On the Hyperfine Structure in the Configurations $4f''6s^2$, $4f''5d6s$, $4f''6s6p$, and $4f''^{-1}5d6s^2$ of the Lanthanides

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A survey of hyperfine analyses in the low-lying configurations $4f''6s^2$, $4f''5d6s$, $4f''6s6p$, and $4f''^{-1}5d6s^2$ of the lanthanides is given. Experimental hf radial integrals $\langle r^{-3}\rangle_{nl}$ are indicated for the configurations under investigation. From a comparison of experimental and theoretical hf radial integrals configuration-interaction contributions $A_{nl}$ to the hfs have been evaluated for the configurations for which corresponding integrals were available. With nuclear electric quadrupole moments from muonic x-ray investigations and radial integrals $\langle r^{-3}\rangle_{nl}$ and $\langle r^{-3}\rangle_{nl'}$ from experimental hfs quadrupole shielding corrections $K_{nl}$ have been obtained. The variation of hyperfine radial integrals, configuration-interaction contributions and quadrupole shielding corrections over the $4f$ shell in the configurations under study is discussed. Trends of these quantities in different configurations are compared.

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1. Introduction

Hyperfine structure (hfs) has been discovered experimentally at the end of the last century by Michelson [1] and Fabry and Perot [2], and has attracted the attention of physicists ever since. The hfs in atomic spectral lines is due to the interaction between the electrons in the atom and the electromagnetic moments of the nucleus and consequently can provide information on nuclear as well as electronic properties of the atom. In early years hfs has been studied with the emphasis on obtaining information on the nuclear structure [3]. In order to evaluate nuclear quantities the electronic part of the hyperfine (hf) interaction was usually calculated semi-empirically from e.g. experimental fine-structure constants or the nuclear quantities had to be known for at least one isotope of the same element. Due to the high sensitivity and resolution of optical methods optical hfs and isotope shift have opened an access to the investigation of nuclear properties in long isotopic sequences, including short-lived nuclides [4].

In the last years the electronic aspect has become the main concern in optical hf investigations. Knowing the nuclear magnetic dipole and the electric quadrupole moments from e.g. nuclear magnetic resonance, atomic-beam magnetic resonance, muonic x-ray, Coulomb excitation techniques, the electronic part in the experimental hf constants can be determined directly. The hfs can therefore be used as a sensitive tool for the investigation of electronic properties of the atom.

The starting point for a deeper understanding of hfs is the knowledge of precise experimental hf constants. This requires high-resolution spectroscopy. One of the historical keystones was certainly the development of the atomic-beam magnetic-resonance method by Rabi and co-workers [5, 6] which allowed to obtain very accurate hf constants for ground and low-lying metastable states. Another keystone was the development of narrow-bandwidth, tunable lasers. Indeed, the development of Doppler-free laser spectroscopic methods (laser atomic-beam, atomic-beam laser-rf double-resonance techniques etc.) and their improvement in application, sensitivity and resolution over the last decade has opened a new chapter for hf investigations. One should not forget the development and improvement
of population techniques for higher lying, especially metastable atomic states which gives an access for high-resolution spectroscopy to a variety of atomic levels in particular of numerous levels belonging to the same configuration.

The great advances in theory, in particular new developments in e.g. many-body perturbation and multi-channel quantum defect theory, often stimulated or permitted by the development of large and fast computers and powerful computer codes had a major impact on the treatment and understanding of electronic-structure problems over the last years.

The main difficulty in analyzing experimental hf data arises from the influence of relativistic and configuration-interaction effects. In order to take into account these effects, the hfs is normally treated within an effective tensor operator formalism. Within this formalism the hf constants can be expressed as function of effective electronic radial integrals, denoted \( (r^-3) \) \[7, \text{e.g.} \ 8\]. These radial integrals are normally interpreted as free parameters which are assumed to be constant for all the levels of a configuration and are determined from a fit to the experimental hf constants. This allows a prediction of the hfs of (principally) all the levels of a configuration and are determined from a fit to the experimental hf constants. This allows a prediction of the levels in particular of numerous levels belonging to the same configuration.

From an interpretation of hf radial integrals continuously the hfs of the configurations \( nd^n(n+1)s^2 \), \( nd^{n+1}(n+1)s \) and \( nd^{n+2} \) of the 3d-, 4d- and 5d-shell atoms has been discussed by Olsson and Rosén \[10, 11\] and Bütgenbach \[12\]. An investigation of hfs in the configurations \( 4f^n6s^2 \) of the 4f-shell atoms has been published in the 1974-review by Lindgren and Rosén \[9\]. Over the last years the knowledge of the experimental hfs in the 4f-shell atoms in the low lying configurations \( 4f^n6s^2 \), \( 4f^n5d6s \), \( 4f^n6s6p \) and \( 4f^{n-1}5d6s^2 \) has increased considerably. Especially in the configurations \( 4f^n6s^2 \) extensive work has been accomplished: in the last three years precise hf data have been determined for Tb, Dy, Ho, Er and Tm \[13-16\]. This has prepared the foundation for a new systematic analysis of hfs in this configuration type (which does not mean that there are no important experimental topics left in the configurations \( 4f^n6s^2 \)). Quite recently semi-empirical Sternheimer correction factors for 4f-shell atoms and ab initio hf constants for the lowest multiplets of the \( 4f^n6s^2 \) configurations have been calculated with multiconfiguration Dirac-Fock (MCDF) methods by Cheng and Childs \[17, 18\].

The configurations \( 4f^n6s^2 \) are the lowest lying configurations of the 4f-shell atoms apart from Ce, Gd and Lu. Since only the 4f-electron shell is unfilled the hfs of the pure configuration can be treated, within the effective tensor operator formalism, with only three hf parameters which simplifies considerably the analysis of the experimental data. For this configuration type systematic ab initio calculations for the hfs by Lindgren and Rosén \[9\] exist and enable a detailed interpretation of the hfs. The results obtained in this “easy” configuration type can serve as a guide-line for an interpretation of experimental hfs in other configuration types. The hfs in the configurations \( 4f^n5d6s \), \( 4f^n6s6p \) and \( 4f^{n-1}5d6s^2 \) is more difficult to investigate theoretically. This is not only due to the additional hf parameters of 5d-, 6p- respectively 6s-electrons but also and mainly due to configuration interaction which puts higher demands on the intermediate-coupling wavefunctions used in the hf analyses.

The emphasis of the present work is to give a survey of the results of hf analyses in the configurations \( 4f^n6s^2 \), \( 4f^n5d6s \), \( 4f^n6s6p \) and \( 4f^{n-1}5d6s^2 \) of the lanthanides. The author approached the subject from the point of view of an atomic spectroscopist who tried to find general trends, systematics in the variation of electronic hf quantities in low-lying configurations of the lanthanides. From a consideration of systematics of electronic properties in the hfs additional guidance for the interpretation of (experimental) hf data, additional criterions for testing the reliability of hf analyses etc. can be obtained.