CHINESE JOURNAL OF PHYSICS VOL. 52, NO. 5 October 2014

Calculations of the High Lying (2pns) ^{1,3}P$^\circ$ and (2pnd) ^{1,3}P$^\circ$ Rydberg States of the Be Atom via the Modified Atomic Orbital Theory

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(Received March 4, 2013; Revised February 25, 2014)

We report in this paper on the energy positions of the (2pns) ^{1,3}P$^\circ$ and (2pnd) ^{1,3}P$^\circ$ and the resonance widths of the (2pns) ^{1}P$^\circ$ (n = 3–25) doubly excited states of the beryllium atom. The calculations are performed using the modified atomic orbital theory (MAOT). The present results compared very well with the available theoretical and experimental literature values. The high precision data presented in this work may be a useful guideline for those studying the photoabsorption spectra of Be.

DOI: 10.6122/CJP.20140313 PACS numbers: 31.15.bu, 31.15.vj, 32.80.Zb, 32.80.Ee

I. INTRODUCTION

While the photoionization of helium has been studied thoroughly, the beryllium atom considered as a supra helium-atom has been investigated marginally by comparison. Double excitations in the Be valence-shell region have been studied experimentally as well as theoretically in the past. As the $1s^2$ electrons do not actively participate in the autoionization process, Be appears to be a system only slightly more complicated than He and is an attractive candidate for the study of electronic correlation effects in four electron systems. On the experimental side, Mehlman-Balloffet and Steva [1] and Esteva *et al.* [2] used vacuum sparks to photoexcite and ionize the Be atom, and absorption spectra were recorded on high-sensitive film. These authors reported energy resonances for a few $1s^2 2pns$ ^{1}P$^\circ$ and $1s^2 2pnd$ ^{1}P$^\circ$ doubly excited states of Be. In addition, Wehlitz *et al.* [3] presented the energy positions of the $1s^2 2pns$ ^{1}P$^\circ$ and $1s^2 2pnd$ ^{1}P$^\circ$ autoionizing states of Be from monochromatized synchrotron radiation (MSR). On the theoretical side, energy positions of the $1s^2 2pns$ ^{1}P$^\circ$ (n = 3–5) and $1s^2 2pnd$ ^{1}P$^\circ$ (n = 3–4) states of Be were first calculated by Moores, as stated by Woodruff and Samson [4] using the close-coupling method. Besides, Lin [5] reported results for the $1s^2 2pns$ ^{1}P$^\circ$ (n = 3–4) and $1s^2 2pnd$ ^{1}P$^\circ$ (n = 3–4) levels em-

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ploying the hyperspherical (HS) method. For the high-lying states, Kim *et al.* [6] reported energies of the $1s^2 2p ns\ ^1P^\circ$ and $1s^2 2p nd\ ^1P^\circ$ levels up to $n = 15$ using the hyperspherical close-coupling (HSCC) method, whereas Ju-Tang Hsiao *et al.* [7] applied the multiconfiguration relativistic randon-phase approximation (MCRRPA) to tabulate energies for both singlet and triplet $1s^2 2p ns\ ^{1,3}P^\circ$ and $1s^2 2p nd\ ^{1,3}P^\circ$ doubly excited states of Be up to $n = 20$. Employing the screening constant unit nuclear charge (SCUNC) method, Sakho [8] reported high lying energy positions of the $(2p ns)\ ^{1,3}P^\circ$ and $(2p nd)\ ^{1,3}P^\circ$ autoionizing states and resonance widths of the $(2p ns)\ ^1P^\circ$ excited states of Be up to $n = 20$. In addition, the B-spline-based configuration interaction procedure for the continuum (CIC) has been used by Chang and Zhu [9] to compute energy positions and width resonances of the $2p nl\ ^1P^\circ$ states of Be, whereas Chen [10] applied the B-spline-based complex rotation (BSCR) along with the stabilization method (SM) to calculate energy and width resonances of the $1s^2 2p ns\ ^{1,3}P^\circ$ and $1s^2 2p nd\ ^{1,3}P^\circ$ states of Be. On the other hand, the stabilization method has been used by Pong and Ho [11, 12] in the calculation of the $1s^2 3l3l'\ ^1D^e$ doubly excited states of the beryllium-like ions for $Z = 5$–10 and Z = 12 [11], and in the investigation of the $1s^2 3lnl'\ ^1G^e$ resonance states of the four-electron beryllium-like B^+, C^{2+}, N^{3+}, O^{4+}, and Ne^{6+} ions below the $N = 3$ thresholds of the three-electron systems [12]. Recently, the MAOT formalism has been applied successfully in the studies of high lying $^{1,3}P^\circ$ states of He-like ions [13], of He and H^- [14], and in the photoionization study of the Kr^+ and Xe^+ ions [15]. In this paper, we apply the MAOT formalism to report high precision energy positions for the $1s^2 2p ns\ ^{1,3}P^\circ$ and $1s^2 2p nd\ ^{1,3}P^\circ$ levels of Be along with resonance widths of the $1s^2 2p ns\ ^1P^\circ$ states up to $n = 25$. In Section II we give a brief description of the MAOT formalism and the theoretical part adopted in this work. Section III presents the results obtained along with comparisons with various theoretical and experimental data.

II. THEORY

II-1. Brief description of the MAOT formalism

In the framework of the modified atomic orbital theory (MAOT), the total energy of a $(\upsilon\ell)$-given orbital is expressed in the form [13, 14]

$$E(\upsilon\ell) = -\frac{[Z - \sigma(\ell)]^2}{\upsilon^2}. \tag{1}$$

For an atomic system of several electrons M, the total energy is given by (in Rydberg units)

$$E = -\sum_{i=1}^{M} \frac{[Z - \sigma_i(\ell)]^2}{\upsilon_i^2}.$$

For the $(N\ell, n\ell')\ ^{2S+1}L^\pi$ doubly excited states, the total energy of an atomic system of many M electrons is expressed as follows:

$$E = -\sum_{i=1}^{M} \frac{\left[Z - \sigma_i(^{2S+1}L^\pi)\right]^2}{\upsilon_i^2}. \tag{2}$$

In the photoionisation study, energy resonances are generally measured relatively to the E_∞ converging limit of a given $(^{2S+1}L_J)nl$-Rydberg series. For these states, the general expression of the energy resonances is given by the formula of Sakho presented previously [15] (in Rydberg units):

$$E_n = E_\infty - \frac{1}{n^2} \quad \left\{ Z - \sigma_1(^{2S+1}L_J) - \sigma_2(^{2S+1}L_J) \times \frac{1}{n} \right. \\ \left. - \sigma_2^{\alpha}(^2P^0_{3/2},^1 D_2) \times (n-m) \times (n-q) \sum_k \frac{1}{f_k(n,m,q,s)} \right\}^2 . \qquad (3)$$

In this equation, m and q $(m < q)$ denote the principal quantum numbers of the $(^{2S+1}L_J)nl$-Rydberg series of the considered atomic system used in the empirical determination of the $\sigma_i(^{2S+1}L_J)$-screening constants, s represents the spin of the nl-electron $(s = \frac{1}{2})$, E_∞ is the energy value of the series limit generally determined from the NIST atomic database, E_n denotes the corresponding energy resonance, and Z represents the nuclear charge of the considered element. The only problem that one may face by using the MAOT formalism is linked to the determination of the $\sum_k \frac{1}{f_k(n,m,q,s)}$ term. The correct expression of this term is determined iteratively by imposing general Eq. (3) to give high precision data with a constant quantum defect values along all the considered series. The value of α is fixed to 1 and/or 2 during the iteration. The quantum defect is calculated from the standard formula

$$E_n = E_\infty - \frac{RZ^2}{(n-\delta)^2}.$$

II-2. Energy of the 2pns ^{1,3}P$^\circ$ and 2pnd ^{1,3}P$^\circ$ doubly excited states of Be

Using Eq. (3) we find

• For the 2pns ^{1,3}P$^\circ$ levels:

$$E\left(2pns;^{2S+1}P^\circ\right) = E_\infty - \frac{1}{n^2}\left\{ Z - \sigma_1(s) - \frac{\sigma_2(s)}{n} \right. \\ -\sigma_2(n-m)(n-q)\left[\frac{1}{(n+q-m+s)(n-s)^2} + \frac{1}{(n+2m-q)^3}\right] \\ \left. -\frac{\sigma_2 \times (S+1) \times S}{(n+q-m+s)^2} + \frac{\sigma_2 \times S \times (n-m)^2}{(n+m)^3} \right\}^2 . \qquad (4)$$

• For the 2pnd ^{1,3}P^o levels:

$$E\left(2pnd;^{2S+1}P^\circ\right) = E_\infty - \frac{1}{n^2}\left\{ Z - \sigma_1(d) - \frac{\sigma_2(d)}{n} \right. \\ -\sigma_2(n-m)(n-q)\left[\frac{1}{(n-s)^2} + \frac{1}{(n-q+m)(n+s)^2}\right] \\ \left. +\frac{S \times \sigma_2 \times (n-m)}{(n+q)^2} \right\}^2 . \qquad (5)$$

To evaluate the σ_i-screening constants, we use the $E_{\rm exp}(2pnl)$ experimental data of the monochromatized synchrotron radiation (MSR) of Wehlitz *et al.* [3]. From Kramida and Martin [16] we get (in Rydberg units) $E_\infty = 0.97620699$. For the (2pns) ^{1}P$^\circ$ and (2pnd) ^{1}P$^\circ$ excited states, we get in Rydberg units [3]

- $E_{\rm exp}(2p3s) = 0.800326451$ $(m = 3)$, $\quad E_{\rm exp}(2p4s) = 0.890215261$ $(q = 4)$,
- $E_{\rm exp}(2p3d) = 0.870223637$ $(m = 3)$, $\quad E_{\rm exp}(2p4d) = 0.915792780$ $(q = 4)$.

Using Equations (3) and (4), we find the empirical values of the screening constants:

- $\sigma_1(s) = 3.0825 \pm 0.0012$, $\quad \sigma_2(s) = 1.0220 \pm 0.0029$,
- $\sigma_1(d) = 2.9973 \pm 0.0083$, $\quad \sigma_2(d) = 0.0782 \pm 0.0190$.

The $E_{\rm exp}(2pnl)$ experimental energy values of Wehlitz *et al.* [3] are converted into Rydberg units using 1 Ry = 13.60569 eV.

II-3. Resonance widths of the 2pns ^{1}P$^\circ$ doubly excited states of Be

The resonance widths of the 2pns ^{1}P$^\circ$ doubly excited states of the beryllium atom are given by (in Rydberg units)

$$\Gamma\left(2pns;^1P^0\right) = \frac{1}{n^2}\left\{Z - \sigma_1(s) - \frac{\sigma_2(s)}{n} - \sigma_2(n-m)(n-q)\left[\frac{1}{(n+m-s)^3}\right]\right\}^2. \quad (6)$$

The σ_i-screening constants in Eq. (6) are evaluated using the experimental widths (in meV) $\Gamma_{\rm exp}$ (2p3s ^{1}P$^\circ$) $= 531 \pm 10$ and $\Gamma_{\rm exp}$ (2p4s ^{1}P$^\circ$) $= 174 \pm 10$ $(m = 3;\ q = 4)$ of Be measured by Wehlitz *et al.* [3]. Eq. (6) provides then $\sigma_1(s) = 3.969 \pm 0.035$ and $\sigma_2(s) = -1.684 \pm 0.089$.

III. RESULTS AND DISCUSSIONS

III-1. Comparison with literature data published in atomic units

The results obtained in this work are quoted in Tables V–VI and compared with the available literature data. In Tables I and II, we present comparisons of the energy positions of the (2pns) ^{1}P$^\circ$ (Table I) and of the (2pnd) ^{1}P$^\circ$ (Table II) excited states of Be obtained from the present modified atomic orbital theory (MAOT) with the experimental data of Mehlman-Balloffet and Esteva [1], Esteva *et al.* [2], Wehlitz *et al.* [3], the theoretical screening constant by unit nuclear charge (SCUNC) values of Sakho [8], the hyper-spherical close-coupling (HCC) calculations of Kim *et al.* [6] as quoted in Ju-Tang Hsiao *et al.* [7], and with the multi-configuration relativistic random-phase approximation (MCRRPA) values of Ju-Tang Hsiao *et al.* [7]. It can be seen that the MAOT results agree very well with the listed literature data. The very good agreement between the calculations up to high n values should be mentioned. For $n = 15$, the MAOT data and the SCUNC, MCRRPA, and HCC results are respectively at (in a.u.) 0.485644, 0.485741, 0.485675, and 0.48468 for the

2p15s $^1P^\circ$ level and at 0.485655 (MAOT), 0.485985 (SCUNC), 0.485912 (MCRRPA), and 0.48487 (HCC) for the 2p15d $^1P^\circ$ level. These results show that the MAOT calculations match more with those from the SCUNC and MCRRPA formalisms. Table III indicates the present calculations for the doubly (2pns) $^3P^\circ$ and (2pnd) $^3P^\circ$ states of Be compared with the MCRRPA values [7] and with the SCUNC data [8]. For both the (2pns) $^3P^\circ$ and (2pnd) $^3P^\circ$ states, the agreements between the calculations are seen to be very good up to $n = 15$. For the (2pns) $^3P^\circ$ and (2pnd) $^3P^\circ$ levels ($n > 15$), the MAOT results up to $n = 20$ are compared with the only existing SCUNC values [8] and good agreements are obtained. These agreements allow us to list our results up to $n = 25$. As far as the resonance widths of the (2pns) $^1P^\circ$ states are concerned, the results obtained in this work are listed in Table IV and comparisons are done with the SCUNC values [8], the MCRRPA data [7], the HCC results [6], the generalized hyperspherical coordinate (GHSC) results of Greene [17], and the close-coupling (CC) data of Moores as quoted in Woodruff and Samson [4]. Here, the agreements between the current results and all the listed literatures values are seen to be good except for the HCC results [6]. In their study, Ju-Tang Hsiao *et al.* [7] mentioned that their calculations, which include more correlation and relativistic effects than all the other calculations [4, 6, 13], should in principal provide the most precise lifetimes theoretically. It should be mentioned that our results match well with those of Ju-Tang Hsiao *et al.* [7] up to $n = 15$. These good agreements enable one to expect our results up to $n = 25$ to be fairly accurate.

III-2. Comparison with literature data published in eV

Table V shows the present calculations of the energy positions for the (2pns) $^1P^\circ$ and (2pnd) $^1P^\circ$ states and of the width resonances for the (2pns) $^1P^\circ$ levels of Be. Comparisons are done with the experimental data [3] and with the SCUNC calculations [8]. The experimental measurements [3] are published in eV and the uncertainties have been quoted. Hence our results are converted into eV for a direct comparison and the uncertainties are also quoted. Comparison indicates that our results agree well with the experimental data of Wehlitz *et al.*, [3] and with the SCUNC calculations [8] for both energy and the width resonances of the (2pns) $^1P^\circ$ states. For the (2pns)$^1P^\circ$ levels ($n > 12$), our results are compared with the only existing SCUNC values [8] and good agreements are obtained up to $n = 20$. In addition, the literature widths values have been published in meV. Our results are thus converted to meV and good agreement is then seen between the MAOT widths and both the experimental data [3] and the SCUNC values [8] for the (2pns) $^1P^\circ$ levels up to $n = 9$ except for the experimental data for $n = 8$. As far as the (2pnd) $^1P^\circ$ states are concerned, the excellent agreement between the MAOT result at 12.742 (7) eV and the experimental data [3] at 12.742 (6) for the (2p5d) $^1P^\circ$ level should be mentioned. For $n > 5$ our results are compared with the only available values [8]. The agreements between the MAOT and the SCUNC calculations are then seen to be satisfactory when n ranges between 3 and 13. But, when $n > 13$, the MAOT and SCUNC results come closer to each other. This may allow us to extend our calculations up to $n = 25$. In general, if the agreements between theory and the experiments are good for the energy positions as shown by the data quoted in Tables I–V, discrepancies are observed for the widths. New

schemes of experiments are needed to solve the large discrepancies observed for widths. In Table VI, we compare the present results for the energy positions of the doubly (2pns) ^{1,3}P$^{\circ}$ and (2pnd) ^{1,3}P$^{\circ}$ excited states and for the widths of the (2pns) ^{1}P$^{\circ}$ states of Be with the B-spline-based configuration interaction procedure for the continuum (CIC) calculations of Chang and Zhu [9] and with the results from B-spline-based complex rotation (BSCR) along with the stabilization method (SM) of Chen [10]. For the energy positions, the theoretical results [9, 10] are listed in eV. For the width resonances, the data are quoted in meV for the BSCR calculations [10] and in Ry for the SM [10] and CIC [9] computations. Our results are then converted either into eV, meV, or Ry for direct comparison with the cited literature data. Comparisons indicate that the MAOT calculations agree very well with the theoretical results [9, 10] for both energy and the width resonances. It should be underlined that, for the 2p3s ^{1}P$^{\circ}$ level, the MAOT value (in Ry) at 3.89 [-2] matches better with the CIC data at 3.81 [-2] than with the SM result [10] at 1.56 [-2]. In addition, for this same level, it is seen that the MAOT data (in meV) at 530 agree well with the BSCR result at 526 [10]. This may indicate that the SM value [10] at 1.56 [-2] can be regarded as probably being lower than the actual value.

IV. CONCLUSION

Energy positions of the (2pns) ^{1,3}P$^{\circ}$ and (2pnd) ^{1,3}P$^{\circ}$ autoionizing states and resonance widths of the (2pns) ^{1}P$^{\circ}$ excited states of the beryllium atom are reported applying the modified atomic orbital theory (MAOT). The energy positions of the resonances investigated are in good agreement with various experiments [1–3] and theoretical calculations [7–10]. The high accuracy obtained in this work indicates that the MAOT formalism can be applied usefully in the investigations of the Rydberg series of many electrons atomic systems in connection with the Opacity Project, which is an extensive international collaboration to calculate and compile a database of the collisional and radiative properties of all the ionization stages of many electrons systems.

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TABLE I: Energy positions (E) of the (2pns) ^{1}P° doubly excited states of Be. The present results (MAOT) are compared with various other results. SCUNC: screening constant by unit nuclear charge data of Sakho [8]; MCRRPA: multiconfiguration relativistic random-phase approximation values of Ju-Tang Hsiao *et al.* [7]; HCC: hyperspherical close-coupling calculations of Kim *et al.* [6]; M-BE: experimental data of Mehlman-Balloffet, and Esteva [1]; ES: experimental data of Esteva *et al.* [2]; MSR: experimental data of Monochromatized Synchrotron Radiation of Wehlitz [3]. The results are expressed in atomic units.

	Theory				Experiment		
States	MAOT	SCUNC	MCRRPA	HCC	MSR	ES	M-BE
(2p3s) ^{1}P°	0.400160	0.401800	0.401143	0.40094	0.400163	0.4018	0.3935
(2p4s) ^{1}P°	0.445106	0.444500	0.444445	0.44436	0.445108	0.4445	0.4398
(2p5s) ^{1}P°	0.461957	0.461842	0.462043	0.46149	0.461976	0.4620	0.4606
(2p6s) ^{1}P°	0.470468	0.470613	0.470813	0.47006	0.470832	0.4708	0.4697
(2p7s) ^{1}P°	0.475430	0.475659	0.475803	0.47494	0.475683	0.4757	0.4749
(2p8s) ^{1}P°	0.478583	0.478821	0.478907	0.47799	0.478549	0.4788	0.4781
(2p9s) ^{1}P°	0.480709	0.480930	0.480968	0.48003	0.480607	0.4808	
(2p10s)^{1}P°	0.482208	0.482404	0.482406	0.48145	0.482262	0.4822	
(2p11s)^{1}P°	0.483302	0.483472	0.483449	0.48247	0.482996	0.4833	
(2p12s)^{1}P°	0.484123	0.484271	0.484229	0.48324	0.484282	0.4840	
(2p13s)^{1}P°	0.484754	0.484882	0.484829	0.48384			
(2p14s)^{1}P°	0.485249	0.485361	0.485233	0.48430			
(2p15s)^{1}P°	0.485644	0.485741	0.485675	0.48468			
(2p16s)^{1}P°	0.485964	0.486049					
(2p17s)^{1}P°	0.486226	0.486301					
(2p18s)^{1}P°	0.486444	0.486510					
(2p19s)^{1}P°	0.486626	0.486686					
(2p20s)^{1}P°	0.486781	0.486834					
(2p21s)^{1}P°	0.486912						
(2p22s)^{1}P°	0.487026						
(2p23s)^{1}P°	0.487124						

continued ...

	Theory				Experiment		
States	MAOT	SCUNC	MCRRPA	HCC	MSR	ES	M-BE
(2p24s)^{1}P°	0.487209						
(2p25s)^{1}P°	0.487284						

TABLE II: Present MAOT energy positions (E) of the (2pnd) ^{1}P° doubly excited states of Be. Same as in Table I for explanation of the literature data.

	Theory				Experiment		
States	MAOT	SCUNC	MCRRPA	HCC	MSR	ES	M-BE
(2p3d) ^{1}P°	0.435114	0.435700	0.437546	0.43478	0.435112	0.4357	0.4359
(2p4d) ^{1}P°	0.457898	0.459500	0.458992	0.45706	0.457896	0.4595	0.4581
(2p5d) ^{1}P°	0.468260	0.469916	0.469214	0.46771	0.468260	0.4700	0.4688
(2p6d) ^{1}P°	0.474008	0.475451	0.474858	0.47356		0.4760	0.4748
(2p7d) ^{1}P°	0.477559	0.478763	0.478303	0.47711			
(2p8d) ^{1}P°	0.479914	0.480911	0.480559	0.47942			
(2p9d) ^{1}P°	0.481558	0.482386	0.482116	0.48102			
(2p10d) ^{1}P°	0.482752	0.483446	0.483236	0.48215			
(2p11d) ^{1}P°	0.483646	0.484234	0.484068	0.48300			
(2p12d) ^{1}P°	0.484333	0.484835	0.484704	0.48365			
(2p13d) ^{1}P°	0.484873	0.485306	0.485199	0.48415			
(2p14d) ^{1}P°	0.485305	0.485681	0.485594	0.48455			
(2p15d) ^{1}P°	0.485655	0.485985	0.485912	0.48487			
(2p16d) ^{1}P°	0.485944	0.486235					
(2p17d) ^{1}P°	0.486184	0.486443					
(2p18d) ^{1}P°	0.486387	0.486618					
(2p19d) ^{1}P°	0.486559	0.486766					
(2p20d) ^{1}P°	0.486706	0.486893					
(2p21d) ^{1}P°	0.486833						
(2p22d) ^{1}P°	0.486944						
(2p23d) ^{1}P°	0.487041						
(2p24d) ^{1}P°	0.487126						
(2p25d) ^{1}P°	0.487201						

TABLE III: Energy positions (E) of the ($2pns$) $^3P^\circ$ and ($2pnd$) $^3P^\circ$ doubly excited states of Be. The present results (MAOT) are compared with the screening constant by unit nuclear charge (SCUNC) data of Sakho [8] and with the multiconfiguration relativistic random-phase approximation (MCRRPA) values of Ju-Tang Hsiao *et al.* [7].

	Theory				Theory		
States	MAOT	SCUNC	MCRRPA	States	MAOT	SCUNC	MCRRPA
(2p3s) ^{3}P°	0.385483	0.386515	0.385166	(2p3d) ^{3}P°	0.435114	0.435700	0.435196
(2p4s) ^{3}P°	0.440240	0.440347	0.440153	(2p4d) ^{3}P°	0.457823	0.458846	0.457713
(2p5s) ^{3}P°	0.460077	0.460097	0.460260	(2p5d) ^{3}P°	0.468183	0.469358	0.468476
(2p6s) ^{3}P°	0.469718	0.469714	0.469898	(2p6d) ^{3}P°	0.473943	0.475015	0.474406
(2p7s) ^{3}P°	0.475157	0.475134	0.475266	(2p7d) ^{3}P°	0.477506	0.478420	0.478010
(2p8s) ^{3}P°	0.478523	0.478489	0.478563	(2p8d) ^{3}P°	0.479871	0.480636	0.480359
(2p9s) ^{3}P°	0.480746	0.480706	0.480733	(2p9d) ^{3}P°	0.481523	0.482163	0.481975
(2p10s)^{3}P°	0.482287	0.482246	0.482237	(2p10d) ^{3}P°	0.482723	0.483260	0.483133
(2p11s) ^{3}P°	0.483397	0.483357	0.483322	(2p11d) ^{3}P°	0.483622	0.484077	0.483991
(2p12s) ^{3}P°	0.484221	0.484184	0.484131	(2p12d) ^{3}P°	0.484313	0.484702	0.484645
(2p13s) ^{3}P°	0.484850	0.484816	0.484749	(2p13d) ^{3}P°	0.484856	0.485191	0.485154
(2p14s) ^{3}P°	0.485339	0.485308	0.485233	(2p14d) ^{3}P°	0.485290	0.485581	0.485559
(2p15s) ^{3}P°	0.485726	0.485699	0.485619	(2p15d) ^{3}P°	0.485643	0.485897	0.485885
(2p16s) ^{3}P°	0.486039	0.486015		(2p16d) ^{3}P°	0.485933	0.486157	
(2p17s) ^{3}P°	0.486294	0.486273		(2p17d) ^{3}P°	0.486175	0.486373	
(2p18s) ^{3}P°	0.486506	0.486487		(2p18d) ^{3}P°	0.486379	0.486555	
(2p19s) ^{3}P°	0.486682	0.486666		(2p19d) ^{3}P°	0.486552	0.486710	
(2p20s) ^{3}P°	0.486831	0.486817		(2p20d) ^{3}P°	0.486700	0.486842	
(2p21s) ^{3}P°	0.486958			(2p21d) ^{3}P°	0.486828		
(2p22s) ^{3}P°	0.487067			(2p22d) ^{3}P°	0.486939		
(2p23s) ^{3}P°	0.4871462			(2p23d) ^{3}P°	0.487036		
(2p24s) ^{3}P°	0.487244			(2p24d) ^{3}P°	0.487122		
(2p25s) ^{3}P°	0.487316			(2p25d) ^{3}P°	0.487198		

TABLE IV: Resonance widths (Γ) of doubly (2pns) ^{1}P° excited states of Be. The present results (MAOT) are compared with various literature data. SCUNC: screening constant by unit nuclear charge data of Sakho [8]; MCRRPA: multiconfiguration relativistic random-phase approximation values of Ju-Tang Hsiao *et al.* [7]; HCC: hyperspherical close-coupling calculations of Kim *et al.* [6]; GHSC: generalized hyperspherical coordinate results of Green [17]; CC: close-coupling data of Moores as quoted in Ref. [4]. The results are expressed in atomic units. The notation $a(b)$ means $a \times 10^b$.

		Theory				
States	MAOT	SCUNC	MCRRPA	HCC	GHSC	CC
(2p3s) ^{1}P°	1.9492 (−2)	1.9514 (−2)	2.3205 (−2)	5.2206 (−2)	1.9477 (−2)	1.34 (−2)
(2p4s) ^{1}P°	6.3845 (−3)	6.3943 (−3)	6.8000 (−3)	1.8183 (−2)	6.1738 (−3)	4.78 (−3)

continued ...

		Theory				
States	MAOT	SCUNC	MCRRPA	HCC	GHSC	CC
(2p5s) ^{1}P°	2.8243 (−3)	2.8360 (−3)	2.8927 (−3)	8.2208 (−3)	2.7929 (−3)	2.22 (−3)
(2p6s) ^{1}P°	1.4953 (−3)	1.5056 (−3)	1.5021 (−3)	4.3952 (−3)		
(2p7s) ^{1}P°	8.8886 (−4)	9.0168 (−4)	8.8218 (−4)	2.6239 (−3)		
(2p8s) ^{1}P°	5.7204 (−4)	5.8859 (−4)	5.6340 (−4)	1.6905 (−3)		
(2p9s) ^{1}P°	3.8991 (−4)	4.0967 (−4)	3.8228 (−4)	1.1539 (−3)		
(2p10s) ^{1}P°	2.7757 (−4)	2.9952 (−4)	2.7147 (−4)	8.2318 (−4)		
(2p11s) ^{1}P°	2.0442 (−4)	2.2761 (−4)	1.9970 (−4)	6.0636 (−4)		
(2p12s) ^{1}P°	1.5474 (−4)	1.7841 (−4)	1.5109 (−4)	4.5936 (−4)		
(2p13s) ^{1}P°	1.1981 (−4)	1.4342 (−4)	1.1704 (−4)	3.5647 (−4)		
(2p14s) ^{1}P°	9.4553 (−5)	1.1772 (−4)	9.2534 (−5)	2.8297 (−4)		
(2p15s) ^{1}P°	7.5845 (−5)	9.8325 (−5)	7. 4511 (−5)	2.2784 (−4)		
(2p16s) ^{1}P°	6.1703 (−5)					
(2p17s) ^{1}P°	5.0823 (−5)					
(2p18s) ^{1}P°	4.2322 (−5)					
(2p19s) ^{1}P°	3.5589 (−5)					
(2p20s) ^{1}P°	3.0191 (−5)					
(2p21s) ^{1}P°	2.5816 (−5)					
(2p22s) ^{1}P°	2.2235 (−5)					
(2p23s) ^{1}P°	1.9277 (−5)					
(2p24s) ^{1}P°	1.6813 (−5)					
(2p25s) ^{1}P°	1.4747 (−5)					

TABLE V: Energy positions (E) of the (2pns) ^{1}P° and (2pnd) ^{1}P° doubly excited states and widths (Γ) of the (2pns) ^{1}P° states of Be. The present results (MAOT) are compared with the screening constant by unit nuclear charge (SCUNC) data of Sakho [8] and with the monochromatized synchrotron radiation (MSR) data of Wehlitz *et al.* [3] published in eV. For energy conversion the infinite Rydberg 1 Ry = 13.605698 eV (1 eV = 1.602189×10^{-19} J) is used. The uncertainties in the MAOT results and in the experimental energy positions and widths are given in parentheses.

	Energy positions (eV)			Widths (meV)		
	Theory		Experiment	Theory		Experiment
States	MAOT	SCUNC	MSR	MAOT	SCUNC	MSR
(2p3s) ^{1}P°	10.8889 (10)	10.933	10.889 (1)	530 (10)	531	531 (10)
(2p4s) ^{1}P°	12.1119 (10)	12.095	12.112 (1)	174 (10)	174	174 (10)
(2p5s) ^{1}P°	12.5705 (7)	12.567	12.571 (1)	77 (7)	77	77 (10)
(2p6s) ^{1}P°	12.8021 (5)	12.808	12.812 (1)	41 (5)	41	47 (3)
(2p7s) ^{1}P°	12.9371 (4)	12.943	12.944 (1)	24 (3)	24	29 (3)
(2p8s) ^{1}P°	13.0229 (3)	13.029	13.022 (1)	16 (3)	16	16 (3)
(2p9s) ^{1}P°	13.0808 (3)	13.087	13.078 (1)	11 (2)	11	3 (5)
(2p10s) ^{1}P°	13.1215 (2)	13.117	13.123 (1)	8 (2)		

continued ...

	Energy positions (eV)			Widths (meV)		
	Theory		Experiment	Theory		Experiment
States	MAOT	SCUNC	MSR	MAOT	SCUNC	MSR
(2p11s) ^{1}P°	13.1513 (2)	13.156	13.143 (1)	6 (1)		
(2p12s) ^{1}P°	13.1737 (2)	13.178	13.178 (1)	4 (1)		
(2p13s) ^{1}P°	13.1908 (1)	13.194				
(2p14s) ^{1}P°	13.2043 (1)	13.207				
(2p15s) ^{1}P°	13.2151 (1)	13.218				
(2p16s) ^{1}P°	13.2238 (1)	13.226				
(2p17s) ^{1}P°	13.2309 (1)	13.233				
(2p18s) ^{1}P°	13.2368 (1)	13.239				
(2p19s) ^{1}P°	13.2418 (1)	13.243				
(2p20s) ^{1}P°	13.2460 (1)	13.247				
(2p21s) ^{1}P°	13.2496 (1)					
(2p22s) ^{1}P°	13.2526 (1)					
(2p23s) ^{1}P°	13.2553 (1)					
(2p24s) ^{1}P°	13.2576 (1)					
(2p25s) ^{1}P°	13.2597 (1)					
(2p3d) ^{1}P°	11.840 (6)	11.856	11.840 (6)			
(2p4d) ^{1}P°	12.460 (6)	12.504	12.460 (6)			
(2p5d) ^{1}P°	12.742 (7)	12.787	12.742 (6)			
(2p6d) ^{1}P°	12.898 (7)	12.938				
(2p7d) ^{1}P°	12.995 (6)	13.028				
(2p8d) ^{1}P°	13.059 (6)	13.086				
(2p9d) ^{1}P°	13.104 (5)	13.126				
(2p10d) ^{1}P°	13.136 (4)	13.155				
(2p11d) ^{1}P°	13.161 (4)	13.177				
(2p12d) ^{1}P°	13.179 (3)	13.193				
(2p13d) ^{1}P°	13.194 (3)	13.206				
(2p14d) ^{1}P°	13.206 (3)	13.216				
(2p15d) ^{1}P°	13.215 (2)	13.224				
(2p16d) ^{1}P°	13.223 (2)	13.231				
(2p17d) ^{1}P°	13.230 (2)	13.237				
(2p18d) ^{1}P°	13.235 (2)	13.242				
(2p19d) ^{1}P°	13.240 (2)	13.246				
(2p20d) ^{1}P°	13.244 (2)	13.249				
(2p23d) ^{1}P°	13.253 (1)					
(2p24d) ^{1}P°	13.255 (1)					
(2p25d) ^{1}P°	13.257 (1)					

TABLE VI: Energy positions (E) of the (2pns) ^{1,3}P$^\circ$ and (2pnd) ^{1,3}P$^\circ$ doubly excited states and widths (Γ) of the (2pns) ^{1}P$^\circ$ states of Be. The present results (MAOT) are compared with the B-spline-based configuration interaction procedure for the continuum (CIC) results of Chang and Zhu [9] and with the calculations from both the B-spline-based complex rotation (BSCR) formalism and the stabilization method (SM) of Chen [10].

	E (eV)				Γ (meV)		Γ ($a \times 10^b$ Ry)		
	MAOT	BSCR	SM	CIC	MAOT	BSCR	MAOT	SM	CIC
(2p3s) ^{1}P$^\circ$	10.89	10.95	11.08	10.93	530	526	3.89 [-2]	1.56 [-2]	3.81 [-2]
(2p4s) ^{1}P$^\circ$	12.11	12.12	12.11	12.10	174	175	1.28 [-2]	1.29 [-2]	1.24 [-2]
(2p5s) ^{1}P$^\circ$	12.57	12.59	12.58	12.57	77	79	5.66 [-3]	5.38 [-3]	5.54 [-3]
(2p6s) ^{1}P$^\circ$	12.80	12.82	12.82	12.81	41	42	3.01 [-3]	2.83 [-3]	2.98 [-3]
(2p7s) ^{1}P$^\circ$	12.94	12.95	12.95	—	24	25	1.76 [-3]	1.71 [-3]	—
(2p3d) ^{1}P$^\circ$	11.84	11.87	11.86	11.86					
(2p4d) ^{1}P$^\circ$	12.46	12.47	12.47	12.47					
(2p5d) ^{1}P$^\circ$	12.74	12.76	12.76	12.76					
(2p6d) ^{1}P$^\circ$	12.90	12.92	12.93	—					
(2p3s) ^{3}P$^\circ$	10.49	10.61	10.61						
(2p4s) ^{3}P$^\circ$	11.98	12.02	12.01						
(2p5s) ^{3}P$^\circ$	12.52	12.54	12.54						
(2p6s) ^{3}P$^\circ$	12.78	12.80	12.80						
(2p7s) ^{3}P$^\circ$	12.93	12.94	12.94						
(2p8s) ^{3}P$^\circ$	13.02	13.03	13.04						
(2p3d) ^{3}P$^\circ$	11.84	11.81	11.80						
(2p4d) ^{3}P$^\circ$	12.46	12.44	12.44						
(2p5d) ^{3}P$^\circ$	17.74	17.74	17.74						
(2p6d) ^{3}P$^\circ$	12.90	12.91	12.91						
(2p7d) ^{3}P$^\circ$	13.00	13.01	13.01						
(2p8d) ^{3}P$^\circ$	13.06	—	—						