

Shiro L. Saito

Multireference configuration interaction calculations for complexes of positronium and B, C, N, and O atoms

Received: 3 March 2005 / Accepted: 28 July 2005 / Published online: 10 December 2005
© Springer-Verlag 2005

Abstract Positronium (Ps) binding energies for complexes of Ps and atoms with open shell electrons, PsX (X=B, C, N, and O), are calculated using the multireference singly and doubly excited configuration interaction (MRSDCI) method. The effectiveness of this method for the complexes is verified. The MRSDCI calculations are carried out with a frozen-core approximation so as to incorporate only the most important valence correlation effects. Many-body correlation effects and contributions from higher angular momentum orbitals are estimated by extrapolation techniques. The resulting Ps binding energies agree well with the results of diffusion Monte Carlo simulations by Bressanini et al. (J Chem Phys 108:4756,1998) and by Jiang and Schrader (Phys Rev Lett 81:511332,1998). For PsO the Ps binding energy obtained by Jiang and Schrader is about 1.8 times larger than that of Bressanini et al.; the present calculated value is close to that of Jiang and Schrader.

Keywords Positron-atom complex · PsB-PsO · MRSDCI · Positronium binding energy · Positron ionization energy

1 Introduction

Positron and positronium chemistry is an area of radiation chemistry, where the interaction of positrons and matters is studied. In particular, the study of bound states of positrons and atoms, molecules, or their ions is one of important subjects in positron and positronium chemistry [1–4]. We refer to these bound states as positron–atom complexes or positron–molecule complexes. There have been many experimental and theoretical studies of these complexes.

The last decade has seen high quality theoretical calculations for several positron–atom complexes and positron–molecule complexes, and the positronium (Ps) binding energies

have been evaluated accurately [5]. The Ps binding energy of PsX is calculated by

$$\text{BE} = E_{\text{Ps}} + E_{\text{X}} - E_{\text{PsX}}, \quad (1)$$

where E_{Ps} , E_{X} , and E_{PsX} are the total energies for Ps, X, and PsX, respectively. The Ps binding energy can also be estimated using the electron affinity (EA) of X and the positron ionization energy (PI) of PsX as follows :

$$\begin{aligned} \text{BE} &= E_{\text{Ps}} + (E_{\text{X}} - E_{\text{X}^-}) + (E_{\text{X}^-} - E_{\text{PsX}}) \\ &= E_{\text{Ps}} + \text{EA} + \text{PI}. \end{aligned} \quad (2)$$

Accurate determination of Ps binding energies requires wave functions which can provide accurate electron affinities and positron ionization energies. To calculate accurate positron ionization energies, positron–electron correlations must be incorporated. In fact, it has been shown that the Hartree–Fock (HF) method provides negative Ps binding energies [6, 7].

Computational methods with explicitly correlated functions, e.g., Hylleraas-type functions or explicitly correlated Gaussians (ECG), are best suited to incorporation of the positron–electron correlation effects. Although such methods are very powerful and are suitable for positron–atom complexes, they are not practical for many-body systems because of their heavy computational cost. Mitroy et al. [5] have applied the stochastic variational method (SVM) with ECG to many-electronic positron–atom complexes with one or two valence electrons using a model potential. For positron–atom complexes with many valence electrons, density functional theory (DFT), quantum Monte Carlo (QMC), or configuration interaction (CI) methods have been applied. DFT has recently grown into a method which efficiently calculates accurate energy values of atoms or molecules. However, there are only a few DFT calculations for positron–atom complexes [8–10]. QMC is a method which stochastically solves the Schrödinger equation and is capable of giving accurate results. The diffusion Monte Carlo (DMC) method, which is a variant of QMC, has been employed by Schrader and co-workers [11–13] and by Bressanini et al. [14].

The CI is a standard method which is extensively used for calculating atomic or molecular wave functions because of

S. L. Saito
Faculty of Liberal Arts,
Chukyo University,
Toyota 470-0393, Japan
E-mail: ssaito@sccs.chukyo-u.ac.jp

its simplicity. CI calculations of many-electronic positron-atom complexes have been carried out by the present author [15–17]. Unfortunately, the convergence of CI expansions is very slow, because the effects of the higher partial wave component of the positron–electron pair and of the many-body excitation are large. The CI method often gives unsatisfactory results owing to such slow convergence. It would nevertheless be possible to obtain good results with the help of an appropriate extrapolation procedure.

Our previous work [17] applied the multireference singly and doubly excited CI (MRSDCI) method to positronium halides, and showed that the many-body correlation effects contribute greatly to the results. The present work investigates the effectiveness of the MRSDCI method for positron–atom complexes with open shell electrons. We apply the MRSDCI method to the ground states of the positron–atom complexes PsB ($2,3P$), PsC ($3,4S$), PsN ($2,3P$), and PsO ($1,2P$), the neutral atoms B ($2P$), C ($3P$), N ($4S$), and O ($3P$), and their anions B $^-$ ($3P$), C $^-$ ($4S$), N $^-$ ($3P$), and O $^-$ ($2P$), and give Ps binding energies and positron ionization energies for these positron–atom complexes. These species have previously been studied using HF calculation by Patrick and Cade [7], DFT by Harrison [8] and Kanhere et al. [9], and DMC by Jiang and Schrader [13] and Bressanini et al. [14]. PsN has been studied by HF only. The present MRSDCI calculations use a frozen-core approximation so as to incorporate only the most important valence correlation effects. We estimate the full CI (FCI) limits of the total energies by extrapolation against the weight of reference space (w_{ref}). In addition, by analyzing energy lowering with respect to angular momentum (λ), we estimate the contributions to the total energies from higher angular momentum orbitals. Hereafter, we refer to the effect of the higher angular momentum orbitals as the ‘higher λ effect.’

The next section explains the computational method, which is the same as in the previous work [17]. The third section summarizes the results of the Ps binding energies and positron ionization energies for PsB, PsC, PsN, and PsO, and discusses them in comparison with the works of other researchers.

2 Computational method

For atomic systems, Slater- or Gaussian-type basis sets are usually employed. Unfortunately, their linear dependence often disturbs the calculations. In the present work we use the B -spline set which is one of piecewise polynomials, because this set is free from computational linear dependence and is very flexible. The present basis set consists of N K th-order B -splines [18, 19] on a knot sequence defined on an interval $[0, R]$. A knot sequence was used with endpoints of K -fold multiplicity :

$$0, R_1, R_1(1 + \beta), R_1(1 + \beta + \beta^2), \dots, R, \quad (3)$$

where R_1 is the initial interval and β is the parameter characterizing the distribution of the knots. Here, β is chosen to

satisfy the following condition :

$$R = R_1(1 + \beta + \beta^2 + \dots + \beta^{N-K+2}), \quad (\beta \geq 1). \quad (4)$$

Values used were $N = 40$, $R = 40$, and $K = 9$. The R_1 values were optimized by singly and doubly excited CI (SDCI) calculations with the HF reference configuration in the $spdf$ -space for each system individually. Since the B -spline set is very flexible, all atomic radial orbitals of each system were expanded using a common B -spline set regardless of the symmetry of the atomic orbitals.

Configuration state functions were constructed using the natural orbitals (NOs) with λ up to 8. The NOs used were generated by a series of MRSDCI calculations with reference spaces consisting of principal configurations of the SDCI wave functions (a ‘minimal reference space’). The minimal reference configurations are listed in Table 1.

First, MRSDCI calculations were performed with the HF orbitals in the spd -space, to obtain spd -NOs. Subsequently, f -NOs were generated by MRSDCI calculations with the spd -NOs. The NOs with higher angular momentum than f were generated in the same way, step by step. To reduce the computational cost, those NOs whose occupation number was less than 5.0×10^{-7} were truncated at each step.

To estimate the FCI limits and the higher λ effects for the total energies, a further series of MRSDCI calculations was performed, increasing the reference configurations which were selected for the largest weight in the previous CI wave functions. By analyzing the convergence patterns of the total energies (E_{CI}) provided by these calculations with respect to w_{ref} and λ , it was possible to estimate the FCI limits and the higher λ effect.

Table 1 Minimal reference configurations

System	PsX	X $^-$	X
X = B	$1s^2 2s^2 2p^2 1s_+$	$1s^2 2s^2 2p^2$	$1s^2 2s^2 2p$
	$+ 2s 1s_+ \rightarrow 2p 2p_+$	$+ 2s^2 \rightarrow 2p^2$	$+ 2s^2 \rightarrow 2p^2$
	$+ 2p 1s_+ \rightarrow 3s 2p_+, 3d 2p_+$	$+ 2p^2 \rightarrow 3p^2$	$+ 2s \rightarrow 3d$
	$+ 2s^2 \rightarrow 2p^2$	$+ 2s 2p \rightarrow 3s 3p$	
	$+ 1s_+ \rightarrow 3d_+$	$+ 2s \rightarrow 3d$	
	$+ 2s \rightarrow 3d$		
X = C	$1s^2 2s^2 2p^3 1s_+$	$1s^2 2s^2 2p^3$	$1s^2 2s^2 2p^2$
	$+ 2s 1s_+ \rightarrow 2p 2p_+$	$+ 2p^2 \rightarrow 3p^2$	$+ 2s^2 \rightarrow 2p^2$
	$+ 2p 1s_+ \rightarrow 3s 2p_+, 3d 2p_+$	$+ 2s 2p \rightarrow 3s 3p$	$+ 2s \rightarrow 3d$
	$+ 2p^2 \rightarrow 3p^2$	$+ 2s \rightarrow 3d$	
	$+ 2s 2p \rightarrow 3s 3p$		
X = N	$1s^2 2s^2 2p^4 1s_+$	$1s^2 2s^2 2p^4$	$1s^2 2s^2 2p^3$
	$+ 2p^2 \rightarrow 3p^2$	$+ 2p^2 \rightarrow 3p^2$	$+ 2s \rightarrow 3d$
	$+ 2p \rightarrow 3p$	$+ 2p \rightarrow 3p$	
X = O	$1s^2 2s^2 2p^5 1s_+$	$1s^2 2s^2 2p^5$	$1s^2 2s^2 2p^4$
	$+ 2p 1s_+ \rightarrow 3d 2p_+$	$+ 2p^2 \rightarrow 3p^2$	$+ 2s \rightarrow 3d$
	$+ 2p^2 \rightarrow 3p^2$	$+ 2p \rightarrow 3p$	

The subscript ‘+’ stands for a positronic orbital

Table 2 Results of MRSDCI with minimal reference configurations. N_{CI} , E_{CI} , and $\Delta\epsilon$ respectively denote the dimension of the configuration interaction (CI) wave function, total energy, and loss of total energy due to the natural orbital (NO) truncation procedure

System	N_{CI}	E_{CI} (au)	$\Delta\epsilon$ (au)
B	930	-24.602152	-0.000076
B ⁻	6,977	-24.612035	-0.000054
PsB	88,539	-24.819986	-0.000152
C	3,025	-37.788909	-0.000118
C ⁻	6,819	-37.835132	-0.000111
PsC	67,493	-38.047655	-0.000207
N	1,940	-54.528075	-0.000167
N ⁻	21,763	-54.517939	-0.000179
PsN	145,346	-54.723448	-0.000248
O	11,867	-74.998715	-0.000280
O ⁻	37,013	-75.050242	-0.000283
PsO	289,549	-75.266345	-0.000399

With E_{CI} as a function of w_{ref} , the FCI limits of E_{CI} were estimated by extrapolating E_{CI} to $w_{\text{ref}} = 1$. To do this, the convergence patterns of $E_{\text{CI}+\text{Q}}$ and E_{av} were also analyzed. Here, $E_{\text{CI}+\text{Q}}$ is E_{CI} plus the Davidson correction [20], and $E_{\text{av}} = \frac{1}{2}(E_{\text{CI}} + E_{\text{CI}+\text{Q}})$.

The higher λ effect for the total energies was also estimated by extrapolating the energy contributions due to the respective λ -NOs to $\lambda \rightarrow \infty$. To treat the systems on equal footing, we extrapolated the total energies to $\lambda \rightarrow \infty$ using the results of the largest-scale CI calculations with approximately the same w_{ref} . The energy contribution (ΔE_{λ}) was fitted by the following relation with two parameters a and b :

$$-\Delta E_{\lambda} = a\lambda^{-b}. \quad (5)$$

The contribution from the NOs having angular momentum greater than 8 was estimated as $-\sum_{\lambda=9}^{\infty} \Delta E_{\lambda}$. This extrapolation was carried out by assuming linearity of the contribution pattern. We finally obtained the FCI limits including the higher λ effect.

The HF calculations with the B -spline set were carried out using our atomic self-consistent field program code based on the algorithm of Roothaan and Bagus [21,22]. All CI calculations were performed by the program ATOMCI [23,24] modified for atomic systems containing positrons.

3 Results and discussion

Table 2 summarizes the total energies provided by MRSDCI with minimal reference space, together with their losses due to the NO truncation. The energy loss is of the order ~ 0.002 – 0.003 eV. To reduce the energy loss, it is desired that the NO truncation threshold be reduced. However, the reduction of the truncation threshold increases the computational cost greatly. The present threshold provides a good balance between the computational cost and accuracy.

We estimated the FCI limits of the total energies by analyzing the convergence patterns of the total energies against w_{ref} . As an example, the energies E_{CI} , $E_{\text{CI}+\text{Q}}$, and E_{av} for PsC, C, and C⁻ are plotted against w_{ref} in Fig. 1. E_{CI} at $w_{\text{ref}} = 1$ is the FCI limit of the total energy. As shown in Fig. 1, w_{ref} values of CI wave functions for PsC are much smaller than unity relative to those for C and C⁻. This situation appears also in the other systems. Thus, it is often difficult to accurately determine the FCI limit for positronium-atom complexes, i.e., to find a point where E_{CI} and $E_{\text{CI}+\text{Q}}$

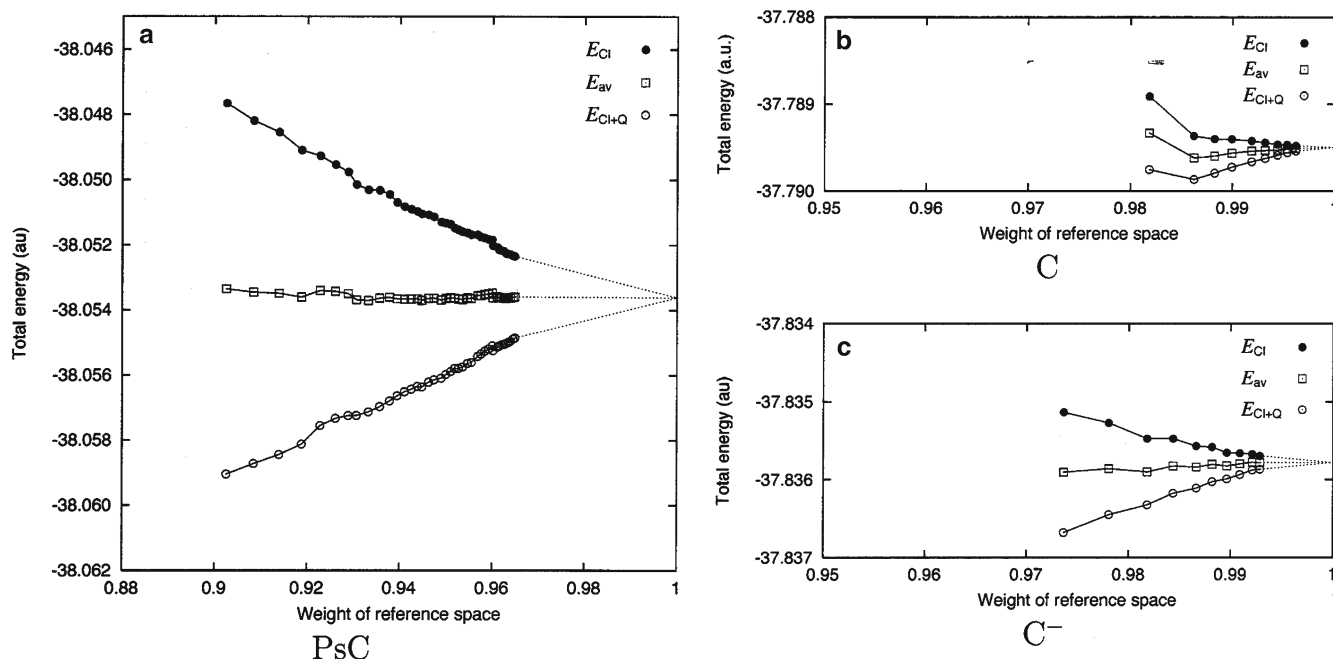


Fig. 1 Convergence of configuration interaction energies for PsC, C, and C⁻ with respect to the weight of the reference space

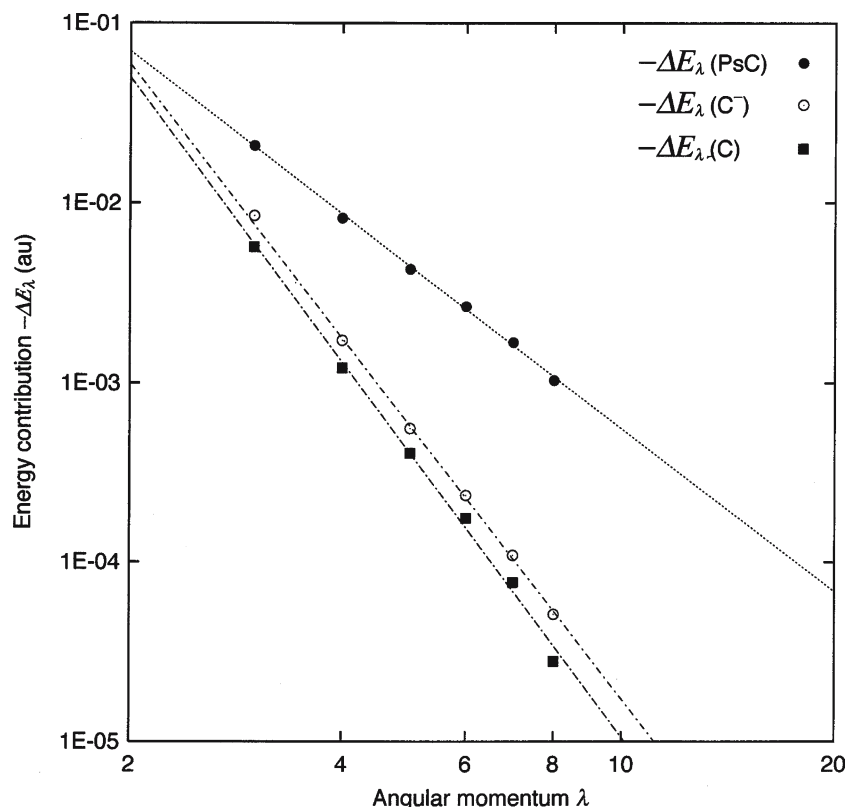


Fig. 2 Contributions to the total energies for PsC, C, and C^- from the respective λ orbitals

meet at $w_{\text{ref}} = 1$. As we showed previously [17], since the E_{av} curve tends to rapidly approach a constant value, E_{av} is very useful for estimating the FCI limit.

The contributions to the total energies from the NOs with larger angular momentum than 8 were estimated by extrapolation. Figure 2 shows the contribution to the total energies for PsC, C, and C^- from the respective λ -NOs on a log-log scale. The energy contribution converges linearly at $\lambda \geq 5$. Figure 2 also shows that the energy convergence for PsC is slower than that of C^- and C. This means that the effects of the higher partial wave components of the positron–electron pair are important. The FCI limits and the higher λ contributions for the total energies are summarized in Table 3. The convergence pattern for the other systems is similar to that for the species of carbon.

Table 4 summarizes the Ps binding energies and positron ionization energies for PsX and the electron affinities of X, together with results of other researchers. The positron ionization energies and the electron affinities were used to analyze their contribution to the Ps binding energies by Eq. (2). The higher λ corrected FCI limits of these energies constitute the present results.

All the present electron affinities are in good agreement with the measured values [25]. Accordingly, the precision of the present Ps binding energies depends almost only on that of the positron ionization energies. The higher λ effect for the electron affinities is small; the values are 0.004 eV or less. The many-body correlation effect is also small except for nitrogen.

Table 3 Full CI (FCI) limits (E_{FCI}) and higher λ contributions ($E_{\lambda>8}$) for total energies (in au)

System	E_{FCI}	$E_{\lambda>8}$
B	-24.60226	-0.00002
B^-	-24.61243	-0.00004
PsB	-24.83056	-0.00883
C	-37.78950	-0.00005
C^-	-37.83578	-0.00008
PsC	-38.05362	-0.00380
N	-54.52974	-0.00011
N^-	-54.52634	-0.00019
PsN	-54.74961	-0.00415
O	-75.00406	-0.00026
O^-	-75.05718	-0.00038
PsO	-75.28127	-0.00231

The present positron ionization energies for PsB, PsC, PsN, and PsO are 6.176, 6.029, 6.183, and 6.150 eV, respectively; these are almost the same values regardless of systems. The higher λ effect greatly increases the positron ionization energies; the increments for PsB, PsC, PsN, and PsO are respectively 0.241, 0.121, 0.108, and 0.052 eV. Increase due to the many-body effect is also large. The increases for PsB, PsC, PsN, and PsO are 0.276, 0.145, 0.218, and 0.270 eV, respectively. Thus, in order to calculate accurate positron ionization energies, it is important to incorporate not only the higher λ effect but also the many-body effect.

Table 4 Electron affinity (EA) of *X* atom, positron ionization energies (PI) and Ps binding energies (BE) for Ps*X* (in eV)

Method	Reference	EA	PI	BE
<i>X</i> = B				
HF	[7]	-0.268	3.642	-3.428
DFT	[8]	-0.144	3.519	-3.207
DFT	[9]	0.164	9.583	2.662
DMC	[14]	0.351	6.01	-0.44
MRSDCI ^a	Present work	0.269	5.659	-0.874
FCI limit	Present work	0.277	5.935	-0.590
FCI limit + higher λ	Present work	0.277	6.176	-0.350
Experiment	[25]	0.277		
<i>X</i> = C				
HF	[7]	0.550	4.141	-2.112
DFT	[8]	0.991	4.028	-1.784
DFT	[9]	1.294	9.837	4.328
DMC	[14]	1.342	5.940	0.479
MRSDCI ^a	Present work	1.258	5.783	0.238
FCI limit	Present work	1.259	5.928	0.384
FCI limit + higher λ	Present work	1.260	6.029	0.486
Experiment	[25]	1.263		
<i>X</i> = N				
HF	[7]	-2.149	4.419	-4.533
MRSDCI ^a	Present work	-0.320	5.592	-1.486
FCI limit	Present work	-0.092	6.075	-0.820
FCI limit + higher λ	Present work	-0.090	6.183	-0.710
Experiment	[25]	-0.072		
<i>X</i> = O				
HF	[7]	-0.535	4.716	-2.622
DFT	[8]	0.267	4.584	-1.952
DFT	[9]	2.751	10.841	9.564
DMC	[14]	1.374	5.940	0.479
DMC ^b	[13]	1.38	6.26	0.84
MRSDCI ^a	Present work	1.402	5.880	0.480
FCI limit	Present work	1.445	6.098	0.740
FCI limit + higher λ	Present work	1.449	6.150	0.796
Experiment	[25]	1.461		

^aCalculation with minimal reference space^bUncertainties of EA and BE are ± 0.05 and ± 0.18 eV, respectively

The present Ps binding energies for PsB, PsC, PsN, and PsO are respectively -0.350, 0.486, -0.710, and 0.796 eV. The positive Ps binding energies indicate that PsC and PsO exist stably. This result is consistent with the DMC simulations performed by Jiang and Schrader [13] and by Bressanini et al. [14]. For PsN, theoretical calculation has been performed only by the HF method [7] so far, and has given negative value. The present Ps binding energy for PsN is also negative Ps binding energy. If the positron ionization energy of PsN exceeds ~ 6.9 eV, the Ps binding energy of PsN will be positive. However, since this value is too large relative to the other systems, PsN will not exist stably. The contributions of the higher λ effect and the many-body effect to the Ps binding energies are large. As seen above, these effects mainly result from the positron ionization energies. For PsN, the many-body effect of the electron affinity considerably contribute to the Ps binding energy.

Let us compare the present Ps binding energies, positron ionization energies, and electron affinities with the results of

DMC and DFT. In particular, it is expected that DMC simulations give reliable results. For example, DMC Ps BEs for PsH obtained by Jiang and Schrader [27] and by Bressanini et al. [26] are in excellent agreement with accurate variational calculations [28]. The DMC simulations for PsB and PsC were carried out by Bressanini et al. [14] only. For PsC, the present Ps binding energy is in good agreement with the DMC result, but the present positron ionization energy is larger than that of the DMC by 0.089 eV. The poor result for the positron ionization energy would be ascribed to the error of the carbon electron affinity provided by the DMC. The DMC overestimates the carbon electron affinity by 0.08 eV. For PsB, the present Ps binding energy and positron ionization energy are larger than those of the DMC by 0.09 and 0.17 eV, respectively. This error of positron ionization energy is also mainly due to overestimation of the DMC electron affinity for the boron atom. If DMC simulations of the anions that provide the exact electron affinities were carried out, the DMC positron ionization energies for PsB and PsC would be 6.09 and 6.019 eV, respectively. These values are close to the present positron ionization energies.

For PsO, Jiang and Schrader [13] and Bressanini et al. [14] have made DMC simulations. However, the Ps binding energy found by Jiang and Schrader is about 1.8 times larger than that of Bressanini et al. The difference in Ps binding energies between both DMC simulations is 0.36 eV. The present Ps binding energy (0.796 eV) is quite close to that of Jiang and Schrader (0.84 eV). Both DMC electron affinities for the oxygen atom are almost the same, and are smaller than the experimental value [25] by about 0.08 eV. This means that DMC positron ionization energies include the error of about 0.08 eV at least. The present positron ionization energy for PsO (6.150 eV) is smaller than that of Jiang and Schrader (6.26 eV) by ~ 0.11 eV. If DMC simulation of the oxygen anion was made so as to provide the exact electron affinity, then the DMC positron ionization energy for PsO would be 6.18 eV; this value is close to the present positron ionization energy. On the other hand, the positron ionization energy of Bressanini et al. is slightly smaller than the FCI limit of the energy. Since the FCI limit is smaller than the exact value due to the higher λ effect, the corresponding ionization energy is obviously smaller than the exact value. Therefore, we can conclude that the error in the Ps binding energy of PsO given by Bressanini et al. is caused by failure to account fully for the positron-electron correlation.

Density functional theory calculations for PsB, PsC, and PsO have been performed by Harrison [8] and Kanhere et al. [9]. The energies provided by Harrison [8] are similar to the HF results. Kanhere et al. [9] have carried out the DFT calculation with correlation effects and have obtained very large Ps binding energies. In contrast to the negative Ps binding energy of PsB obtained by CI and DMC, that of Kanhere et al. [9] is positive. The result of Kanhere et al. [9] seems to be unrealistic. For the Ps binding energies of PsC and PsO, the DFT values given by Kanhere et al. [9] are a factor 8.9 and 12.0 times larger than the present results. This is mainly due to the error in positron ionization energies (~ 10 eV).

Their errors are about 1.6–1.8 times larger than ours. The positron–electron correlation is overestimated. If incorporation of the positron–electron correlation is improved, DFT method will grow into a powerful method for atomic and molecular systems with positrons.

4 Summary

We have carried out MRSDCI calculations for positron–atom complexes with open shell electrons, PsB, PsC, PsN, and PsO, and estimated the Ps binding energies and the positron ionization energies with the help of extrapolation techniques. To obtain these accurate values, it has been shown that incorporation of the many-body correlation effect and the higher λ effect are important. Our Ps binding energies agree well with DMC values obtained by Jiang and Schrader and by Bressanini et al. However, the Ps binding energy for PsO considerably differs between both DMC simulations. We have obtained the Ps binding energy which is quite close to the result of Jiang and Schrader. The positron ionization energy for the present complexes is almost the same, regardless of the system. It follows that the Ps binding energy is determined mainly by the electron affinity of the corresponding neutral atom. From this ground, we can predict that complexes of Ps and atoms having large electron affinity, such as sulphur, selenium, platinum, gold, should be stable. The MRSDCI method will reveal the stability of such systems.

References

- Green J, Lee J (1964) Positronium chemistry. Academic, New York
- Schrader DM, Jean YC (ed) (1988) Positron and positronium chemistry. Elsevier, Amsterdam
- Mogensen OE (1995) Positron annihilation in chemistry. Springer, Berlin Heidelberg New York
- Tachikawa M, Shimamura I, Buenker RJ, Kimura M (2001) In: Surko CM, Gianturco FA (eds) New directions in antimatter chemistry and physics. Kluwer, Dordrecht, p 437
- Mitroy J, Bromley MWJ, Ryzhikh GG (2002) J Phys B 35:R81 and references therein
- Cade PE, Farazdel A (1977) J Chem Phys 66:2598
- Patrick AJ, Cade PE (1981) J Chem Phys 75:1893
- Harrison JG (1986) J Chem Phys 84:1659
- Kanhere DG, Kshirsagar A, Bhamre V (1988) Chem Phys Lett 160:526
- Kim K, Harrison J (1996) J Phys B 29:595
- Schrader DM, Yoshida T, Iguchi K (1992) Phys Rev Lett 68:3281
- Schrader DM, Yoshida T, Iguchi K (1993) J Chem Phys 98:7185
- Jiang N, Schrader DM (1998) Phys Rev Lett 81:5113
- Bressanini D, Mella M, Morosi G (1998) J Chem Phys 108:4756
- Miura N, Saito SL (2003) Mol Phys 101:143
- Saito SL (2003) Chem Phys Lett 381:565
- Saito SL (2005) J Chem Phys 122:054302
- de Boor C (2001) A practical guide to splines. Springer, Berlin Heidelberg New York
- Sapirstein J, Johnson WR (1996) J Phys B 29:5213
- Langhoff SR, Davidson ER (1974) Int J Quantum Chem 8:61
- Roothaan CCJ, Bagus PS (1963) Meth Comput Phys 2:47
- Saito SL (2003) Theor Chem Acc 109:326
- Sasaki F (1974) Int J Quantum Chem 8:605
- Sasaki F, Sekiya M, Noro T, Ohtsuki K, Osanai Y (1990) In: Clementi E (ed) Modern techniques in computational chemistry: MO-TECC. ESCOM, Leiden, p 181
- Hotop H, Lineberger WC (1985) J Phys Chem Ref Data 14:731
- Bressanini D, Mella M, Morosi G (1998) Phys Rev A 57:1678
- Jiang N, Schrader DM (1998) J Chem Phys 109:9430
- For example, see Ref. [5]