

## Excited States of Positronic Lithium and Beryllium

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Using a variational method with an explicitly correlated Gaussian basis, we study the  $e^+$ -Li and  $e^+$ -Be complexes in the ground and lowest excited states with higher spin multiplicity. Our calculations provide rigorous theoretical confirmation that a positron can be attached to the excited states:  $1s2s2p^4P^o$  and  $1s^22s2p^3P^o$  for  $e^+$ -Li and  $e^+$ -Be, respectively. The result is particularly notable for the  $e^+$ -Be complex, as the excited  $^3P^o$  state lies below the autoionization threshold. We report accurate binding energies, annihilation rates and structural properties of these positron-atom systems. The existence of the ground and metastable excited states with bound positron opens up a new route to the presently lacking experimental verification of stability of a positron binding to any neutral atom.

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Understanding the mechanisms of the interaction of low energy positrons with matter is one of the main tasks of positron physics and chemistry. In particular, of great interest is the question whether atoms and molecules can capture positrons and form bound states stable against dissociation [1–9]. Since 1997, when the first conclusive and rigorous theoretical confirmation of a possibility of attaching a positron to a neutral lithium was given [1], there have been a number of investigations claiming the dynamical stability of positron-atom complexes. At present, at least a dozen atoms are believed to be capable of binding a positron. In contrast, on the experimental side no evidence has been collected as of yet to demonstrate the existence of positronic atoms. While different experimental approaches to study positron binding to atoms have been proposed, e.g., by measuring resonant positron-atom annihilation [10,11] or by laser-assisted photorecombination [12], the existence of excited states is of crucial importance for detecting positron-atom complexes as it should allow spectroscopic measurements. Just recently such an approach has been used by Cassidy *et al.* [13] to confirm the production of a positronium molecule ( $\text{Ps}_2$ ). The technique employed in Ref. [13] was based on observing small yet detectable changes in the annihilation yield of dense Ps over a narrow range of wavelengths corresponding to a transition between the ground and excited states of  $\text{Ps}_2$ . The existence of a bound excited state of  $\text{Ps}_2$ , in turn, had been previously predicted by numerical calculations [14].

Only a handful of theoretical studies so far have dealt with the investigation of excited states of positronic atoms. The simplest multielectron atom, helium, has been known to attach a positron in its  $1s2s^3S$  state for more than a decade [15] (here and below the term symbol refers to electrons only). Recently, it has also been shown that positron attachment is possible in three doubly excited states [16–18]. Nevertheless, in its ground singlet state He does not form a bound positron-atom complex. There was also an indication based on large configuration

interaction (CI) calculations that Ca and Be might also bind a positron in an excited state [6,19]. These calculations, however, did not yield positive binding energy values. Instead, they relied heavily on asymptotic series analysis and extrapolation, and involved a fixed-core approximation. It is only recently that Bressanini [9] demonstrated convincingly that lithium can attach a positron in the excited  $1s2s2p^4P^o$  state. While an encouraging fact by itself, it is somewhat unfortunate that this quartet state of Li lies far above the autoionization threshold. Its lifetime on the order of microseconds [20] is primarily determined by the relatively quick autoionization process. The question of the existence of positron-atom complexes in metastable states, whose energies are below the autoionization threshold, is much more intriguing from the practical point of view. In this Letter, we report a rigorous confirmation of such possibility for the  $1s^22s2p^3P^o$  state of a Be atom (see Fig. 1). The lowest excited state of Be, it can only decay radiatively to the ground  $^1S$  state by emitting two or more photons. Its lifetime exceeds 2 s [21]. Our calculations allowed us to estimate also the lifetimes of both  $e^+$ -Li

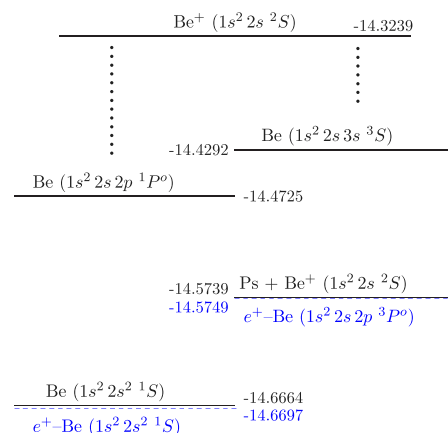


FIG. 1 (color online). Energy levels of Be and Be<sup>+</sup> (solid black lines) and e<sup>+</sup>-Be (dashed blue lines).

and  $e^+$ -Be complexes against electron-positron annihilation.

An accurate description of positronic systems is challenging even in their ground states. The difficulties stem from the presence of a different kind of light particle and weak binding energies. Moreover, due to strong repulsion from nuclei, the positron transforms the system into a clusterlike structure, which may result in poor convergence of traditional quantum-chemical approaches [22,23]. Explicitly correlated Gaussian (ECG) basis sets that depend on all interparticle distances provide effective means for overcoming these obstacles for small systems. For the case of  $L = 0, 1$  considered in this work, where  $L$  is the total orbital angular momentum, a suitable form of the spatial part of ECGs is

$$\phi_k^{(L=0)} = \exp\left[-\sum_i \alpha_{ik} r_i^2 - \sum_{i<j} \beta_{ijk} r_{ij}^2\right], \quad (1)$$

$$\phi_k^{(L=1,M=0)} = z_{pk} \exp\left[-\sum_i \alpha_{ik} r_i^2 - \sum_{i<j} \beta_{ijk} r_{ij}^2\right], \quad (2)$$

where  $\mathbf{r}_i$  are particle coordinates,  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ , and  $\alpha_{ik}$ ,  $\beta_{ijk}$ , and  $p_k$  are variational parameters. The explicit use of the spin part of the wave function can be avoided by employing Young projection operators within spin-free formalism [24]. Variational expansions in terms of ECGs have demonstrated an exceptional performance in calculations of various quantum few-body systems, including those containing positrons [25–28].

It has been known that the condition and likelihood of positron binding to an atom  $A$  depends on the ionization potential (IP) of the atomic state [5]. When the IP is greater than 0.25 hartree (binding energy of Ps), the threshold for the total energy is set by dissociation channel  $e^+ + A$ . In this case the key property affecting the existence of a bound state is the atomic polarizability. When the IP is smaller than 0.25, the dissociation channel  $\text{Ps} + A^+$  becomes more competitive. It has been observed that a positron is more likely to form a bound state with an atom when the IP value is not far from 0.25. The ground and excited states of Li and Be considered in this Letter satisfy that condition fairly well, as demonstrated in Table I. Regardless of the dissociation threshold, a bound

TABLE I. Atomic ionization potentials (in hartree, from Ref. [29]) and dissociation thresholds for positron-atom complexes.

$e^+$ -A(state)	IP[A(state)]	Dissociation threshold
$e^+$ -Li( $1s^2 2s^2 S$ )	0.198	Ps + Li <sup>+</sup> ( $1s^2 1S$ )
$e^+$ -Li( $1s 2s 2p^4 P^o$ )	0.255	$e^+$ + Li( $1s 2s 2p^4 P^o$ )
$e^+$ -Be( $1s^2 2s^2 1S$ )	0.343	$e^+$ + Be( $1s^2 2s^2 1S$ )
$e^+$ -Be( $1s^2 2s 2p^3 P^o$ )	0.242	Ps + Be <sup>+</sup> ( $1s^2 2s^2 S$ )

positron-atom state can be generally viewed as a mixture of two major configurations involving different binding mechanisms, namely, a positron interacting with a polarized atom and a polarized Ps atom interacting with an atomic ion.

The convergence of the total nonrelativistic energies for the  $e^+$ -Li and  $e^+$ -Be positronic complexes and relevant states of the atoms and ions is shown in Table II. We performed calculations using finite masses for the atomic nuclei:  $M(^7\text{Li}) = 12\,786.3933m_e$  and  $M(^9\text{Be}) = 16\,424.2037m_e$ , where  $m_e$  is the electron mass. To enable direct comparison with energies from published works we also recalculated all quantities by setting the nuclear mass to infinity.

TABLE II. Convergence of total nonrelativistic energies and positron binding energies (BE). All values are in hartree.

Basis size	Nucleus	BE		
		Li <sup>+</sup> ( $1S$ )	$e^+$ -Li( $2S$ )	
500	$^7\text{Li}$	-7.279 321 52	-7.531 731 45	0.002 410
1000	$^7\text{Li}$	-7.279 321 52	-7.531 802 42	0.002 481
1500	$^7\text{Li}$	-7.279 321 52	-7.531 811 66	0.002490
2000	$^7\text{Li}$	-7.279 321 52	-7.531 814 32	0.002 493
2500	$^7\text{Li}$	-7.279 321 52	-7.531 815 32	0.002494
3000	$^7\text{Li}$	-7.279 321 52	-7.531 815 73	0.002 494
3000	$^\infty\text{Li}$	-7.279 913 41	-7.532 410 48	0.002 497
Ref. [30] <sup>a</sup>	$^\infty\text{Li}$	-7.279 913 4	-7.532 395 5	0.002 482
		Li( $4P^o$ )	$e^+$ -Li( $4P^o$ )	
500	$^7\text{Li}$	-5.367 605 51	-5.373 199 50	0.005 594
1000	$^7\text{Li}$	-5.367 605 79	-5.373 386 70	0.005 781
1500	$^7\text{Li}$	-5.367 605 81	-5.373 417 78	0.005 812
2000	$^7\text{Li}$	-5.367 605 82	-5.373 427 57	0.005 822
2500	$^7\text{Li}$	-5.3676 058 2	-5.373 431 52	0.005 826
3000	$^7\text{Li}$	-5.367 605 82	-5.373 433 43	0.005 828
3000	$^\infty\text{Li}$	-5.368 010 15	-5.373 835 48	0.005 825
Ref. [9] <sup>b</sup>	$^\infty\text{Li}$	-5.367 33(3)	-5.3710(2)	0.0037(2)
		Be( $1S$ )	$e^+$ -Be( $1S$ )	
500	$^9\text{Be}$	-14.666 428 42	-14.669 153 13	0.002 725
1000	$^9\text{Be}$	-14.666 434 60	-14.669 553 55	0.003 119
1500	$^9\text{Be}$	-14.666 435 25	-14.669 633 47	0.003 198
2000	$^9\text{Be}$	-14.666 435 37	-14.669 662 10	0.003 227
2500	$^9\text{Be}$	-14.666 435 47	-14.669 674 34	0.003 239
2500	$^\infty\text{Be}$	-14.667 356 45	-14.670 592 86	0.003 236
Ref. [31] <sup>c</sup>	$^\infty\text{Be}$	-14.667 338	-14.670 519	0.003 181
		Be <sup>+</sup> ( $2S$ )	$e^+$ -Be( $3P^o$ )	
500	$^9\text{Be}$	-14.323 863 15	-14.572 774 52	-0.001 089
1000	$^9\text{Be}$	-14.323 863 47	-14.574 263 28	0.000 400
1500	$^9\text{Be}$	-14.323 863 49	-14.574 629 84	0.000 766
2000	$^9\text{Be}$	-14.323 863 49	-14.574 784 65	0.000 921
2500	$^9\text{Be}$	-14.323 863 49	-14.574 863 80	0.001 000
2500	$^\infty\text{Be}$	-14.324 763 18	-14.575 764 95	0.001 002

<sup>a</sup>ECG, 1200 basis functions.

<sup>b</sup>Fixed-node diffusion Monte Carlo simulations.

<sup>c</sup>ECG, 2200 basis functions.

The data in Table II exhibit excellent agreement with and marginal improvement over the best previous calculations of the ground states of  $e^+$ -Li and  $e^+$ -Be by Mitroy *et al.* [30,31]. We have confirmed the stability of the excited  $1s2s2p^4P^o$  state of positronic lithium, and significantly increased the accuracy of the binding energy from 0.0037 hartree reported in Ref. [9] to 0.005 827 6(10) hartree obtained in this work. Finally, our efforts to compute the  $1s^22s2p^3P^o$  state of  $e^+$ -Be have provided conclusive evidence that beryllium can attach a positron in an excited triplet state. The positron binding energy in that state is rather small and equal to just 0.001 000 3(400) hartree or 0.027 22(10) eV. Because of tighter energy convergence in the case of bare atoms in comparison with the corresponding positron-atom complexes, our calculated binding energies are undoubtedly bounds from below to the exact nonrelativistic values. The uncertainties are estimated by extrapolating to the limit of the infinite basis size. Given the sufficiently high convergence of the total energies and no approximations involved in the calculations (at the nonrelativistic level), the prediction of the existence of the bound excited state is rigorous. The inclusion of relativistic corrections would not alter this conclusion, as they cancel out to a large extent in weakly bound systems when the energy difference (e.g.,  $e^+$ -A vs Ps +  $A^+$ ) is evaluated. This happens because the largest contribution to the relativistic correction is due to core electrons, which remain essentially undistorted upon binding a positron. Rough estimates suggest that the net effect of relativistic corrections on the positron binding energy in the  $1s^22s2p^3P^o$  state of  $e^+$ -Be is at least 1–2 orders of magnitude smaller than the binding energy itself. We have computed the change in the binding energy due to the inclusion of the two largest corrective terms, the mass velocity and Darwin terms, and obtained a shift of only 0.000 007 hartree.

Table III lists expectation values, which allow us to compare the structure of the excited states of positronic

lithium and beryllium with that of the ground states as well as with the related atoms and ions. As a result of weak binding, positronic atoms typically have a very large spatial extent and possess halolike properties [32]. Remarkably, for both  $e^+$ -Li and  $e^+$ -Be, the size of the system as a whole in the excited state is smaller than in the ground state. The value of the average nucleus-positron distance,  $\langle r_{ne^+} \rangle$ , drops notably in the excited states. This fact can be rationalized in the case of Li by the almost twice higher binding energy in the  $1s2s2p^4P^o$  state compared to the  $1s^22s^2S$  state. For Be, however, where binding in the excited state is extremely weak, the exact reason for such behavior is not immediately clear. The atomic  $^3P^o$  state, i.e., when no positron is attached, is predictably larger than the ground  $^1S$  state. The near equality of  $\langle r_{ne^+} \rangle$  with  $\langle r_{e^+e^-} \rangle$  leads to the conclusion that  $e^+$ -Be ( $1s^22s^2^1S$ ) fits well into the picture of a bare positron interacting with a distant atom. This conclusion becomes even more evident when comparing nucleus-electron and electron-electron pair correlation functions,  $g_{ij}(\mathbf{r}) = \langle \delta(\mathbf{r}_{ij} - \mathbf{r}) \rangle$ , shown in Fig. 2. The change in these two distributions upon going from the Be atom to the  $e^+$ -Be complex is tiny. In contrast, the same two distributions,  $g_{ne^-}(\mathbf{r})$  and  $g_{e^-e^-}(\mathbf{r})$ , exhibit noticeable difference between Li ( $1s^22s^2S$ ) and  $e^+$ -Li ( $1s^22s^2S$ ). The ratio between  $\langle r_{ne^+} \rangle$  and  $\langle r_{e^+e^-} \rangle$  for  $e^+$ -Li ( $1s^22s^2S$ ) suggests that this system can be mainly viewed as a weakly distorted Ps- $A^+$  complex.

The geometric structure interpretation for the excited  $P$  states of positronic atoms is somewhat less straightforward. The value of  $\langle r_{ne^+} \rangle$  is larger for  $e^+$ -Be compared to  $e^+$ -Li. At the same time the average positron-electron distance,  $\langle r_{e^+e^-} \rangle$ , is smaller. While the ratio between the  $\langle r_{ne^+} \rangle$  and  $\langle r_{e^+e^-} \rangle$  in the  $1s^22s2p^3P^o$  state of  $e^+$ -Be is not exactly consistent with a Ps- $A^+$  configuration, the positron-electron correlation function shown in Fig. 3 has a pronounced maximum at small positron-electron separation, which suggests that this configuration dominates.

TABLE III. Expectation values (in atomic units) for the ground and excited states of positronic complexes and relevant atoms and ions. For convenience, we use  $n$ ,  $e^+$ , and  $e^-$  as indices, to denote nucleus, positron, and electron respectively.  $\Gamma$  is the spin-averaged annihilation rate (in  $10^9 \text{ s}^{-1}$ ). All quantities were computed using the largest generated ECG basis. Values in parentheses show estimated remaining uncertainty due to finite size of the basis.

System	$\langle r_{ne^-} \rangle$	$\langle r_{e^-e^-} \rangle$	$\langle r_{ne^+} \rangle$	$\langle r_{e^+e^-} \rangle$	$\langle \delta(\mathbf{r}_{ne^-}) \rangle$	$\langle \delta(\mathbf{r}_{e^-e^-}) \rangle$	$\langle \delta(\mathbf{r}_{ne^+}) \rangle$	$\langle \delta(\mathbf{r}_{e^+e^-}) \rangle$	$\Gamma$
Ps	3.000 000							0.039 789	2.0028
Li $^+(^1S)$	0.572 821(0)	0.862 373(0)			6.850 35(3)	0.533 608(6)			
Li $(^2S)$	1.663 312(0)	2.889 697(0)			4.613 04(5)	0.181 404(10)			
$e^+$ -Li $(^2S)$	3.4112(4)	6.3635(8)	9.9476(11)	7.7773(8)	4.5706(15)	0.178 43(10)	0.000 0018(2)	0.011 582(20)	1.7484(30)
Li $(^4P)$	2.034 578(0)	3.495 662(0)			2.978 053(50)	0(0)			
$e^+$ -Li $(^4P)$	2.272 48(8)	3.913 73(15)	9.0956(8)	8.8956(8)	2.9780(20)	0(0)	0.000 0019(3)	0.003 941(10)	0.595 11(150)
Be $^+(^2S)$	1.033 863(0)	1.755 787(0)			11.699 22(30)	0.526 780(40)			
Be $(^1S)$	1.493 194(0)	2.545 443(0)			8.839 48(15)	0.267 56(4)			
$e^+$ -Be $(^1S)$	1.535 73(2)	2.606 26(4)	9.9998(35)	9.9575(35)	8.819(15)	0.2676(4)	0.000 002 5(10)	0.002 140(10)	0.430 95(200)
Be $(^3P)$	1.556 996(1)	2.693 011(2)			8.7136(15)	0.261 22(10)			
$e^+$ -Be $(^3P)$	2.326(6)	4.148(10)	9.55(8)	8.78(3)	8.710(10)	0.2633(5)	0.000 0016(5)	0.005 05(7)	1.0170(150)

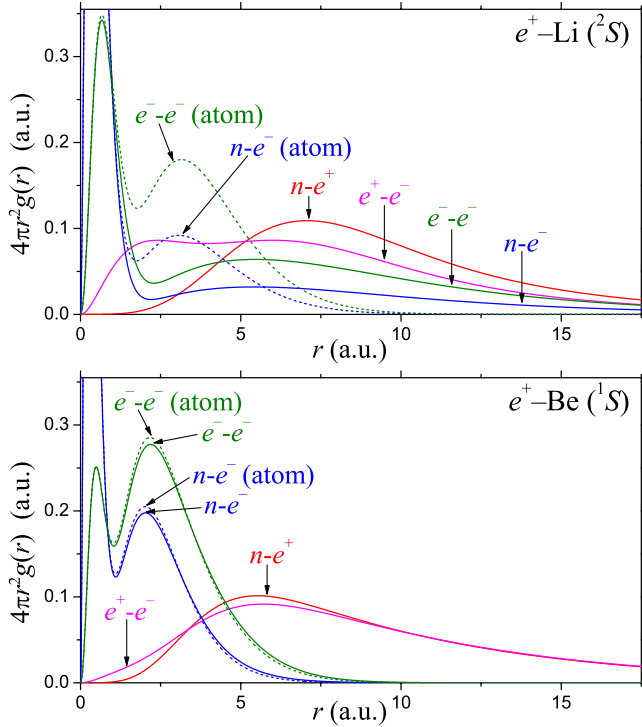


FIG. 2 (color online). Pair correlation functions for the ground  $S$  states of positronic lithium and beryllium. Dashed lines correspond to isolated atoms with no positron.

Interestingly, the positron-electron correlation function for the  $P$  state of positronic lithium also has a noticeable (albeit shorter) peak at small distances. Therefore, there should be certain admixture of  $\text{Ps-A}^+$  configuration in this state as well. Nucleus-positron correlation functions for the  $P$  states of both  $e^+\text{-Li}$  and  $e^+\text{-Be}$  presented in Fig. 3 do not have a node (only a concavity) at  $z = 0$ . The absence of the node suggests that the positron is in a mixture of states with zero and nonzero orbital angular momenta.

In Table III we also show the expectation values of the two-particle delta functions. Knowledge of the average electron-positron densities at coalescence points allows us to predict the lifetimes against annihilation. The total spin-averaged particle-antiparticle annihilation rate (see Ref. [33] for details) is given by

$$\Gamma = \pi \frac{\alpha^4 c}{a_0} \left[ 1 + \left( \frac{19\pi}{12} - \frac{17}{\pi} \right) \alpha - 2\alpha^2 \ln \alpha \right] N_{e^+} N_{e^-} \langle \delta_{e^+e^-} \rangle, \quad (3)$$

where  $\alpha$  is the fine structure constant,  $c$  is the speed of light,  $a_0$  is the Bohr radius, and  $N_{e^+}$  and  $N_{e^-}$  are the number of positrons and electrons in the system. The terms following the unity in the square brackets of Eq. (3) represent the leading radiative corrections [34,35].

It is important to note that the annihilation rates in the ground and excited states of both  $e^+\text{-Li}$  and  $e^+\text{-Be}$  are significantly different. In the case of lithium,  $\Gamma$  is about 3

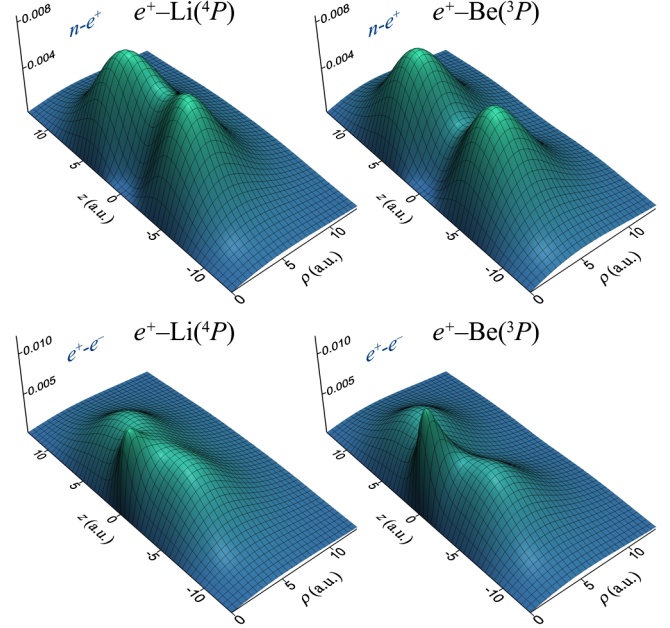


FIG. 3 (color online). Nucleus-positron and positron-electron correlation functions,  $2\pi\rho g(\mathbf{r})$  [ $\mathbf{r} \equiv (\rho, z)$ ,  $\rho = \sqrt{x^2 + y^2}$ ], for the excited  $P$  states of positronic Li and Be.

times smaller in the excited  $4P^o$  state than in the ground  $2S$  state,  $1.7484(30) \times 10^9 \text{ s}^{-1}$  vs  $0.59511(150) \times 10^9 \text{ s}^{-1}$ , respectively. For beryllium, the situation is opposite. The ground state survives for roughly twice longer than the excited state:  $\Gamma(^1S) = 0.43095(200) \times 10^9 \text{ s}^{-1}$ , while  $\Gamma(^3P^o) = 1.0170(150) \times 10^9 \text{ s}^{-1}$ . The lower electron-positron annihilation rate in  $e^+\text{-Li}(4P^o)$  and  $e^+\text{-Be}(^1S)$  should be attributed to the fact that in these states the positron is alone and only weakly interacts with the atom. Hence, the electron and positron components of the wave function overlap little. In contrast, the most significant configuration in  $e^+\text{-Li}(^2S)$  and  $e^+\text{-Be}(^3P^o)$  is  $\text{Ps-A}$ . The electron in the  $\text{Ps}$  atom is the one which most likely annihilates with the positron. A substantial difference in  $\Gamma$  of the ground and excited states should be a welcome fact for possible spectroscopic studies that detect optically induced changes in the annihilation yield.

To summarize, we have investigated positron-atom complexes in excited states  $e^+\text{-Li}(1s2s2p^4P^o)$  and  $e^+\text{-Be}(1s^22s2p^3P^o)$ . Based on the results of variational calculations with all-particle correlated basis sets, we have obtained a rigorous confirmation that both of these states should be dynamically stable. The  $1s^22s2p^3P^o$  state has the advantage of being the lowest excited state of Be and having a long (exceeding seconds) lifetime against radiative decay. Theoretical evidence for the capability of two-to four-electron atoms to form excited states with positrons obtained in Refs. [9,15,16] as well as in this work raise the question as to whether positron binding in excited states should be of common occurrence. Indeed, while the ground state of an atom may not always possess the properties

necessary for attaching a positron, it is more likely that suitable candidates (e.g., those with higher polarizability and ionization potential close to 0.25 hartree) can be found among the multitude of excited states. Routine search for weakly bound positron-atom states, however, remains a difficult task and will require the development of new, reliable, and computationally inexpensive approaches in the future. We hope that the conclusive evidence for the existence of a weakly bound excited state of positronic beryllium may stimulate future experimental efforts to perform spectroscopic measurements that involve the ground to excited state transition in this and other similar systems.

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