Theoretical evaluation of the ^{7,9}Be$^-$ 2s2p^2 ^{4}P$_{1/2,3/2,5/2}$ hyperfine structure parameters and Be 2s2p ^{3}P^o electron-affinity

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Abstract. The hyperfine structures of ^{7,9}Be$^-$ $2s2p^2\ ^4P_{1/2,3/2,5/2}$ are investigated theoretically using the multiconfiguration Hartree-Fock and configuration interaction methods. The effects of the hyperfine mixing between the fine-structure J-levels are discussed. The feasibility of some atomic spectroscopy experiments, allowing the determination of the ^{7}Be quadrupole moment from the observed hyperfine structure of the ^{7}Be$^-$ negative ion and from the present electronic parameters, is investigated. The Be $2s2p\ ^3P^o$ electron-affinity is monitored as a function of the orbital and configuration spaces to assess the reliability of the wave functions of the neutral atom and the negative ion. The theoretical value nicely converges towards the most recent theoretical and experimental results.

1. Introduction

The accuracy of the ^{7}Be$(p,\gamma)^8$B reaction factor is often presented as an important limiting factor in the determination of the flux of high-energy neutrinos generated in the solar core [1]. Although the key to the solar neutrinos problem might have been found recently [2], it is still worthwhile to improve the experimental and theoretical estimates of the relevant low-energy astrophysical S_{17} factor†. In this line, it has been shown that this S factor is linearly correlated with the quadrupole moment of the ^{7}Be nucleus [1]. There is thus some hope to refine the value of the S factor from the knowledge of the nuclear quadrupole moment.

Atomic spectroscopy experiments on unstable beryllium isotopes are performed these days, thanks to the ISOLDE facility at CERN [4]. In this latter reference, isotope shift and hyperfine structure measurements are announced [5] for ^{7,9,10}Be II and a preliminary value of the nuclear magnetic dipole moments of ^{7}Be has been reported in this context [6].

The nuclear quadrupole moment value for ^{9}Be has been extracted by combining the *ab initio* electric field gradient value [7] and the experimental quadrupole coupling constant of the metastable levels ^{9}Be$(2s2p\ ^3P^o_{2,1})$, measured by the atomic-beam magnetic-resonance method [8]. A similar experiment for exploring the hyperfine structure of ^{7}Be in its metastable levels would not be easy to realize on a low produced radioactive element such as ^{7}Be. Therefore, some experiment consisting in measuring the hyperfine structures of the metastable negative ion ^{7}Be$^-(2s2p^2\ ^4P)$ which should allow the extraction of the nuclear moment is hereafter proposed. The feasibility of this determination depends on both the magnitude of the electric quadrupole interaction in the hyperfine structure and on the reliability of the theoretical electric field gradient which can be evaluated from atomic variational calculations. Present work provides the needed ingredients for such an analysis and complete through the negative ion the set of available electronic parameters for Be$^+$ [9] and neutral beryllium [10].

Ab initio determination of the hyperfine parameters of ^{9}Be$^-(2s2p^2\ ^4P_{1/2,3/2,5/2})$ has been reported in the pioneer work of Beck and Nicolaides [11]. We reinvestigate these electronic parameters using the multiconfiguration Hartree-Fock (MCHF) and

† see ref [3] for a definition of the low-energy cross-section S-factor. S_{17} denotes the cross-section factor for the capture of protons by ^{7}Be.

configuration interaction (CI) methods combined with the active space concept to monitor the convergence of the various electronic contributions as a function of the orbital active set.

The multiconfiguration Hartree-Fock method and the computational strategy based on the concept of the orbital active space are described in section 2. The theoretical evaluation of the electron-affinity is considered in section 3 as a quality test of the wave functions describing both the neutral atom and the negative ion. The relevant hyperfine matrix elements are given in section 4.1, together with the theoretical background needed to understand the separation between the nuclear properties and the electronic contributions. The convergence of the hyperfine parameters of the $Be^-(2s2p^2\ ^4P_J)$ levels is investigated in section 4.2. The relative contributions of the electric quadrupole and magnetic dipole interaction terms to the hyperfine splittings and the effect of the J-hyperfine mixing are discussed in section 4.3 for $^9Be^-$ and in section 4.4 for $^7Be^-$. A sketch of an original experimental scheme which should allow the determination of hyperfine structures of the metastable states of the negative ions $^{7,9}Be^-$ is presented in section 4.5.

2. The MCHF computational procedure

The non-relativistic multiconfiguration Hartree-Fock (MCHF) approach is used for calculating the wave function Ψ of the state labeled $\gamma LSM_LM_S\pi$ where γ represents the dominant configuration and π is the parity. The MCHF wave function Ψ is expanded in terms of configuration state functions (CSF) $\{\Phi_i\}$ having the same $LSM_LM_S\pi$ symmetry but arising from different electronic configurations (γ_i)

$$\Psi(\gamma LSM_LM_S\pi) = \sum_{i=1} c_i\ \Phi(\gamma_i LSM_LM_S\pi). \tag{1}$$

The CSF's are built on a basis of one-electron spin-orbital functions

$$\phi_{nlm_lm_s} = \frac{1}{r}P_{nl}(r)Y_{lm_l}(\theta,\varphi)\chi_{m_s}. \tag{2}$$

In the MCHF procedure *both* the sets of radial functions $\{P_{n_il_i}(r)\}$ and mixing coefficients $\{c_i\}$, are optimized to self-consistency by solving numerically and iteratively the multiconfiguration Hartree-Fock differential equations for the former and the configuration interaction (CI) problem for the latter [12].

The active space method is used for building the CSFs expansion (1). The expansion can be produced by considering electron excitations from the reference configuration(s) to a given active set (AS) of orbitals. The rules adopted for generating the configuration space differ according to the correlation model being used. Within a given correlation model, the active set of orbitals spanning the configuration space can be increased in a systematic way to monitor the convergence of the total energy or any other property [13, 14]. The active set is specified by the maximum n-value considered, without any l-restriction (ie. $l_{\max} = n - 1$) if not specified. When a limitation on the allowed angular momentum value is used, the usual symbolic notation is adopted. For instance, the $8g$ active set notation indicates that $n \leq 8$ orbitals are considered, with the restriction $l_{\max} = 4$ corresponding to g-orbitals, ie.

$$8g = \{1s, 2s, 2p, 3s, \ldots, 8s, 8p, 8d, 8f, 8g\}.$$

In the present work, the single and double (SD) excitations from the reference configuration have been used for generating the multiconfiguration space of the MCHF approximation used for the orbital optimization. With a fixed set of radial functions determined from a SD[10g] MCHF calculation, a configuration interaction calculation can be performed over a larger set of configuration states. In our adopted strategy, the configuration lists used in the CI calculations have been produced by merging the configuration subspace created from single- and double-excitations to the $10g$ active set (SD[10g]) with another subspace generated by allowing further triple- and quadruple-excitations (TQ[x]) to smaller orbital active sets (x). This merging of CSF lists is denoted hereafter by the union "$\cup$" symbol. The limited population constraint [13, 14] "at least three electrons with $n \leq 4$" was adopted in this last step in order to keep the size of the multiconfiguration expansions manageable.

3. The Be $2s2p\ ^3P^o$ electron-affinity

The energy levels diagram of beryllium is displayed in fig. 1. The two bounded terms of Be^- appear just below their respective detachment threshold. The fine and hyperfine structures of the lowest bound state of the negative ion ($^9Be^-\ 2s2p^2\ ^4P_{1/2,3/2,5/2}$) are also represented qualitatively in the same figure, together with the beryllium electron-affinity defined by

$$E_a = E(\text{Be } 2s2p\ ^3P^o) - E(\text{Be}^-\ 2s2p^2\ ^4P). \tag{3}$$

The MCHF/CI approaches described above have been used for both the neutral atom and the negative ion, considering increasing orbital active sets up to [10g] for the SD-MCHF calculations and including triple- and quadruple-excitations up to [7g] for the CI calculations.

Combining the total energies of the negative ion with those of neutral beryllium obtained by using the same excitation models, one can monitor the electron affinity of beryllium as a function of the increasing orbital active set within a given correlation model (SD or SDTQ). As illustrated by Table 1, convergence of the electron affinity has not been achieved even with the largest CI calculations considered in the present paper. However, the largest CI active set gives a value in agreement with the theoretical estimation of Olsen et al. [15] and the convergence trend to a somewhat larger value is on line with the theoretical value obtained by Hsu and Chung [16] and with the most recent experimental value [17], taking into account their quoted uncertainty. Table 1 reflects the high quality of the wave functions which are used for estimating the electronic contributions to the hyperfine structure parameters discussed in sections 4 and 5.

4. The hyperfine structure of Be^- $2s2p^2\ ^4P_{1/2,3/2,5/2}$

4.1. Theory

The hyperfine interaction matrix elements, in the $|JIFM_F\rangle$ coupled states basis, are usually expressed in terms of the diagonal ($J = J'$) and off-diagonal ($J \neq J'$) magnetic dipole (A) and electric quadrupole (B) hyperfine parameters:

$$A_J = \frac{\mu_I}{I} \frac{1}{[J(J+1)(2J+1)]^{1/2}} \langle \gamma_J J \| \mathbf{T}^{(1)} \| \gamma_J J \rangle, \tag{4}$$

$$A_{J,J-1} = \frac{\mu_I}{I} \frac{1}{[J(2J-1)(2J+1)]^{1/2}} \langle \gamma_J J \| \mathbf{T}^{(1)} \| \gamma_J (J-1) \rangle, \tag{5}$$

$$B_J = 2Q \left(\frac{J(2J-1)}{(J+1)(2J+1)(2J+3)} \right)^{1/2} \langle \gamma_J J \| \mathbf{T}^{(2)} \| \gamma_J J \rangle, \tag{6}$$

$$B_{J,J-1} = \frac{Q}{2} \left(\frac{J(J-1)}{(J+1)(2J-1)(2J+1)} \right)^{1/2} \langle \gamma_J J \| \mathbf{T}^{(2)} \| \gamma_J (J-1) \rangle, \tag{7}$$

$$B_{J,J-2} = \frac{Q}{4} \left(\frac{J(J-1)(2J-1)}{(2J-3)(2J+1)} \right)^{1/2} \langle \gamma_J J \| \mathbf{T}^{(2)} \| \gamma_J (J-2) \rangle, \tag{8}$$

in which the nuclear magnetic dipole μ_I and electric quadrupole moment Q are the relevant nuclear quantities. The electronic matrix elements are obtained by integrating the irreducible spherical tensors,

$$\mathbf{T}^{(1)} = \frac{\alpha^2}{2}\sum_{i=1}^{N}\big\{2\mathbf{l}^{(1)}(i)r_i^{-3} - g_s\sqrt{10}[\mathbf{C}^{(2)}(i)\times\mathbf{s}^{(1)}(i)]^{(1)}r_i^{-3} + g_s\frac{8}{3}\pi\delta(\mathbf{r}_i)\mathbf{s}^{(1)}(i)\big\} \tag{9}$$

and

$$\mathbf{T}^{(2)} = -\sum_{i=1}^{N}\mathbf{C}^{(2)}(i)r_i^{-3} \tag{10}$$

over the spin and spatial electron coordinates [18]. The rank-one tensor of the magnetic dipole hyperfine interaction represents the magnetic field due to the electrons at the site of the nucleus arising from the orbital motion of the electrons (orbital term), from the dipole field due to the spin motion of the electrons (spin-dipole term), and the Fermi contact contribution which appears only for s-electrons. The rank-two tensor of the electric quadrupole hyperfine interaction is the electric field gradient at the site of the nucleus which interacts with the nuclear quadrupole moment to bring the electric quadrupole hyperfine interaction.

In light atoms where the relativistic effects can be neglected, the diagonal and off-diagonal A and B factors can be expressed in terms of the J-independent hyperfine parameters a_l, a_{sd}, a_c and b_q [19]

$$\begin{aligned}
a_l &= \langle\gamma LSM_LM_S \mid \sum_{i=1}^{N} l_0^{(1)}(i)r_i^{-3} \mid \gamma LSM_LM_S\rangle,\\
a_{sd} &= \langle\gamma LSM_LM_S \mid \sum_{i=1}^{N} 2C_0^{(2)}(i)s_0^{(1)}(i)r_i^{-3} \mid \gamma LSM_LM_S\rangle,\\
a_c &= \langle\gamma LSM_LM_S \mid \sum_{i=1}^{N} 2s_0^{(1)}(i)r_i^{-2}\delta(r_i) \mid \gamma LSM_LM_S\rangle,\\
b_q &= \langle\gamma LSM_LM_S \mid \sum_{i=1}^{N} 2C_0^{(2)}(i)r_i^{-3} \mid \gamma LSM_LM_S\rangle,
\end{aligned}$$

where $M_L = L$ and $M_S = S$. These parameters are usually known as the orbital (a_l), spin-dipole (a_{sd}) and contact (a_c) electronic parameters while the b_q parameter represents the electric field gradient at the nucleus.

4.2. Convergence study of the hyperfine parameters

The basic hyperfine structure (HFS) parameters of Be^- $2s2p^2\ ^4P$ from which the A_J and B_J constants can be evaluated if the nuclear quantities (I, μ_I and Q) are known, are monitored in Table 2 as functions of the active set.

In the MCHF level of approximation used for the orbital optimization with a SD configuration space, the largest orbital space (10g) seems to be complete enough for getting a convergence better than 0.1% in the a_l, a_{sd} and a_c parameters . Convergence of the b_q parameter is more difficult to get, the value being still affected by 1.3% going from the SD[9g] to the SD[10g] MCHF expansion. The inclusion of triple and quadruple excitations through the (SD[10g] $\cup$ TQ[7g]) CI calculations affects the orbital (a_l) and the electric field gradient (b_q) parameters by less than 0.3%. The corresponding variation is somewhat larger (although less than 0.8%) for the spin-dipole and contact hyperfine parameters. For the four parameters, the SD-TQ configuration spaces look complete enough, the largest variation (0.3%) being found for the a_{sd} parameter. Taking all these observations into account, our final hyperfine electronic parameters and associated uncertainties are estimated as $a_l = 0.1732(5)$, $a_{sd} = 0.0378(2)$, $a_c = 7.748(21)$ and $b_q = 0.066(2)$.

We report in the same table the electronic contributions calculated by Beck and Nicolaides [11] using configuration interaction techniques in Slater-type orbital basis sets. Their a_c, a_{sd} and a_c-values † agree well with the present $n = 4 - 6$ SD-MCHF results. This consistency is not surprising after analysing their correlation models using "up to 250 N-electron functions". Their corresponding total energy, $E = -14.573\ 085$ a.u., also falls in the range of the corresponding SD-MCHF energies for these orbital active sets (see Table 1).

4.3. Hyperfine structure of $^9Be^-$

The A_J and B_J parameters calculated for $^9Be^-$ $^4P_{1/2,3/2,5/2}$ using the nuclear data compiled by Raghavan [20] ($I = 3/2, \mu = -1.177492(17)\ \mu_N$), together with the nuclear quadrupole moment value $Q = +0.05288(38)$ b determined by Sundholm and Olsen [7], are reported in Table 3 and Table 4. Note that this $Q(^9\mathrm{Be})$ value results from the combination of the experimental quadrupole coupling constant,

† Tedious angular momentum algebra allowed us to set the relations between our electronic parameters and their "hyperfine reduced matrix elements", only valid for ^4P: $a_l = (1/\sqrt{6})\ \alpha_l, a_{sd} = -(1/10\sqrt{5})\ \alpha_d, a_c = (3\sqrt{3}/2\sqrt{5})\ \alpha_c, b_q = (1/\sqrt{30})\ \alpha_q$.

$B_2 = 1.429(8)$ MHz, measured by the atomic-beam magnetic-resonance technique [8] for $2s2p\ ^3P_2^o$ with the theoretical electric field gradient calculated by Sundholm and Olsen using the finite-element MCHF method, using the relation ‡

$$B(\text{MHz}) = -234.9647\ qQ(b)b_q(a_0^{-3}).$$

Applying the same procedure with the $b_q = -0.1152545\ a_0^{-3}$ value calculated from the present SD[10g] ∪ TQ[7g] MCHF/CI expansion (13278 CFSs), the nuclear quadrupole moment is estimated to be $Q = +0.05277$ b, falling inside the error bars given by Sundholm and Olsen [7].

The diagonal (J, J) and off-diagonal (J, J') magnetic dipole and electric quadrupole hyperfine interaction constants A and B values corresponding to the largest MCHF/CI expansions (SD[10g] ∪ TQ[7g]) are reported in Table 5, along with the detailed balance of the three contributions to the A-parameters. As shown by this table, the contact term is largely dominant in all cases.

The hyperfine splittings $\Delta E_{F,F'} = E_{F'} - E_F$ are reported in Table 6. The first series of results correspond to the first-order perturbation correction, evaluated from the expectation value of the hyperfine interaction perturbation term using the coupled state function $|JIFM_F\rangle$ as zero-order wave functions, i.e.

$$\Delta E(J, I, F) = E_{M1}(J, I, F) + E_{E2}(J, I, F), \tag{11}$$

with

$$E_{M1}(J, I, F) = \frac{1}{2} A_J\ C \tag{12}$$

and

$$E_{E2}(J, I, F) = B_J\ \frac{\frac{3}{4}C(C+1) - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)} \tag{13}$$

in which

$$C = F(F+1) - J(J+1) - I(I+1).$$

The magnetic dipole (M1) and electric quadrupole (E2) contributions are given separately in the table. In this scheme, the hyperfine structure of $^9\text{Be}^-\ 2s2p^2\ ^4P_{1/2}$ is only due to the dipole magnetic interaction. If the correction is limited to the M1

‡ $q(^3P_2) = 1.$ as calculated from [19].

contribution, the hyperfine splittings strictly obey the Landé interval rule for the three J-values considered, i.e.

$$\Delta E^J_{F-1,F} \equiv E^J_F - E^J_{F-1} = F\ A_J.$$

To the knowledge of the authors, there is no observed hyperfine structure data to compare with. The only comparison which can be done is with the pioneer theoretical work of Beck and Nicolaides [11] for the basic hyperfine parameters (see Table 2). Off-diagonal hyperfine effects between different fine-structure levels have been considered by these authors. Unfortunately, owing to space limitations in their published work, explicit results for $Be^-\ ^4P$ were not presented and the reader is left with the interesting comment that "off-diagonal effects will be significant", without any further quantitative discussion of these effects for this system.

The second set of results presented in Table 6 takes into account the hyperfine coupling between J-levels having the same F-value. Using the *ab initio* hyperfine parameters, the hyperfine structures have been evaluated by diagonalizing the interaction matrix built from equations (12) and (13) for the diagonal matrix elements, and from similar expressions [18, 21] for the off-diagonal J-coupling terms. The experimental fine structure of Andersen *et al.* [22] has been used for setting the zero-order interaction matrix. The differences between the hyperfine splittings obtained using the first-order perturbation and the diagonalization models are very similar if restricting the hyperfine interaction to the M1 contribution (differences between columns 8 and 4) or if including the E2 contribution (M1+E2) (differences between columns 9 and 7). This illustrates that the J-hyperfine coupling is mainly due to the magnetic dipole interaction. The same observation can be done on the basis of the differences between the M1 and (M1+E2) results in the diagonalization model which almost reproduce the first order electric quadrupole correction. The effect of this (J, J') off-diagonal M1 coupling, which can be realized from a comparison of columns 4 and 8, is of the same order of magnitude than the diagonal E2 corrections, i.e. in the range of $0.2-1\%$ of the diagonal magnetic dipole contribution.

The fine structure of $Be^-\ ^4P$ sets the zero-order energy separation for building the hyperfine interaction matrix inducing the J-coupling. The present non-relativistic MCHF wave functions have been used to evaluate the fine structure splittings using the Breit-Pauli Hamiltonian. The corresponding results (MCHF+BP) are reported

in Table 9 and compared with other theories and observation. The computational task is huge: the calculation of the non-fine and fine-structure corrections took 156h CPU-time on a Compaq AlphaServer GS140 for the largest MCHF/CI expansion. The only observed values available for these splittings are those measured by Andersen *et al* [22] using state-selective stepwise two-photon detachment. On the theoretical side, relativistic corrections have been calculated using first-order perturbation theory by Beck and Nicolaides in their pioneer work [11] and by Hsu and Chung [16] from their "full core plus correlation" (FCPC) wave functions. As for the hyperfine structure parameters, the present results for which correlation is limited to $n = 4 - 6$ orbital active sets are consistent with Nicolaides and Beck. However, the convergence pattern shows that these limited orbital active sets in the SD expansion multiconfiguration Hartree-Fock model do not make the complete story of the fine structure splittings and that their evaluation still requires larger expansions. More surprising is the large difference found for the $5/2 - 3/2$ energy separation between the present results and those reported by Hsu and Chung. The agreement between FCPC and MCHF+BP was indeed found to be gratifying for three-electron ions [23]. The present MCHF+BP $3/2 - 1/2$ fine structure splitting, although sensitively larger than the FCPC result, is closer to observation.

4.4. Hyperfine structure of $^7Be^-$

^{7}Be has a rather long half-life ($T_{1/2} = 53.29$ d) and is a good candidate for performing atomic spectroscopy measurements. Like the stable isotope ^{9}Be, its nuclear spin is $I = 3/2$. The magnetic moment has been estimated recently by comparing hyperfine structures of $2s\ ^2S_{1/2} - 2p\ ^2P^o_{1/2}$ for ^{7}Be$^+$ and ^{9}Be$^+$, as obtained from collinear fast-beam laser spectroscopy with optical detection. The preliminary value reported in [6] is $\mu = -1.398(15)\ \mu_N$. The quadrupole moment of this isotope has been estimated to be $-0.060 \leq Q(^7\text{Be}) \leq -0.069$ b [1] from a set of parameters that reproduce simultaneously the most important properties of ^{7}Be, ^{7}Li and ^{8}B. We adopted the mean value, i.e. $Q(^7\text{Be}) = -0.0645$ b.

The hyperfine parameters and splittings calculated with these nuclear data and the electronic parameters of the present work are reported in Table 7 and Table 8, respectively. All the comments made for the stable isotope ^{9}Be$^-$ concerning the effect of the mixing of fine-structure levels, apply for ^{7}Be$^-$. One major difference however is

the opposite sign of the electric quadrupole interaction term relatively to the magnetic dipole contribution, due to the negative sign of the $Q(^7\mathrm{Be})$ quadrupole moment.

4.5. On the possible extraction of $Q(^7Be)$ from a spectroscopic study of the negative ion

The quadrupole moment of the nucleus can be deduced from hyperfine structure analysis provided that the studied atomic level has a J-value higher than 1/2. The case of neutral beryllium is difficult because the J-value of its ground state is $J = 0$ and furthermore, as in light atoms, the hyperfine splitting constant is very small which makes attempts to measure excited level HFS through optical spectroscopy hazardous, the structure being comparable to the natural linewidth of the level. In 1967, Blachman and Lurio [8] studied the HFS of the metastable level $1s^2 2s2p\ ^3P_1^o$. In this case, the long lifetime of the level made it possible to perform radiofrequency spectroscopy and to determine the hyperfine structure with a very high accuracy. However, this experiment required a peculiar source using electron bombardment of a thermal Be atomic beam, which would not be easy to realize on a low produced radioactive element such as ^{7}Be.

An alternative way is to perform an experiment on the ground term $2s2p^2\ ^4P$ of the negative ion $^7\mathrm{Be}^-$. This term consists of three metastable levels $J = 1/2, 3/2, 5/2$. The lifetime of the $J = 3/2$ level is of 42 μsec [24] which allows measurements in the kHz precision range; the other two, $J = 1/2$ and 5/2 have lifetime much shorter, respectively 0.73 and 0.33 μsec [22]. We can take advantage of this lifetime difference to imagine a detection scheme of a RF resonance between HFS levels of the J=3/2 state.

The scheme of the proposed experiment is sketched in Fig. 2. We need to start with a source of negative ions at low energy, in order to get a low velocity beam (no more than a few tens Km/sec). This may be obtained using a sputter source or a laser plasma source with a post acceleration of a few eV. The negative ions from the beam, preferably in pulsed operation, are deflected by electric field plates to separate ions from neutrals and then detected after a time of flight of around 30 μsec using a channel-plate detector. As the metastable state $2s2p^2\ ^4P$ of Be^- has only the $J = 3/2$ level with a long lifetime, one will get rapidly a beam of Be^- ions in the level $2s2p^2\ ^4P_{3/2}$. The principle of the experiment is to measure precisely the

frequencies of the different transitions $F \rightarrow F \pm 1 (F = 2, 1)$. This can be done using RF excitations and magnetic resonance. The detection of resonance will be performed thanks to the great difference in lifetime of the levels $J = 3/2$ ($\tau = 42$ μsec) and $J = 5/2$ ($\tau = 0.3$ μsec). Using a first RF loop in the A-region, tuned on the transition $(J = 3/2, F = 2) \rightarrow (J = 5/2, F = 3)$ at around 17.1 GHz, one depopulates the level $(J = 3/2, F = 2)$, reducing the signal of Be^- to 11/16 of its maximum value when taking into account the multiplicity of the different F-levels. In the B-region, an identical loop is used to analyze the population of ions in the $(J = 3/2, F = 2)$ level after crossing the C-region. If no excitation occurs in this region, the signal on the detector will stay unchanged. In the C-region the RF excitation between levels $J = 3/2, F = 2 \rightarrow F = 3, 1$ will be performed using two Ramsey loops. At resonance, if the RF power in the Ramsey loops is properly adjusted, all the population of the level $F = 3$ (or 1) is transferred to the level $F = 2$. This level will then be emptied by the B-loop and the signal on the detector will be further reduced to either 4/16 or 8/16 of its maximum value, depending on the excitation to the $F = 3$ or $F = 1$ level, respectively. It is also possible to detect electrons resulting from the autodetachment following excitation by the B-loop. In this case, the resonance signal will appear on a zero level. This increases the sensitivity of the detection but certainly would require to add an acceleration voltage for the electrons just behind the B-loop where they are created. For $^7Be^-$, the splitting between HFS levels $\Delta E_{F-1,F}$ has been estimated by the *ab initio* calculations presented in this paper (see Table 8), for the transitions $J = 3/2, F = 2 \rightarrow F = 3, 1$. They are respectively given by $3A + B$ and $2A - B$ where A and B are respectively the magnetic dipole and the electric quadrupole coupling constant. The relatively large $A_{3/2}$ factor (-111.5 MHz) should allow to well separate the two resonances of interest. However, the $B_{3/2}$ factor, from which one can extract the quadrupole moment, is much smaller, being estimated to be -0.8 MHz from the present work. Despite its smallness, this quantity should be still large enough to allow its determination using the experiment described above: with a distant between the Ramsey loops of 10 cm, the interaction time is of the order of 10 μsec, and the linewidth of the resonance is of the order of 65 kHz. The central position of the resonance could then still be measured with an accuracy of the order of the kHz, quite sufficient to extract a reliable value of the B factor.

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Figure captions

- **Fig. 1**: Schematic diagram of the ^{7,9}Be$^-$ $2s2p^2\ ^4P_J$ fine and hyperfine structures, with their detachment treshold Be $2s2p\ ^3P^o$.
- **Fig. 2**: Schematic diagram of an experiment designed to measure HFS splitting in Be$^-$. The level scheme, in the upper part of the drawing, indicates the transitions excited using RF loops A, B and C.

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Tables and table captions

Table 1. Total energies of Be $2s2p\ ^3P^o$ and Be $2s2p^2\ ^4P$ together with the electron-affinity of Be $2s2p\ ^3P^o$ as functions of the active set.

	Be($1s^2 2s2p\ ^3P^o$)		Be$^-$($1s^2 2s2p^2\ ^4P$)		
Active set	$E_{tot}(a.u.)$	NCSF	$E_{tot}(a.u.)$	NCSF	EA(eV)
HF	-14.5115018	1	-14.5090277	1	-0.0673
2	-14.5115767	4	-14.5090395	4	-0.0690
3	-14.5533693	56	-14.5527630	78	-0.0165
4	-14.5597543	208	-14.5661729	313	0.1746
5	-14.5636590	502	-14.5713284	784	0.2087
6g	-14.5652854	942	-14.5733203	1493	0.2186
7g	-14.5658835	1528	-14.5742324	2440	0.2272
8g	-14.5661239	2260	-14.5746172	3625	0.2311
9g	-14.5662361	3138	-14.5748012	5048	0.2331
10g	-14.5662905	4162	-14.5748912	6709	0.2340
SD[10g] ∪ TQ[3]	-14.5665738	4230	-14.5753383	6919	0.2385
SD[10g] ∪ TQ[4]	-14.5666494	5238	-14.5764941	11062	0.2679
SD[10g] ∪ TQ[5]	-14.5667212	7918	-14.5768124	35699	0.2746
SD[10g] ∪ TQ[6g]	-14.5667304	10598	-14.5770444	85976	0.2807
SD[10g] ∪ TQ[7g]	-14.5667336	13278	-14.5772259	161893	0.2855
other theory [15]					0.285(5)
other theory [16]					0.2891(10)
obs. [17]					0.29099(10)

Table 2. Hyperfine electronic parameters (all in a.u.) for Be$^-$ $2s2p^2\ ^4P$

active set	a_l	a_{sd}	a_c	b_q
HF	0.1652998	0.0330600	6.5025430	0.0661199
2	0.1653476	0.0330695	6.5044221	0.0661388
3	0.1684524	0.0348313	7.3509623	0.0693240
4	0.1706113	0.0384247	7.6458337	0.0602512
5	0.1727152	0.0365575	7.6022947	0.0633231
6g	0.1736252	0.0375705	7.6428579	0.0696089
7g	0.1736801	0.0378516	7.6899468	0.0666196
8g	0.1736053	0.0373309	7.6805143	0.0649583
9g	0.1735641	0.0374753	7.6859930	0.0666256
10g	0.1735259	0.0375060	7.6916313	0.0657945
SD[10g] ∪ TQ[3]	0.1732088	0.0375499	7.6905958	0.0658541
SD[10g] ∪ TQ[4]	0.1735688	0.0378480	7.7167935	0.0656721
SD[10g] ∪ TQ[5]	0.1735219	0.0376892	7.7305532	0.0658304
SD[10g] ∪ TQ[6g]	0.1733976	0.0377008	7.7314404	0.0660029
SD[10g] ∪ TQ[7g]	0.1732338	0.0378126	7.7492123	0.0659507
other theory [11]	0.17171	0.03698	7.5646	0.06401

Table 3. Hyperfine magnetic dipole A (MHz) parameters of $^9Be^-$.

active set	$A_{1/2}$ (MHz)	$A_{3/2}$ (MHz)	$A_{5/2}$ (MHz)
HF	-175.0877540	-79.0137399	-70.9550723
2	-175.1383492	-79.0365733	-70.9755794
3	-198.6400065	-89.2433182	-79.5849990
4	-207.0206921	-92.4824669	-82.7055323
5	-205.5509157	-92.2040347	-82.2772620
6g	-206.7163926	-92.6030897	-82.7404506
7g	-208.0448113	-93.1477419	-83.2213146
8g	-207.7432084	-93.0899853	-83.1091527
9g	-207.9094513	-93.1397471	-83.1670223
10g	-208.0705003	-93.2044076	-83.2231685
SD[10g] ∪ TQ[3]	-208.0612288	-93.1804486	-83.2046335
SD[10g] ∪ TQ[4]	-208.7956421	-93.4739892	-83.4862797
SD[10g] ∪ TQ[5]	-209.1668877	-93.6591829	-83.6176776
SD[10g] ∪ TQ[6g]	-209.1987027	-93.6662208	-83.6231748
SD[10g] ∪ TQ[7g]	-209.7097497	-93.8674495	-83.7993000

Table 4. Hyperfine electric quadrupole B (MHz) parameters of $^9Be^-$.

active set	$B_{3/2}$ (MHz)	$B_{5/2}$ (MHz)
HF	0.657229	-0.821536
2	0.657416	-0.821769
3	0.689077	-0.861346
4	0.598894	-0.748617
5	0.629429	-0.786786
6g	0.691909	-0.864885
7g	0.662195	-0.827744
8g	0.645682	-0.807102
9g	0.662255	-0.827818
10g	0.653994	-0.817492
SD[10g] ∪ TQ[3]	0.654587	-0.818233
SD[10g] ∪ TQ[4]	0.652777	-0.815971
SD[10g] ∪ TQ[5]	0.654351	-0.817938
SD[10g] ∪ TQ[6g]	0.656065	-0.820082
SD[10g] ∪ TQ[7g]	0.655546	-0.819433

Table 5. Contributions to the diagonal and off-diagonal $A_{J,J'}$ and $B_{J,J'}$ parameters (MHz) of $^9Be^-$.

J	J'	A_{orb}	A_{sd}	A_{cont}	A	B
1/2	1/2	8.6497814	-3.1503649	-215.2091662	-209.7097497	0.0
3/2	3/2	-3.4599126	4.2844962	-94.6920331	-93.8674495	0.6555465
5/2	5/2	-5.1898688	-1.1341313	-77.4752998	-83.7993000	-0.8194331
1/2	3/2	-6.8382526	3.2377567	68.0551139	64.4546180	0.0561028
1/2	5/2	0.0	0.0	0.0	0.0	-0.4858641
3/2	5/2	-3.1781326	-1.2732698	31.6291587	27.1777563	-0.2172850

Table 6. Hyperfine splittings of $^9Be^-$.

			first-order perturbation theory				hfs matrix diagonalization	
J	$\Delta E_{F-1,F}$ (MHz)		$M1$	$E2$		$M1+E2$	$M1$	$M1+E2$
1/2	$\Delta E_{1,2}$	$2A_{1/2}$	-419.4195	0.0	0.0	-419.4195	-420.1512	-420.1573
3/2	$\Delta E_{2,3}$	$3A_{3/2}$	-281.6024	$B_{3/2}$	0.6555	-280.9468	-283.3927	-282.7258
	$\Delta E_{1,2}$	$2A_{3/2}$	-187.7349	$-B_{3/2}$	-0.6555	-188.3904	-187.4982	-188.1476
	$\Delta E_{0,1}$	$A_{3/2}$	-93.8674	$-B_{3/2}$	-0.6555	-94.5230	-93.3030	-93.9688
5/2	$\Delta E_{3,4}$	$4A_{5/2}$	-335.1972	$4/5B_{5/2}$	-0.6555	-335.8527	-336.1864	-336.8346
	$\Delta E_{2,3}$	$3A_{5/2}$	-251.3979	$-9/20B_{5/2}$	0.3687	-251.0292	-251.2758	-250.9207
	$\Delta E_{1,2}$	$2A_{5/2}$	-167.5986	$-4/5B_{5/2}$	0.6555	-166.9430	-167.1035	-166.4481

Table 7. Contributions to the diagonal and off-diagonal $A_{J,J'}$ and $B_{J,J'}$ parameters (MHz) of $^7Be^-$.

J	J'	A_{orb}	A_{sd}	A_{cont}	A	B
1/2	1/2	10.2696192	-3.7403313	-255.5112174	-248.9819295	0.0
3/2	3/2	-4.1078477	5.0868504	-112.4249356	-111.4459329	-0.7995981
5/2	5/2	-6.1617715	-1.3465192	-91.9840382	-99.4923290	0.9994976
1/2	3/2	-8.1188468	3.8440889	80.7997415	76.5249836	-0.0684309
1/2	5/2	0.0	0.0	0.0	0.0	0.5926292
3/2	5/2	-3.7732990	-1.5117140	37.5523264	32.2673133	0.2650318

Table 8. Hyperfine splittings of $^7Be^-$.

			first-order perturbation theory				hfs matrix diagonalization	
J	$\Delta E_{F-1,F}$ (MHz)		$M1$	$E2$		$M1+E2$	$M1$	$M1+E2$
1/2	$\Delta E_{1,2}$	$2A_{1/2}$	-497.9639	0.0	0.0	-497.9639	-498.9907	-498.9819
3/2	$\Delta E_{2,3}$	$3A_{3/2}$	-334.3378	$B_{3/2}$	-0.7996	-335.1374	-336.8561	-337.6720
	$\Delta E_{1,2}$	$2A_{3/2}$	-222.8919	$-B_{3/2}$	0.7996	-222.0932	-222.5612	-221.7706
	$\Delta E_{0,1}$	$A_{3/2}$	-111.4459	$-B_{3/2}$	0.7996	-110.6463	-110.6492	-109.8350
5/2	$\Delta E_{3,4}$	$4A_{5/2}$	-397.9693	$4/5B_{5/2}$	0.7996	-397.1697	-399.3602	-398.5713
	$\Delta E_{2,3}$	$3A_{5/2}$	-298.4770	$-9/10B_{5/2}$	-0.4498	-298.9268	-298.3057	-298.7358
	$\Delta E_{1,2}$	$2A_{5/2}$	-198.9847	$-4/5B_{5/2}$	-0.7996	-199.7843	-198.2884	-199.0878

Table 9. MCHF+BP fine structure splittings (in cm^{-1}) of Be^- $2s2p^2\ ^4P$ as a function of the active set.

Active set	$5/2-3/2$	$3/2-1/2$
HF	0.273	0.595
2	0.273	0.595
3	0.298	0.600
4	0.539	0.672
5	0.597	0.709
6g	0.613	0.717
7g	0.636	0.728
8g	0.643	0.731
9g	0.647	0.733
10g	0.649	0.734
SD[10g] $\cup$ TQ[3]	0.649	0.733
SD[10g] $\cup$ TQ[4]	0.687	0.750
SD[10g] $\cup$ TQ[5]	0.703	0.757
SD[10g] $\cup$ TQ[6g]	0.718	0.764
SD[10g] $\cup$ TQ[7g]	0.732	0.771
other theory [11]	0.5695	0.6914
other theory [16]	0.6151	0.7024
obs. [22]	0.59(7)	0.74(7)