



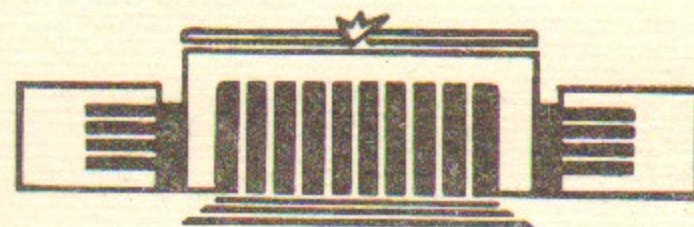
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AND NUCLEAR MAGNETIC MOMENTS
OF RADIUM ISOTOPES

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HYPERFINE STRUCTURE OF Ra⁺ AND NUCLEAR MAGNETIC MOMENTS OF RADIUM ISOTOPES

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Abstract

The energy levels, fine- and hyperfine-structure intervals in the Ra⁺ ion have been calculated using the relativistic Hartree-Fock method with the core polarization and correlation corrections taken into account. The accuracy of calculation is ~ 1%. The calculation enables us to improve the accuracy of determination of the radium isotopes (A = 211 - 229) magnetic moments from the data on hyperfine structure (Ref.1).

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In the Ref. [1] the hyperfine-structure (HFS) of odd isotopes of the Ra^+ ion have been measured, and the magnetic moments of the Ra nuclei with $A = 211 - 229$ have been obtained using the semiempirical formulae. Because of the uncertainty in atomic calculations, the accuracy in the determination of the magnetic moments ($\sim 5\%$) proved to be considerably worse than the accuracy of the HFS measurement (0.1 - 0.01%).

The better accuracy of calculation can be achieved by using the relativistic Hartree-Fock (RHF) method with the correlation correction being taken into account by means of the many-body perturbation theory. It is the method by which the nuclear magnetic moments of the Fr isotopes have previously been determined (Ref. 2,3). In the present work a calculation ^{similar} to that of Ref. [3] has been made for the Ra^+ ion.

The Hamiltonian of an atom is convenient to represent as follows:

$$\hat{H} = \sum_{i=1}^N (H_0(\vec{r}_i) + H_{HFI}(\vec{r}_i)) + V_{corr} \quad (1)$$

where H_0 is the relativistic Hartree-Fock Hamiltonian, H_{HFI} is the hyperfine interaction (HFI) operator, V_{corr} is the residual electron-electron interaction (not taken into account in H_0), and N is the number of electrons in the atom.

The self-consistent field $V_0^{N-1} = V_d + V_{ex}$ (V_d and V_{ex} are the direct and exchange interactions, respectively) of $N-1$ electrons from the closed shells is included

$$H_0 = \vec{\alpha} \cdot \vec{p} + \beta(m_e - 1) - \frac{Ze^2}{r} + V_0^{N-1} \quad (2)$$

Here $\vec{\alpha}$ and β are Dirac matrices and m_e is the mass of the electron. The solution of the Dirac equation with the Hamiltonian H_0 allows one to obtain the complete orthonormalized set of orbitals, which includes both the occupied and unoccupied states of the discrete and continuous spectra. The HFI is convenient to take into account in single-particle orbitals rather than by means of the many-body per-

turbation theory. The equations for the HFI induced corrections to energy $\delta\varepsilon$ and to the wavefunction $\delta\psi$ are of the form

$$(H_0 - \varepsilon) \delta\psi = -H_{HFI} \psi - \delta V_{ex} \psi + \delta\varepsilon \psi \quad (3)$$

Here δV_{ex} is HFI induced correction to the exchange interaction, which is due to the corrections to wavefunctions of the core electrons. (The correction to the direct potential does not appear). The self-consistent solution of equations (3) for all the core electrons corresponds to exact account of the core polarization. The HFS of an external electron level is determined by the formula

$$\delta\varepsilon = \langle \psi | H_{HFI} | \psi \rangle + \langle \psi | \delta V_{ex} | \psi \rangle \quad (4)$$

where ψ is the wavefunction of the electron. The second term is contribution of the core polarization. Note that the finite size of the nucleus should be taken into account. For S -electrons, the nuclear finite size effect decreases the HFS by 15%.

The most complicated calculation is that dealing with the correlation correction which is due to the residual interaction V_{corr} . By definition, V_{corr} is equal to the difference between the exact and Hartree-Fock Hamiltonians:

$$V_{corr} = \sum_{i < k}^N \frac{e^2}{r_{ik}} - \sum_{i=1}^N V^{N-1}(r_i) \quad (5)$$

In the considered scheme the first-order correction with respect to V_{corr} does not arise. The second-order corrections are determined by 16 diagrams presented in Ref. [3]. The detailed description of this correction calculation method as well as method of core polarization calculation are presented in Ref. [3].

Variation of the nuclear radius from $A = 211$ to $A = 229$ gives rise to only a 0.3% change of the hyperfine splitting. The differences in the distribution of the magnetic moment inside the nuclei turns out to be insignificant as well (see

Ref. [3]). Therefore, the HFS constant A is proportional to the g -factor of the nucleus ($g = \frac{\mu}{I}$, μ is the magnetic moment in nuclear magnetons, I is the nuclear spin). Table 1 lists the Hartree-Fock values of ratio A/g (the contribution $\langle \psi | H_{HFI} | \psi \rangle$), the contributions of the core polarization $\langle \psi | \delta V_{ex} | \psi \rangle$ and of the correlation correction for the $7s$, $7p_{3/2}$, $7p_{1/2}$ -states of the Ra^+ ion. The experimental values of the HFS constants of $7s$ and $7p_{1/2}$ levels from Ref. [1] for Ra^+ with $A = 211 - 229$ are presented in Table 2. The nuclear magnetic moments for these isotopes obtained from the HFS by means of Table 1 are presented in the Table 2 as well.

The values of the magnetic moments, which have been derived from the $7s$ -level HFS constants, proved to be 2% lower in comparison with those based on the $7p_{1/2}$ -level HFS constants. Our calculations for caesium (Ref. 3) have shown that we somewhat overestimate the magnitude of the HFS for the s -levels and underestimate it for the $p_{1/2}$ -levels. Perhaps it is the case for Ra^+ too. Therefore we take the average values of the magnetic moments as a result ($\mu = (\mu(7p_{3/2}) + \mu(7s))/2$). The accuracy of these values is $\sim 1\%$. Table 2 also presents the magnetic moments obtained in Ref. [1]. These are larger, by 3% in comparison with our values.

Using the values of the magnetic moments, it is possible to predict the HFS constants of the $7p_{3/2}$ -levels. These constants are relatively small and therefore are more sensitive to the neglected higher-order correlation corrections. Calculated constants of the $p_{3/2}$ -levels (Ref. 3) exceed the experimental values in Cs by 3.5% for the $6p_{3/2}$ and $7p_{3/2}$ levels and in Fr by 8% for the $7p_{3/2}$ level. It is therefore probable that the calculated values of the HF constants in the Ra^+ , $A(7p_{3/2}) = \frac{\mu}{I} 315$ MHz, are a few per cent overestimated.

In order to check accuracy of our calculation, we have also calculated the energies of the lower s and p levels with the correlation corrections taken into account. The result is given in Table 3. Comparison with the experimental data shows that the accuracy is 0.1% for energy and 0.5 - 1% for fine structure intervals of the p -levels.

Table 1. Contributions to the HFI constants of the 7s, 7p_{1/2} and 7p_{3/2} levels divided by the g-factor of the nucleus (in MHz). Values of $M=gI$ are presented in Table 2.

	RHF $\langle \psi H_{\text{HFI}} \psi \rangle$	Polarization $\langle \psi \delta V_{\text{ex}} \psi \rangle$	Correlations	Sum
7s	14590	2414	2297	19300
7p _{1/2}	2446	451	801	3698
7p _{3/2}	188	119	8	315

Table 2. Experimental HFI constants (in MHz) Ref. [1] and nuclear magnetic moments determined from these data

Mass number	I	A(7s _{1/2})[1]	A(7p _{1/2})[1]	M[1]	Our values
211	5/2	6624,8(1.0)	1299.7(8)	0.90	0.870(9)
213	1/2	22920(6)	4525(5)	0.62	0.603(8)
221	5/2	-1345.0(1.8)	-266,3(1.5)	-0.18	-0.177(3)
223	3/2	3398,3(2.9)	667,1(2.1)	0.28	0.267(3)
225	1/2	-27684(13)	-5446(7)	-0.75	-0.727(9)
227	3/2	-5063.5(3.1)	-996.2(2.3)	-0.41	-0.399(5)
229	5/2	3789.7(2.3)	743,9(1.2)	0.51	0.497(5)

Table 3. Calculated and experimental energy levels and fine structure intervals for Ra⁺ (in cm⁻¹)

	RHF	Correlations	Sum	Experiment [5]
7s	-75652 ^{*)}	-6244	-81896	-81842
7p _{1/2}	-56874	-3615	-60489	-60491
8p _{1/2}	-30052	-1205	-31257	-31236
9p _{1/2}	-18748	-585	-19333	-
7p _{3/2}	-52896	-2711	-55607	-55633
8p _{3/2}	-28498	-953	-29451	-29450
9p _{3/2}	-17973	-469	-18442	-18432
Fine structure				
7p	3978	904	4882	4858
8p	1554	252	1806	1786
9p	775	116	891	-

*) Just as in the Ref. [4] the Lamb-shift of the 7s-level, equal to 160 cm⁻¹, is taken into account.

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МАГНИТНЫЕ МОМЕНТЫ ЯДЕР ИЗОТОПОВ РАДИЯ И
СВЕРХТОНКАЯ СТРУКТУРА Ra^{226}

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