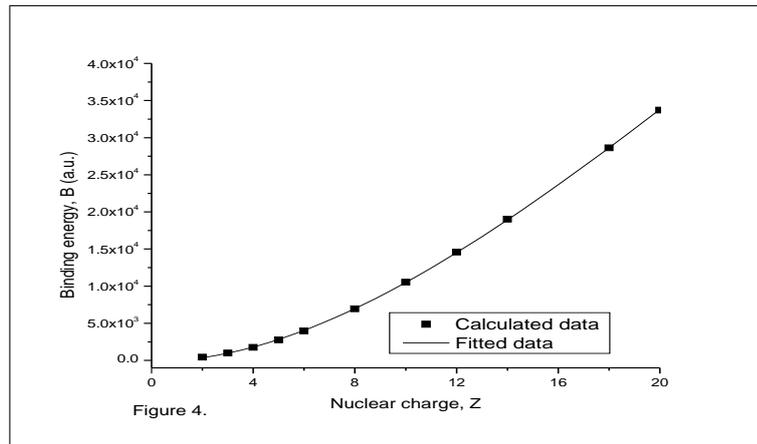


Figure 4. Pattern of dependence of the ground-state energy (B) of muonic atom/ions on the increase in nuclear charge Z .

S-state of several muonic three-body systems obtained by numerical solution of the coupled differential equations by the renormalized Numerov method [35] have been compared with the ones of the literature wherever available. Since reference values are not available for systems having nuclear charge $Z > 3$, we made a crude estimation of the ground-state ($1s_e 1s_\mu$) energies following the relation

$$B_{est}^{3B} = \frac{Am_N Z^2}{2} \left[\frac{1}{1 + Am_N} + \frac{m_\mu}{m_\mu + Am_N} \right] \quad (13)$$

where $m_N = 1836$, muon mass $m_\mu = 206.762828$ (in atomic unit) and A is mass number of the nucleus. Here we assumed two hydrogen-like subsystems for the muonic atom/ions. This estimate can further be improved by assuming a compact $(A(Z), \mu^-)_{1s}$ positive muonic ion and an electron in the $1s$ state, "feeling" a $(Z-1)$ charge and an $Am_N + m_\mu$ mass. For this case the estimation formula (Eq. (13)) can be replaced by

$$B_{est}^{2B} = \frac{1}{2} \left[\frac{Am_N + m_\mu}{1 + Am_N + m_\mu} (Z-1)^2 + \frac{Am_N m_\mu}{m_\mu + Am_N} Z^2 \right] \quad (14)$$

4. Conclusion

In conclusion, we note that the calculated ground-state energy of muonic helium and muonic lithium at $K_m = 28$ listed in column 4 of Table 2 are greater than the corresponding reference values listed in column 5 of Table 2. This discrepancies may have arose due to the CUSP conditions applicable to Coulomb systems which have not been accommodated in the present calculations. It can be seen that the estimated energies (B_{est}) in columns 2 & 3 of Table 2 are less than the corresponding calculated energies (B_{calc}) in column 4 of Table 2 for systems having $Z \leq 10$ while the same for $Z > 10$ becomes larger than B_{calc} . This may happen due to weaker correlation between electron-muon pair in systems having nuclear charge $Z < 10$ while a stronger correlation in systems having $Z > 10$. It may also be noted that estimated energy listed in column 3 of Table 2 agrees fairly with the reference values

Table 1. Energy (B) of the lowest bound S-state of electron-muon three-body systems at different K_{max} along with the corresponding relative energy difference η .

System K_{max}	Binding energies (B) and corresponding relative energy difference (η)					
	${}^{\infty}\text{He}^{2+}\mu^{-}e^{-}$		${}^{\infty}\text{Li}^{3+}\mu^{-}e^{-}$		${}^{\infty}\text{Be}^{4+}\mu^{-}e^{-}$	
	B	η	B	η	B	η
0	217.78577	0.352207	490.78306	0.360783	798.35396	0.385798
4	336.19645	0.110907	767.78745	0.116652	1299.82240	0.146813
8	378.13435	0.055125	869.17847	0.052009	1523.49147	0.065150
12	400.19520	0.033222	916.86372	0.029708	1629.66350	0.033758
16	413.94723	0.022228	944.93547	0.019627	1686.59904	0.020329
20	423.35753	0.015913	963.85254	0.014046	1721.59813	0.013800
24	430.20330	0.011949	977.58415	0.010573	1745.68917	0.010153
28	435.40598	0.006945	988.03084	0.005984	1763.59496	0.006227

Table 2. Energy (B) of the lowest bound S-state of electron-muon-nucleus three-body systems.

System	Binding energies expressed in atomic unit (a.u.)			
	Estimated		Calculated	Other Results
	$B_{est}^3[Eq.(13)]$	$B_{est}^2[Eq.(14)]$	$B_{K_m=28}$	
$e^{-}\mu^{-3}\text{He}^{2+}$	400.574	399.064	420.424	399.042 ^a , 399.043 ^b
$e^{-}\mu^{-4}\text{He}^{2+}$	404.212	402.702	424.017	402.637 ^c , 402.641 ^d
$e^{-}\mu^{-\infty}\text{He}^{2+}$	415.537	414.026	435.406	414.036 ^e , 414.037 ^f
$e^{-}\mu^{-6}\text{Li}^{3+}$	917.814	915.291	970.737	915.231 ^e , 915.231 ^g
$e^{-}\mu^{-7}\text{Li}^{3+}$	920.224	917.701	973.166	917.649 ^e , 917.650 ^g
$e^{-}\mu^{-\infty}\text{Li}^{3+}$	934.957	932.433	988.031	932.457 ^e
$e^{-}\mu^{-9}\text{Be}^{4+}$	1641.703	1638.161	1745.087	
$e^{-}\mu^{-\infty}\text{Be}^{4+}$	1662.146	1658.603	1763.595	
$e^{-}\mu^{-10}\text{B}^{5+}$	2568.319	2563.753	2732.374	
$e^{-}\mu^{-\infty}\text{B}^{5+}$	2597.104	2592.535	2761.200	
$e^{-}\mu^{-12}\text{C}^{6+}$	3705.224	3699.628	3937.535	
$e^{-}\mu^{-\infty}\text{C}^{6+}$	3739.829	3734.231	3971.528	
$e^{-}\mu^{-16}\text{O}^{8+}$	6602.337	6594.666	6907.068	
$e^{-}\mu^{-\infty}\text{O}^{8+}$	6648.585	6640.910	6949.141	
$e^{-}\mu^{-20}\text{Ne}^{10+}$	10330.524	10320.754	10486.654	
$e^{-}\mu^{-\infty}\text{Ne}^{10+}$	10388.414	10378.641	10534.362	
$e^{-}\mu^{-24}\text{Mg}^{12+}$	14889.783	14877.894	14539.329	
$e^{-}\mu^{-\infty}\text{Mg}^{12+}$	14959.316	14947.424	14590.826	
$e^{-}\mu^{-28}\text{Si}^{14+}$	20280.115	20266.085	18956.238	
$e^{-}\mu^{-\infty}\text{Si}^{14+}$	20361.291	20347.257	19010.171	
$e^{-}\mu^{-32}\text{S}^{16+}$	26501.520	26485.328	23653.644	
$e^{-}\mu^{-\infty}\text{S}^{16+}$	26594.340	26578.142	23709.055	
$e^{-}\mu^{-40}\text{Ar}^{18+}$	33564.416	33546.038	28574.033	
$e^{-}\mu^{-\infty}\text{Ar}^{18+}$	33658.461	33640.078	28624.646	
$e^{-}\mu^{-40}\text{Ar}^{18+}$	33564.416	335546.038	28574.033	
$e^{-}\mu^{-\infty}\text{Ar}^{18+}$	33658.461	33640.078	28624.646	
$e^{-}\mu^{-40}\text{Ca}^{20+}$	41437.550	41416.966	33152.978	
$e^{-}\mu^{-\infty}\text{Ca}^{20+}$	41553.656	41533.066	33709.888	

^aRef[2, 10, 11, 37], ^bRef[38], ^cRef[2, 10, 11, 38, 39], ^dRef[1, 20, 40], ^eRef[2],
^fRef[11], ^gRef[18]

for for $Z=2,3$. Finally, it can also be added that in the cases of highly charged muonic ions relativistic correction together with proper inclusion of Kato's cusp conditions [36] (in the limit $r_{jk} \rightarrow 0$) is important for obtaining improved results.

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