Transition wavelength and fine structure for the quartet states of Be^+

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(Received 19 October 1983)

Twenty-four quartet states of Be^+ are calculated using configuration-interaction wave functions. Relativistic and mass polarization corrections are included. The relativistic corrections considered are mass correction to the kinetic energy, Darwin term, and retardation effect. The fine structure is calculated using spin-orbit, spin-other-orbit, and spin-spin operators. The transition wavelengths calculated in this work improve the agreement between theory and experiment in most cases. The lifetimes computed in the present work generally agree with those of the experiment. However, we also point out that the observed line at 3530 Å may have been misidentified in the literature.

I. INTRODUCTION

Recently, the doubly excited, quartet states of Be^+ have attracted a great deal of interest, both experimentally and theoretically. Since these states lie in the elastic scattering energy region, they are metastable against autoionization in the LS coupling scheme. Therefore, the dipole transitions become the dominate decay mechanism. Experimentally, this spectrum has been observed using the beam-foil technique by Hontzeas *et al.*[1] More recently, Bentzen *et al.*[2–4] and Mannervik *et al.*[5] have obtained more data with improved accuracy. The wavelength range investigated experimentally is 600—5000 Å, which corresponds to transitions among $(1s\,2l_1nl_2)^4L$ states with $n \leq 5$.

Theoretically, these quartet levels have been calculated by several methods. Holøien and Geltman[6] and Lunell and Beebe[7] performed Rayleigh-Ritz calculations with a configuration-interaction (CI) basis. Laughlin[8] used a model potential to include the effects of the valence electrons' interaction with the 1s electron; Larsson[9] used the Hylleraas method; Ali[10] has done some Hartree-Fock calculations; Froese Fischer[11] has performed multiconfiguration Hartree-Fock (MCHF) calculations for a large number of states; and finally Galán and Bunge[12] have done accurate CI calculations for a few states.

Among the theoretical works, Froese Fischer[11] has considered the relativistic mass correction and Darwin term whereas Galán and Bunge have estimated the relativistic contribution using two-electron results.[13] No explicit calculation on the orbit-orbit interaction (retardation effect) and mass polarization effect has been reported for Be^+ in the literature.

In this work, the energies for the quartet states of Be^+ are calculated using configuration-interaction wave functions. The relativistic effects are calculated using first-order perturbation theory. The relativistic effects considered in this work are mass correction to kinetic energy, Darwin term, retardation term, spin-orbit, spin-other-orbit and spin-spin effects. Mass polarization effect is also considered.

Using the calculated energies and wave functions in this work, the transition wavelengths, oscillator strengths, and lifetimes are reported. These results are compared with the theoretical and experimental data in the literature.

II. COMPUTATION PROCEDURE

The wave functions for the Be^+ quartet states are expanded in terms of configuration-interaction basis functions. In the LS coupling scheme, we have

$$\Psi_{LMSS_z} = \mathscr{A} \sum C_{mnk}^{l_1 l_2 l_3 L_{12}} \phi_{mnk}(r_1, r_2, r_3) \times Y_{l_1 l_2 L_{12}}^{l_3 LM}(\hat{r}_1, \hat{r}_2, \hat{r}_3) \chi_{SS_z}(1,2,3) \,. \quad (1)$$

Here $\mathscr{A}$ is the antisymmetrization operator and the C's are linear parameters. The explicit forms for ϕ_{mnk} and $Y_{l_1 l_2 L_{12}}^{l_3 LM}$ are given in Davis and Chung.[14] We refer the interested reader to this reference. The spin function is given by

$$\chi_{SS_z}(1,2,3) = \sum_{m_1, m_2, m_3, \mu_z} \langle s_3 \mu m_3 \mu_z \mid S S_z \rangle \times \langle s_1 s_2 m_1 m_2 \mid \mu \mu_z \rangle \times f_{s_1 m_1}(1) f_{s_2 m_2}(2) f_{s_3 m_3}(3) \,, \quad (2)$$

where s_1, s_2, and s_3 are $\frac{1}{2}$ and f is the corresponding single-particle spin function.

The nonrelativistic energy and wave function are obtained by the standard variation procedure. That is,

$$\delta \frac{\langle \Psi \mid H_0 \mid \Psi \rangle}{\langle \Psi \mid \Psi \rangle} = 0 \,, \quad (3)$$

where

$$H_0 = \sum_{i=1}^{3} \left[-\tfrac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right] + \sum_{i<j}^{3} \frac{1}{r_{ij}} \,. \quad (4)$$

The relativistic perturbation operators are given by[15]

$$H_1=-\tfrac{1}{8}\alpha^2\sum_{i=1}^{3}P_i^4 \quad \text{(mass correction)} \tag{5}$$

$$H_2=\frac{\pi}{2}\alpha^2\sum_i\left[Z\delta(\vec{r}_i)-\sum_{j\neq i}\delta(\vec{r}_{ij})\right] \quad \text{(Darwin term)} \tag{6}$$

$$H_3=\frac{1}{M}\sum_{\substack{i<j\\ i,j=1}}^{3}\vec{P}_i\cdot\vec{P}_j \quad \text{(mass polarization)} \tag{7}$$

$$H_4=-\tfrac{1}{2}\alpha^2\sum_{\substack{i<j\\ i,j=1}}^{3}\frac{1}{r_{ij}}\left[\vec{P}_i\cdot\vec{P}_j+\frac{\vec{r}_{ij}\cdot(\vec{r}_{ij}\cdot\vec{P}_i)\vec{P}_j}{r_{ij}^2}\right] \quad \text{(retardation)} \tag{8}$$

$$H_{\text{s.o.}}=\frac{\alpha^2}{2}Z\sum_{i=1}^{3}\frac{\vec{l}_i\cdot\vec{s}_i}{r_i^3} \quad \text{(spin-orbit)} \tag{9}$$

$$H_{\text{s.s.}}=\alpha^2\sum_{\substack{i<j\\ i,j=1}}^{3}\left[-\frac{8\pi}{3}\vec{s}_i\cdot\vec{s}_j\delta(\vec{r}_{ij})+\frac{1}{r_{ij}^3}\left[\vec{s}_i\cdot\vec{s}_j-\frac{3(\vec{s}_i\cdot\vec{r}_{ij})(\vec{s}_j\cdot\vec{r}_{ij})}{r_{ij}^2}\right]\right] \quad \text{(spin-spin)} \tag{10}$$

and

$$H_{\text{s.o.o.}}=-\tfrac{1}{2}\alpha^2\sum_{\substack{i\neq j\\ i,j=1}}^{3}\left[\frac{\vec{r}_{ij}}{r_{ij}^3}\times\vec{P}_i\right]\cdot(\vec{s}_i+2\vec{s}_j) \quad \text{(spin-other-orbit)} . \tag{11}$$

In these equations, α is the fine-structure constant, Z is the nuclear charge, and M is the nuclear mass for $^4Be^9$. It should be pointed out that for quartet states of three-electron systems, the expectation value of $\delta(\vec{r}_{ij})$ is identical to zero.

Among the relativistic corrections, H_1 and H_2 are by far the largest. These expectation values are evaluated using the first-order perturbation theory. The contributions from the other operators are evaluated by diagonalizing the Hamiltonian with the perturbations included.

For calculating the fine-structure splitting, eigenfunctions with total angular momentum J are formed by[16]

$$|JM_JLS\rangle=\sum_{M_L,M_S}|LSM_LM_S\rangle\langle LSM_LM_S|JM_J\rangle . \tag{12}$$

The expectation values of Eqs. (9)—(11) can be rewritten as[17]

$$\langle H_{\text{s.o.}}\rangle=C_{\text{s.o.}}\cdot 2\vec{L}\cdot\vec{S} , \tag{13}$$

$$\langle H_{\text{s.s.}}\rangle=C_{\text{s.s.}}[\tfrac{3}{2}\vec{L}\cdot\vec{S}+3(\vec{L}\cdot\vec{S})^2-L(L+1)S(S+1)] , \tag{14}$$

TABLE I. Energies for the Be^+ quartet states. $J=L+S$ is used for the fine structure (in a.u.). For notation see text.

	$\langle H_0\rangle$	$\langle H_1+H_2\rangle$ (10^{-3})	$\langle H_3\rangle$ (10^{-5})	$\langle H_4\rangle$ (10^{-5})	$\langle H_{\text{s.o.}}\rangle$ (10^{-5})	$\langle H_{\text{s.s.}}\rangle$ (10^{-6})	$\langle H_{\text{s.o.o.}}\rangle$ (10^{-5})	E_{tot}[c]
$(1s2s3s)^4S$	−9.619 706	−2.0585	0.174	0.106				−9.621 762
$(1s2s4s)^4S$	−9.462 304	−1.9967	−0.170	0.473				−9.464 298
$(1s2p3p)^4S$	−9.430 344	−1.8437	−3.945	4.068				−9.432 186
$(1s2s5s)^4S$	−9.394 206	−2.0218	0.014	0.067				−9.396 227
$(1s2s6s)^4S$	−9.362 613	−2.0207	0.123	−0.025				−9.364 633
$(1s2s2p)^4P^o$	−10.066 454	−2.0085	−3.233	3.453	5.995	4.385	−4.864	−10.068 460
$(1s2s3p)^4P^o$	−9.569 405	−2.0030	−0.779	0.796	1.226	0.887	−0.973	−9.571 408
$(1s2p3s)^4P^o$	−9.476 377	−1.8286	−4.053	4.249	7.298	4.600	−5.602	−9.478 204
$(1s2s4p)^4P^o$	−9.441 344	−2.0071	−0.278	0.346	0.3819	0.337	−0.302	−9.443 350
$(1s2p2p)^4P$	−9.870 676	−1.8063	−6.059	6.900	5.928	−4.170	−5.225	−9.872 474
$(1s2p3p)^4P$	−9.428 604	−1.7829	−4.616	4.946	4.351	−2.799	−3.511	−9.430 384
$(1s2p4p)^4P$	−9.312 297	−1.7860	−4.404	4.609	4.096	−2.564	−3.202	−9.314 081
$(1s2s3d)^4D$	−9.540 789	−1.9903	0.221	0.175	0.730	0.619	−0.689	−9.542 775
$(1s2p3p)^4D$	−9.447 881	−1.8152	−4.473	4.539	8.221	5.044	−6.283	−9.449 696
$(1s2s4d)^4D$	−9.428 765	−1.9987	−0.142	0.168	0.488	0.375	−0.452	−9.430 763
$(1s2s5d)^4D$	−9.380 737	−2.0115	0.185	−0.064	0.090	0.086	−0.095	−9.382 747
$(1s2p3d)^4D^o$	−9.406 198	−1.7813	−3.638	4.273	2.800	−4.699	−2.221	−9.407 973
$(1s2p4d)^4D^o$	−9.303 416	−1.7763	−4.035	4.338	2.700	−4.769	−2.086	−9.305 189
$(1s2p5d)^4D^o$	−9.256 562	−1.7821	−4.164	4.365	2.667	−4.799	−2.044	−9.258 342
$(1s2p4f)^4F^e$	−9.302 062	−1.7785	−4.254	4.373	2.011	−5.945	−1.560	−9.303 839
$(1s2p5f)^4F^e$	−9.255 940	−1.7834	−4.268	4.377	1.992	−5.983	−1.530	−9.257 722
$^4F^o(1)$[a]	−9.435 622	−1.8998	−2.646	1.946	3.573	2.304	−2.846	−9.437 529
$^4F^o(2)$[b]	−9.411 012	−1.9022	−2.320	1.972	3.667	2.351	−2.928	−9.412 918
$(1s2s5f)^4F^o$	−9.376 018	−2.0062	−0.006	0.099	0.341	0.229	−0.288	−9.378 023

[a] $(1s2s4f-1s2p3d)^4F^o$.
[b] $(1s2s4f+1s2p3d)^4F^o$.
[c] $E_{\text{tot}}=\langle H_0\rangle+\langle H_1+H_2\rangle+\langle H_3\rangle+\langle H_4\rangle$.

and

$$\langle H_{\text{s.o.o.}} \rangle = C_{\text{s.o.o.}} 2\vec{L}\cdot\vec{S} , \tag{15}$$

where

$$2\vec{L}\cdot\vec{S} = J(J+1) - L(L+1) - S(S+1) ,$$

and the C's are reduced matrix elements.[16]

In computing the nonrelativistic energy, we have used anywhere from 50 to 110 linear parameters and 7 to 13 angular partial waves depending on the convergence of the particular state of interest. The calculated energies are given in Table I together with the relativistic contributions. It is interesting to note that the result for $\langle H_1 + H_2 \rangle$ is very clear in deciding whether this quartet system has a $2s$ or a $2p$ electron. If the $2s$ electron is present this expectation value is approximately -0.002 a.u. If the $2p$ electron is present, this expectation value is about -0.0018 a.u. On the other hand, the two $^4F^o$ states have $1s\,2s\,4f$ and $1s\,2p\,3d$ configurations with roughly the same weight. In this case, $\langle H_1 + H_2 \rangle$ is approximately -0.0019 a.u.

While the $2s$ electron is more effective in lowering the energy, the $2p$ electrons are most effective in contributing to the other relativistic effects such as retardation, fine structure, as well as mass polarization effects. This is also clearly demonstrated in Table I.

TABLE II. Comparison of nonrelativistic energies for Be^+ quartet states (in a.u.).

States	This work	MCHF[a]	Other theory
$(1s\,2s\,3s)^4S$	−9.619 706	−9.619 46	−9.619 49[b]
$(1s\,2s\,4s)^4S$	−9.462 304	−9.462 23	−9.461 69[b]
$(1s\,2p\,3p)^4S$	−9.430 344	−9.430 02	−9.428 11[b]
$(1s\,2s\,5s)^4S$	−9.394 206		−9.393 11[b]
$(1s\,2s\,6s)^4S$	−9.362 613		−9.361 43[b]
$(1s\,2s\,2p)^4P^o$	−10.066 454	−10.065 57	−10.066 41[b]
			−10.064 92[c]
$(1s\,2s\,3p)^4P^o$	−9.569 405	−9.568 70	−9.568 93[b]
$(1s\,2p\,3s)^4P^o$	−9.476 377	−9.475 69	−9.475 74[b]
$(1s\,2s\,4p)^4P^o$	−9.441 344	−9.441 65	−9.440 18[b]
$(1s\,2p\,2p)^4P$	−9.870 676	−9.870 27	−9.868 36[c]
$(1s\,2p\,3p)^4P$	−9.428 604	−9.427 39	−9.423 97[c]
$(1s\,2p\,4p)^4P$	−9.312 297	−9.311 93	
$(1s\,2s\,3d)^4D$	−9.540 789	−9.540 56	−9.540 923[d]
$(1s\,2p\,3p)^4D$	−9.447 881	−9.446 81	
$(1s\,2s\,4d)^4D$	−9.428 765	−9.428 74	
$(1s\,2s\,5d)^4D$	−9.380 737		
$(1s\,2p\,3d)^4D^o$	−9.406 198	−9.405 93	−9.406 340[d]
$(1s\,2p\,4d)^4D^o$	−9.303 416	−9.303 24	
$(1s\,2p\,5d)^4D^o$	−9.256 562		
$(1s\,2p\,4f)^4F$	−9.302 062	−9.301 85	−9.302 142[d]
$(1s\,2p\,5f)^4F$	−9.255 940	−9.255 80	
$^4F^o(1)$	−9.435 622	−9.435 21	−9.435 789[d]
$^4F^o(2)$	−9.411 012	−9.410 42	−9.411 235[d]
$(1s\,2s\,5f)^4F^o$	−9.376 018	−9.375 59	

[a]Froese Fischer, Ref. 11.
[b]Larsson *et al.*, Ref. 9.
[c]Lunell and Beebe, Ref. 7.
[d]Galán and Bunge, Ref. 12.

III. RESULTS AND DISCUSSION

To assess the accuracy of the present work, we compare the nonrelativistic energies in Table I with results from the literature. This comparison is given in Table II. Among the earlier works on Be^+, the most extensive study is probably that of Froese Fischer[11] using the MCHF approach. Compared with the results of Ref. 11, our energies are substantially lower. According to the theorem by MacDonald,[18] all the energies calculated in this work are upper bounds to the true nonrelativistic eigenvalue. Hence, the fact that our energies are lower implies that these energies are more accurate. The only exception is the $1s\,2s\,4p\,^4P^o$ for which the result of MCHF is lower than this work by $-0.000\,31$ a.u. Since this is the fourth lowest state with the $^4P^o$ symmetry, it is not clear whether the MCHF result given here is an upper bound to the true eigenvalue. Larsson *et al.*[9] use r_{ij} coordinates explicitly and up to 97 linear parameters in their wave functions in a variation calculation. Their results are only slightly higher than this work for the lowest ^4S and $^4P^o$. But for higher excited states, the difference in energy becomes more substantial. The present values are slightly higher than those of Galán and Bunge for the five states calculated in Ref. 12. A good portion of this energy difference can be attributed to the extrapolation procedure taken in Ref. 12.

Few fine-structure measurements have been made for the quartets of Be^+ in the literature. To stimulate more interest in this area, the results calculated in this work are presented in Table III. It is clear from this table that only those states with $2p$ electrons give substantial fine-structure splitting. The maximum splitting of the Be^+ system is about 11.25 cm^{-1}. Recently, the fine structures for the $1s\,2s\,2p\,^4P^o$ and $1s\,2p\,2p\,^4P$ states of Be^+ have been calculated by Hata and Grant[19] using the multiconfiguration Dirac-Fock (MCDF) method. Their results deviate

TABLE III. Fine structures for the quartet states of Be^+ (in cm^{-1}). $J = L + 1.5$, $J_1 = L + 0.5$, $J_2 = L - 0.5$, $J_3 = L - 1.5$.

	$E_J - E_{J_1}$	$E_{J_1} - E_{J_2}$	$E_{J_2} - E_{J_3}$
$1s\,2p\,2p\,^4P$	−2.007	9.779	
$1s\,2p\,3p\,^4P$	0.003	7.374	
$1s\,2p\,4p\,^4P$	0.456	7.025	
$1s\,2s\,2p\,^4P^o$	8.951	−6.177	
$1s\,2s\,3p\,^4P^o$	1.898	−1.197	
$1s\,2p\,3s\,^4P^o$	11.253	−5.362	
$1s\,2s\,4p\,^4P^o$	0.663	−0.491	
$1s\,2s\,3d\,^4D$	0.580	−0.265	−0.431
$1s\,2p\,3p\,^4D$	8.838	0.778	−1.747
$1s\,2s\,4d\,^4D$	0.380	−0.141	−0.249
$1s\,2s\,5d\,^4D$	0.0528	−0.0566	−0.0717
$1s\,2p\,3d\,^4D^o$	−2.129	3.636	4.244
$1s\,2p\,4d\,^4D^o$	−2.092	3.739	4.337
$1s\,2p\,5d\,^4D^o$	−2.092	3.772	4.370
$1s\,2p\,4f\,^4F$	−2.924	2.596	4.464
$1s\,2p\,5f\,^4F$	−2.926	2.627	4.502
$^4F^o(1)$	3.111	0.532	−0.631
$^4F^o(2)$	3.170	0.539	−0.647
$(1s\,2s\,5f)^4F^o$	0.268	0.021	−0.086

TABLE IV. Transition wavelengths (in Å) and ocsillator strengths for the quartet states of Be^+.

Transition	Wavelengths	Oscillator strength	MCHF (Ref. 11)	Other theory	Experiment
$2p\,4p\ ^4P-2s\,2p\ ^4P^o$	604.02	0.924 02(−2)	604.4		604.1±0.4[e]
$2s\,6s\ ^4S-2s\,2p\ ^4P^o$	647.40	0.553 07(−2)		646.3[a]	
$2s\,5d\ ^4D-2s\,2p\ ^4P^o$	664.51	0.318 66(−1)		665.4[b]	664.5±0.2[f]
$2s\,5s\ ^4S-2s\,2p\ ^4P^o$	677.83	0.730 55(−2)		676.8[a]	
$2p\,3p\ ^4P-(2s\,2p)^4P^o$	714.12	0.230 32(−1)	713.8	710.9[c]	714.2±0.2[f]
				715.1[d]	
$2s\,4d\ ^4D-2s\,2p\ ^4P^o$	714.54	0.620 16(−1)	715.5	717.2[d]	714.6±0.2[f]
				714.6[b]	
$2p\,3p\ ^4S-2s\,2p\ ^4P^o$	716.14	0.169 62(−1)	716.8	713.9[a]	716.4±0.2[f]
				718.5[d]	
$2p\,3p\ ^4D-2s\,2p\ ^4P^o$	736.40	0.218 52(−1)	736.2	739.3[d]	736.4±0.3[g]
				738.6[b]	
$2p\,5d\ ^4D^o-2p\,2p\ ^4P$	741.96	0.444 12(−1)		739.7[b]	742.0±0.3[f]
$2s\,4s\ ^4S-2s\,2p\ ^4P^o$	754.20	0.500 71(−1)	755.2	753.5[a]	754.4±0.2[f]
					755 ±3[h]
$2p\,4d\ ^4D^o-2p\,2p\ ^4P$	803.23	0.104 04	803.6	799.9[b]	803.1±0.2[f]
$2s\,3d\ ^4D-2s\,2p\ ^4P^o$	866.80	0.313 20	867.9	869.8[d]	867.1±0.2[f]
				851.7[b]	865.3±1[h]
$2p\,3d\ ^4D^o-2p\,2p\ ^4P$	980.97	0.367 76	981.3	973.7[b]	981.7±0.2[f]
				968.2[d]	981.4±1.0[h]
$2s\,3s\ ^4S-2s\,2p\ ^4P^o$	1020.1	0.150 08	1021.5	1020[a]	1020.1±1.0[h]
$2p\,3s\ ^4P^o-2p\,2p\ ^4P$	1155.7	0.126 10	1154.9		1155.9±1.0[h]
$2s\,6s\ ^4S-2s\,3p\ ^4P^o$	2203.7	0.219 38(−1)		2195[a]	
$2p\,2p\ ^4P-2s\,2p\ ^4P^o$	2325.0	0.257 21	2331	2318[c]	2324.60±0.03[i]
					2324.6±0.3[h]
$2p\,5d\ ^4D^o-2p\,3p\ ^4D$	2381.3	0.704 48(−2)			2382.0[h]
$2s\,5d\ ^4D-2s\,3p\ ^4P$	2415.2	0.575 90(−1)			
$2p\,5f\ ^4F-{}^4F^o(1)$	2534.2	0.140 63(−1)	2538		
$2s\,4p\ ^4P^o-2s\,3s\ ^4S$	2554.0	0.250 88(−1)	2562	2540[a]	2563±1[f]
					2562.9±0.2[i]
$2s\,5s\ ^4S-2s\,3p\ ^4P^o$	2601.1	0.502 45(−1)		2591[a]	2599.2±0.5[i]
$2p\,5d\ ^4D^o-2p\,3p\ ^4P$	2648.6	0.463 64(−1)			
$2s\,5f\ ^4F^o-2s\,3d\ ^4D$	2765.7	0.151 08	2762	2783[d]	2764 ±1[g]
					2764.2±1.0[h]
$2p\,4p\ ^4P-2p\,3s\ ^4P^o$	2776.3	0.157 85(−1)	2782		2775 ±1[e]
$2p\,5f\ ^4F-{}^4F^o(2)$	2936.0	0.207 10(−1)	2944		
$2p\,5f\ ^4F-2p\,3d\ ^4D^o$	3032.7	0.987 40(−1)	3035	3058[d]	3031 ±1[g]
$2p\,4d\ ^4D^o-2p\,3p\ ^4D$	3153.2	0.104 14(−1)	3173		
$2p\,3s\ ^4P^o-2s\,3s\ ^4S$	3174.1	0.725 82(−1)	3165	3169[a]	3179.87±0.06[i]
					3180.7±1.0[h]
$2p\,3p\ ^4P-2s\,3p\ ^4P^o$	3231.1	0.821 52(−1)	3219		3231 ±1[f]
$2s\,4d\ ^4D-2s\,3p\ ^4P^o$	3239.8	0.987 30(−1)	3255		3240 ±1[f]
$2p\,3p\ ^4S-2s\,3p\ ^4P^o$	3272.9	0.218 29(−1)	3282	3235[a]	3261 ±1[f]
$2p\,3d\ ^4D^o-2s\,3d\ ^4D$	3380.2	0.115 18	3379.4	3380.6[j]	3380 ±1[f]
				3379.4[d]	3379.9±0.2[i]
$2p\,4f\ ^4F-{}^4F^o(1)$	3408.4	0.143 33	3414	3406.0[j]	3405.4±0.1[i]
					3405.6±0.6[h]
$^4F^o(2)-2s\,3d\ ^4D$	3508.9	0.261 06	3499	3510.8[j]	3510.52±0.05[i]
				3526.4[d]	3510.8±0.5[h]
$2p\,4p\ ^4P-2s\,4p\ ^4P^o$	3524.9	0.635 50(−1)	3507		3530±1[e]
$2p\,4d\ ^4D^o-2s\,4d\ ^4D$	3628.6	0.103 17	3625		3624±1[f]
$2p\,4d\ ^4D^o-2p\,3p\ ^4P$	3639.6	0.155 08	3670		3636±1[f]
$2p\,5d\ ^4D^o-2s\,5d\ ^4D$	3662.7	0.763 34(−1)			3660±1[f]
$2p\,3p\ ^4D-2s\,3p\ ^4P^o$	3743.7	0.171 36	3732	3776.9[d]	3749±1[g]
					3749.3[h]
$2p\,5f\ ^4F-2s\,5f\ ^4F^o$	3787.7	0.557 21(−1)	3797	3793.0[d]	3785±1[g]
$2s\,4s\ ^4S-2s\,3p\ ^4P^o$	4254.1	0.407 12	4279	4248[a]	4252±1[f]
					4252.1±0.3[i]

TABLE IV. (*Continued.*)

Transition	Wavelengths	Oscillator strength	MCHF (Ref. 11)	Other theory	Experiment
$^4F^o(1)$–$2s\,3d\,^4D$	4329.5	0.280 16	4322	4330.1[j]	4329.55±0.07[i] 4330.2±0.5[h]
$2p\,4f\,^4F$–$2p\,3d\,^4D^o$	4375.7	0.610 66	4378	4371.8[j]	4371.1±0.1[i]
$2s\,4p\,^4P^o$–$2s\,3d\,^4D$	4583.0	0.862 65(−1)	4608		4596±1[f]
$2p\,4p\,^4P$–$2p\,3d\,^4D^o$	4853.0	0.462 08(−1)	4848		

[a]Larsson *et al.*, Ref. 9.
[b]Ali as quoted in Ref. 2.
[c]Lunell and Beebe, Ref. 7.
[d]Laughlin, Ref. 8.
[e]Bentzen *et al.*, Ref. 4.
[f]Bentzen *et al.*, Ref. 2.
[g]Bentzen *et al.*, Ref. 3.
[h]Hontzeas *et al.*, Ref. 1.
[i]Mannervik *et al.*, Ref. 5.
[j]Galán and Bunge, Ref. 12.

from those of Table III by about 0.1 to 1.8 cm^{-1}. Since correlation is very important for this system and the calculated transition wavelengths in this work are far more accurate, it is possible that the results in Table III are more reliable.

Using the E_{tot} given in Table I, we tabulate the transition wavelengths for these quartets. This is presented in Table IV. The wavelengths are obtained using the conversion factor 1 a.u. of energy, corresponding to 455.6613 Å. The oscillator strengths for each transition are obtained using nonrelativistic energies and wave functions. Comparison with previous predictions and with experiments are also given in this table.

Generally speaking, the agreement between the present work and experiment is quite good. For the 37 identified lines in Table IV, the agreement between theory and experiment is improved for 27 lines, 15 of which lie within the experimental uncertainty quoted. Most of the 37 lines lie very close to the observed spectra with a few exceptions, notably the $2p\,3p\,^4S$–$2s\,3p\,^4P^o$ at 3272.9 Å (experiment, 3261 Å) and the $2p\,4p\,^4P$–$2s\,4p\,^4P^o$ at 3524.89 Å (experiment, 3530 Å).

For the $2p\,3p\,^4S$–$2s\,3p\,^4P^o$ transition, the calculated wavelength is too long, implying that either the calculated lower-state energy is too high or that of the higher state is too low. The transitions $2p\,3p\,^4P$–$2s\,2p\,^4P^o$ (theory, 714.12 Å, experiment, 714.2 Å), $2p\,3p\,^4P$–$2s\,3p\,^4P^o$ (theory, 3231.08 Å, experiment 3231 Å), $2s\,4d\,^4D$ –$2s\,2p\,^4P^o$ (theory, 714.54 Å, experiment, 714.6±0.2 Å), and $2s\,4d\,^4D$–$2s\,3p\,^4P^o$ (theory 3239.8 Å, experiment, 3240±1 Å) seem to suggest that the calculated $1s\,2s\,3p\,^4P^o$ energy is accurate. Based on the transition $2p\,3p\,^4S$–$2s\,2p\,^4P^o$ (theory, 716.14 Å, experiment, 716.4 Å), the calculated $1s\,2p\,3p\,^4S$ energy is probably slightly too high. This suggests that the observed $2p\,3p\,^4S$ –$2s\,3p\,^4P^o$ transition should be longer than the calculated 3272.92 Å. We note that in Bentzen *et al.*,[4] a strong line have been seen at 3276 Å. It is possible that $2p\,3p\,^4S$–$2s\,3p\,^4P^o$ may have contributed to this line. The line at 3261 Å could have come from other transitions. Very recently, Angentoft *et al.* have reclassified this line and suggested that it may have originated from the $1s(2p\,4d,2s\,14f)^4F^o$ state.[20]

Based on the calculated $2s\,3s\,^4S$–$2s\,2p\,^4P^o$ transition data (theory, 1020.06 Å, experiment, 1020.1 Å), the energies of these two states are probably calculated to similar accuracy. From the $2p\,4p\,^4P$–$2s\,2p\,^4P^o$ transition data (theory, 604.02 Å, experiment, 604.1 Å), the calculated $1s\,2p\,4p\,^4P$ energy is probably reliable. The calculated $2s\,4p\,^4P$–$2s\,3s\,^4S$ transition at 2554.0 Å is too short compared with the measured 2562.9 Å. This implies that the calculated $1s\,2s\,4p\,^4P$ energy is too high. Hence, the experimental result should be shorter than the calculated $2p\,4p\,^4P$–$2s\,4p\,^4P^o$ result of 3524 Å. That is, the 3530 Å may need to be reassigned.

Bentzen *et al.*[2] predict on the basis of a closed-loop energy analysis that a line observed at 3660 Å belongs to the $2p\,5d\,^4D^o$–$2s\,5d\,^4D$ transition. Our calculated result for this transition, 3662.7 Å, confirms this assignment. The weak line at 2382 Å reported by Hontzeas *et al.*[1] is in close agreement with our $2p\,5d\,^4D^o$–$2p\,3p\,^4D$ at 2381.3 Å.

In Table V we present our calculated lifetimes along with those from other theoretical calculations and experiment. The agreement between theory and experiment is good in most cases. The lifetime of the $(1s\,2s\,5d)^4D$ state is calculated here for the first time, and is within the experimental uncertainty quoted by Bentzen *et al.*[2] The lifetime of 5.98 ns for the $(1s\,2s\,5f)^4F^o$ state is in good agreement with the measured value of 5.6±0.5 ns obtained by Bentzen *et al.*[3] and is an improvement over Froese Fischer's result of 7.3 ns.[11] Our result of 3.16 ns for the $(1s\,2p\,2p)^4P^e$ state agrees well with the experimental result of 3.1±0.2 ns by Hontzeas *et al.*[1]

There are a few cases where the theoretical predictions lie outside the experimental uncertainty, e.g., for $^4F^o(1)$, $^4F^o(2)$, and $(1s\,2p\,3d)^4D^o$. In these cases, the agreement between the various calculations is quite good, but they differ significantly from experiment, where the quoted uncertainty is quite small. The reason for this discrepancy is not clear at this time.

IV. SUMMARY

In this work, twenty-four low-lying Be^+ quartet states are calculated along with relativistic and mass polarization effects. The nonrelativistic energy eigenvalues are lower than previous theoretical calculations with the ex-

TABLE V. Lifetimes for the quartet states of Be^+ (in 10^{-9} sec).

State	This work	Other theory MCHF[a]	Laughlin[b]	GB[c]	BAP[d]	Experiment MMJ[e]	HMEB[f]
$(1s\,2s\,3s)^4S$	1.04	1.0					
$(1s\,2s\,4s)^4S$	1.36	1.4			1.6±0.2		
$(1s\,2p\,3p)^4S$	4.03	3.97					
$(1s\,2s\,5s)^4S$	5.45						
$(1s\,2s\,6s)^4S$	6.66						
$(1s\,2s\,3p)^4P^o$	50.0	19.1					
$(1s\,2p\,3s)^4P^o$	1.47	1.5	1.4			1.5±0.1	2.4±0.3
$(1s\,2s\,4p)^4P^o$	10.7	15.1			12±2 13±2		
$(1s\,2p\,2p)^4P$	3.16	5.27					3.1±0.2
$(1s\,2p\,3p)^4P$	2.66	2.7			2.7±0.5		
$(1s\,2p\,4p)^4P$	4.30	4.7	4.3		3.9±0.4 3.7±0.4		
$(1s\,2s\,3d)^4D$	0.359	0.359	0.36		0.64±0.07	0.40±0.03	0.79±0.08
$(1s\,2p\,3p)^4D$	2.83	2.79	2.8		3.9±0.4 3.1±0.3 2.7±0.3		
$(1s\,2s\,4d)^4D$	1.14	1.17	1.16		1.2±0.2		1.3±0.2
$(1s\,2s\,5d)^4D$	1.79				2.2±0.6		
$(1s\,2p\,3d)^4D^o$	0.382	0.378	0.38	0.39	0.45±0.03		1.0±0.1
$(1s\,2p\,4d)^4D^o$	0.824	0.85			0.83±0.06		
$(1s\,2p\,5d)^4D^o$	1.56						
$(1s\,2p\,4f)^4F$	3.39	3.28	3.4	3.3	2.7±0.3	3.0±0.4	
$(1s\,2p\,5f)^4F$	6.01	5.7			6.7±0.5		
$^4F^o(1)$	10.0	10.3	9.6	10		11.7±0.2	
$^4F^o(2)$	6.54	6.24	6.1	5.9		5.3±0.1	
$(1s\,2s\,5f)^4F^o$	5.98	7.3			5.6±0.5		

[a]Froese Fischer, Ref. 11.
[b]Reference 8.
[c]Galán and Bunge, Ref. 12.
[d]Bentzen, Anderson, and Poulson, Refs. 2, 3, and 4.
[e]Mannervik, Martinson, and Jelenkovic, Ref. 5.
[f]Hontzeas *et al.*, Ref. 1.

ception of a few states calculated by Galán and Bunge.[12] Using these energies, the transition wavelengths between 600 and 5000 Å are tabulated. Compared with previous theoretical results, the agreement between theory and experiment is improved in most cases. However, based on the analysis of this work, we find that the 3530 Å line may not be the $2p\,4p\,^4P$–$2s\,4p\,^4P^o$ transition as suggested in a previous work.[2]

The computed lifetimes in this work agree with those of experiment in most cases. However, we find that in several cases the theory disagrees with experiment. Further study is needed to resolve this discrepancy.

To stimulate further experimental interest in making measurements on the fine structure of Be^+, we have tabulated the fine-structure splitting of these quartets. We hope that experiments will be performed and compared with this work in the near future.

ACKNOWLEDGMENTS

We wish to thank Professor T. Andersen for helpful communications. This work is supported by the National Science Foundation, Grant No. PHY-82-06490.

[1]S. Hontzeas, I. Martinson, P. Erman, and R. Buchta, Phys. Scr. 6, 55 (1972).
[2]S. M. Bentzen, T. Anderson, and O. Poulson, J. Phys. B 14, 3435 (1981).
[3]S. M. Bentzen, T. Anderson, and O. Poulson, J. Phys. B 15, L71 (1982).
[4]S. M. Bentzen, T. Anderson, and O. Poulson, Phys. Rev. A 26, 2639 (1982).
[5]S. Mannervik, I. Martinson, and B. Jelenkovic, J. Phys. B 14, L275 (1981).
[6]E. Holøien and S. Geltman, Phys. Rev. 153, 81 (1967).
[7]S. Lunell and N. H. F. Beebe, Phys. Scr. 15, 268 (1977).
[8]C. Laughlin, J. Phys. B 15, L67 (1982); 16, 3329 (1983).
[9]S. Larsson, R. Crossley, and T. Ahlenuis, J. Phys. (Paris) Colloq. 40, C1-6 (1979).
[10]M. A. Ali, J. Quant. Spectrosc. Radiat. Transfer 20, 465 (1978).
[11]C. Froese Fischer, Phys. Rev. A 26, 2627 (1982).

[12]M. Galán and C. F. Bunge, Phys. Rev. A 23, 1624 (1981).
[13]Y. Accad, C. L. Pekeris, and B. Schiff, Phys. Rev. A 4, 516 (1971).
[14]B. F. Davis and K. T. Chung, J. Phys. B 15, 3113 (1982)
[15]H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Plenum, New York, 1977), p. 181.
[16]A. Messiah, *Quantum Mechanics* (Wiley, New York, 1961), Vol. II.
[17]H. Araki, Prog. Theor. Phys. 17, 619 (1957).
[18]J. K. L. MacDonald, Phys. Rev. 43, 830 (1933).
[19]J. Hata and I. P. Grant, J. Phys. B 16, 915 (1983).
[20]M. Agentoft, T. Andersen, C. Froese Fischer, and L. Smentek-Mielczarek, Phys. Scr. 28, 45 (1983).