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CALCULATION OF THE HYPERFINE STRUCTURE OF THE SUPERHEAVY ELEMENTS E113 AND $E114^+$

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ABSTRACT

The hyperfine-structure constants of the lowest s and $p_{1/2}$ states of superheavy elements E113 and $E114^+$ are presented in this article. The relativistic Hartree-Fock method with the core polarization being taken into account by means of the many-body perturbation theory. Breit and quantum electrodynamic (QED) effects are also considered. Similar calculations for Tl and Pb^+ are used to gauge the accuracy of the calculations.

Keywords: hyperfine-structure, relativistic Hartree-Fock, core polarization.

TÓM TẮT

Tính toán cấu trúc siêu tinh tế của nguyên tố siêu nặng E113 và $E114^+$

Trong bài báo này, chúng tôi trình bày hằng số cấu trúc siêu tinh tế của các trạng thái s và $p_{1/2}$ cuả nguyên tố siêu nặng E113 và $E114^+$. Phương pháp Hartree-Fock tương đối tính cùng với sự phân cực lõi được kết hợp với lí thuyết nhiễu loạn cho hệ nhiều hạt. Sự tương tác Breit và bổ chính điện động lực học lượng tử đã được xem xét. Những tính toán tương tự cho Tl và Pb^+ được sử dụng để kiểm soát độ chính xác của việc tính toán.

Từ khóa: cấu trúc siêu tinh tế, Hartree-Fock tương đối tính, sự phân cực lõi.

1. Introduction

The study of the hyperfine structure of superheavy elements is an important source of the information about nuclear structure of these elements (see, e.g., [1]). The hyperfine-structure analysis can be even more important for the superheavy elements (Z>100) where sources of the information are very limited. The study of the superheavy elements are motivated by the hypothetical island of stability in the region Z=114 to Z=126 where shell closures are predicted (see, e.g., [2]). Since superheavy element 113 was synthesized in Japan in 2004 [3], it is of special interest due to its closeness to the hypothetical island of stability and relatively simple electron structure.

Hyperfine-structure intervals are proportional to nuclear moments, such as magnetic dipole moment, electric quadrupole moment, etc. The values of these moments can be

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extracted from the comparison of the calculations and the measurements. Apart from that, the hyperfine-structure intervals are sensitive to electric charge and magnetic moment distributions within the nucleus. Parameters of these distributions can often be extracted from the analysis of the hyperfine structure subject to sufficient experimental data and the accuracy of the calculations. The use of the hyperfine-structure analysis is limited to nuclei with odd number of protons or neutrons.

In the present paper, we perform accurate numerical calculations of the hyperfine structure constants for superheavy element E113 and $E114^+$ applying the same approach as our earlier works for superheavy elements E119 and $E120^+$ [4]. Also, these elements have a very simple electron structure with one external electron above closed shells that ends with the $7s^2$ subshell. Therefore, very accurate calculations are possible for the element. In our previous work [5] we have calculated the energy levels of E113 and E114. Apart from some expected relativistic effects such as larger fine structure and stronger attraction of the *s* states to atomic core, the spectra of this superheavy element are very similar to the spectra of their lighter analogies, Tl, and Pb^+. We expect similar trend for the hyperfine structure and we perform the calculations for the same set of atoms. This gives us an estimate of the accuracy of the results for superheavy elements.

2. Method of calculation

The calculations are performed by using a method developed in the previous works [4,6-8]. It starts from the relativistic Hartree-Fock (RHF) calculations for atomic core and includes dominating correlation and all core polarization corrections to all orders.

Single-electron orbitals are found by solving a system of the RHF equations for $N-1$ electrons of the closed-shell core (the V^{N-1} approximation). The RHF Hamiltonian has a form

$$\hat{h}_o = c\boldsymbol{\alpha}.\mathbf{p} + (\boldsymbol{\beta} - 1)mc^2 + V_{nuc}(r) + V^{N-1}. \quad (1)$$

Here $\boldsymbol{\alpha}$ and β are Dirac matrices, $V_{nuc}(r)$ is nuclear potential, $V^{N-1} = V_{dir} + V_{exch}$ is the sum of the direct and exchange Hartree-Fock potentials, N is the number of electrons, m is the mass of the electron. c is the speed of light.

We included the hyperfine interaction (HFI) in a self consistent way as well. The relativistic Hartree-Fock (RHF) method [6], which is equivalent to the well-known random-phase approximation (RPA), is used for this. To take into account finite nuclear size we use a simple model which represents the nucleus as a uniformly magnetized ball. In our calculations the magnetic nuclear radius is the same as the electric one. However, these two parameters can be varied independently.

The Hamiltonian of the HFI between a relativistic electron and point nucleus is given by

$$\hat{H}_{\mathrm{HFI}} = e\mu \cdot \mathbf{F}(\mathbf{r}), \quad (2)$$

$$\mathbf{F}(\mathbf{r}) = \begin{cases} \dfrac{\mathbf{r}\times\boldsymbol{\alpha}}{r_m^3}, & r < r_m \\ \dfrac{\mathbf{r}\times\boldsymbol{\alpha}}{r^3}, & r \geq r_m, \end{cases} \tag{3}$$

where $r_m = 1.1A^{1/3}\text{fm}$, r_m is the magnetic nuclear radius, A is the mass number of the nucleus, μ is the nuclear magnetic moment in nuclear magnetons.

The RHF equations have a form

$$(\hat{H}_0 - \varepsilon_a)\delta\psi_a = (-F_z - \delta V^{N-1} + \delta\varepsilon_a)\psi_a, \tag{4}$$

$$\delta\varepsilon_a = \left\langle \psi_a \left| F_z + \delta V^{N-1} \right| \psi_a \right\rangle. \tag{5}$$

Here, the index a numerates states in the closed-shell core. These equations are solved self-consistently for all states in the core.

States of the valence electron are calculated in the frozen field of atomic core complemented by the correlation potential operator [7],

$$(\hat{H}_0 + \hat{\Sigma} - \varepsilon)\psi_v^{BO} = 0. \tag{6}$$

Here, the index v numerates valence states. The correlation potential includes all lowest second-order correlation corrections and dominating higher-order correlation corrections [8]. These higher-order correlations include screening of Coulomb interaction and hole-particle interaction. They are taken into account in all orders. Solving Eq. (6) for valence states we find the so-called *Brueckner* orbitals (BOs) for the valence states. This is emphasized by using superscript *BO* for the orbitals.

The total-energy shift for the valence state v due to HFI and correlations is given by

$$\delta\varepsilon_v = \left\langle \psi_v^{BO} \left| F_z + \delta V^{N-1} + \delta\hat{\Sigma} \right| \psi_v^{BO} \right\rangle. \tag{7}$$

Here, $\delta\hat{\Sigma}$ is the change to the correlation potential $\hat{\Sigma}$ due to the hyperfine interaction. The term with $\delta\hat{\Sigma}$ is often called the structure radiation. Finally, there is a contribution due to the renormalization of the many-electron wave function (see, e.g., [7])

$$\delta\varepsilon_{norm} = -\left\langle \psi_v \left| F_z + \delta V^{N-1} \right| \psi_v \right\rangle \left\langle \psi_v \left| \partial\hat{\Sigma} / \partial E \right| \psi_v \right\rangle. \tag{8}$$

The magnetic dipole hyperfine-structure constant A_v for the valence state v is given by

$$A_v = \frac{\mu e^2}{2m_p I} \frac{\delta\varepsilon_v}{\sqrt{j_v(j_v+1)(2j_v+1)}}. \tag{9}$$

Here I is the nuclear angular momentum, m_p is the mass of proton, j_v is the angular momentum of the state for which the correction is calculated.

2.1. Breit interaction

The Breit interaction is included in a very accurate way described in the previous works [9]. The Breit operator in the zero-energy-transfer approximation has the form

$$h^B = -\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 + (\boldsymbol{\alpha}_1 \cdot \mathbf{n})(\boldsymbol{\alpha}_2 \cdot \mathbf{n})}{2r}, \tag{10}$$

where $\mathbf{r} = \mathbf{n}\, r$, r is the distance between electrons, and $\boldsymbol{\alpha}$ are the Dirac matrices.

Similar way to the hyperfine interaction, Breit operator induces a correction to the self-consistent Hartree-Fock potential, which is taken into account in all orders in Coulomb interaction by iterating the RHF equations with the potential.

$$V^{N-1} = V^C + V^B, \tag{11}$$

here, V^C is the Coulomb potential, V^B is the Breit potential. The same potential (11) goes to the left- and right- hand sides of the RHF equations (4).

2.2. QED corrections

The QED corrections are introduced approximately via the QED potential suggested in Ref. [10] to include quantum electrodynamics radiative corrections to the hyperfine structure. The radiative potential has the form

$$V_{rad}(r) = V_U(r) + V_g(r) + V_e(r), \tag{12}$$

where V_U is the Uehling potential, V_g is the potential arising from the magnetic formfactor and V_e is the potential arising from the electric formfactor.

As for the case of Breit interaction, this potential is added to the Hartree-Fock potential,

$$V^{N-1} \equiv V^{N-1} + V_{rad}. \tag{13}$$

This potential was chosen to fit accurate calculations of the QED corrections to the energies. It may give less accurate results for the hyperfine structure. Therefore, we consider current calculations of the QED corrections as rough estimations only.

3. Results

The results of the calculations are presented in the Table. Here, RHF corresponds to the $\langle \psi_v | F_z | \psi_v \rangle$ matrix elements with the Hartree-Fock wave functions ψ_v; RPA corresponds to the $\langle \psi_v | F_z + \delta V^{N-1} | \psi_v \rangle$ matrix elements; BO and RPA (BO) columns correspond to the same matrix elements but with Hartree-Fock wave function replaced

with Brueckner orbitals; and the "Str." column includes structure radiation and renormalization.

As can be seen from the table, the most important corrections are the many-body corrections associated with the core polarization effect RPA and with the correlation interaction of the external electron with the core BO. These effects follow approximately the same pattern when moving from light to heavy atoms. This means that the accuracy of the results should be about the same for all atoms and ions.

Breit contribution is small and can be neglected in all cases. This is because Breit contributions are proportional to lower powers of *Z* than other relativistic effects. The QED corrections are large for *s* states and small for *p* states. They reduce the hyperfine structure constants of these states by about 1%. The deviation from experiment for the *ab initio* results of Tl and Pb+ are approximately 1%, thus the accuracy of E113 and E114+ are estimated within 1% to 2%.

Table. *Hyperfine-structure constants of the lowest $s_{1/2}$ and $p_{1/2}$ states of Tl, Pb^+, E113 and $E114^+$ in different approximations in MHz*

Atom	Sta.	RHF	RPA	BO	RPA (BO)	Breit	QED	Str.	Total	Expt.
Tl	7s	563400	732400	835710	954779	3150	-16902	-12207	928820	939000[a]
	$6p_{1/2}$	169560	210380	263760	324420	1256	-385	-1132	324159	314000[a]
E113	8s	1969098	2526390	3195140	3901044	-2811	12930	-195883	3715280	
	$7p_{1/2}$	729357	1021100	1239908	1400366	-937	39586	19700	1458715	
Pb+	7s	50433	59087	59305	68448	-276	-1308	-1240	65624	65374[b]
	$6p_{1/2}$	50405	60192	65975	77999	247	126	-465	77907	75706[b]
E114+	8s	213205	248967	231024	266909	1011	-2405	-8016	257499	
	$7p_{1/2}$	184689	217136	243795	286809	-1279	-1006	130	284654	

[a]Reference [11]

[b]Reference [12]

4. Conclusion

The hyperfine structures of lowest s and $p_{1/2}$ states of the superheavy elements E113 and $E114^+$ have been calculated with an uncertainty approximation 2%. The results may be used for experimental studies of nuclear, spectroscopic, and chemical properties of the elements.

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