

SEMI-EMPIRICAL INVESTIGATIONS OF THE IONIC BISMUTH (BI II) ENERGY STRUCTURE FOR ELECTRIC QUADRUPOLE MOMENT CALCULATION

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The history of the bismuth electric quadrupole moment (Q) investigation have begun in 1960 with the R. S. Title and K. F. Smith publication titled: *The hyperfine structure of ^{209}Bi* [1]. In that paper, authors estimated the value of the bismuth electric quadrupole moment as $Q = -0,360 \pm 0,001b$. Since then, the numerous amount of authors [2, 3, 4, 5], have tried to calculate the value of Q for bismuth. Unfortunately, those investigations led to the divergent results and currently there is no agreement within atomic physicists society about the bismuth quadrupole moment value. Developed by us the parameterization method of the fine- (fs) and hyperfine structure (hfs)[6, 7], makes one able to calculate the electric quadrupole moment. For the bismuth ion, the finally obtained values for one-body hfs parameters a_{6p}^{01} and b_{6p}^{02} and two-body hfs parameters were used to calculate the electric quadrupole moment. However, to perform semi-empirical hfs analysis both the accurate values of hyperfine structure constants A and B and the correct fine structure eigenvectors describing electronic system of BiII are needed.

On the basis of the experimental results [8, 9, 10, 11] concerning the fine structure literature data and the hyperfine structure literature data, a parametric studies of the atomic structure for the odd and even parity configurations system of the ionic bismuth (Bi II) were performed. The present paper is the application of our many-body parametrization method allowing the analysis of complex electronic configurations system containing up to four open shells by taking into account all electromagnetic interactions expected in an atom, in accordance with the second-order perturbation theory. The above mentioned theory is described in general terms in the first work of the series under the common title *Construction of the energy matrix for complex atoms* [7].

The odd-parity configurations system contains following 81 configurations: $6p^36s$, $\sum_{n=7}^{40}6s^26pns$, $\sum_{n=7}^{40}6s^26pnd$, $\sum_{n=5}^{15}6s^26png$. For the even-parity configurations system, calculations were carried out within the basis of 71 configurations: $6p^26s^2$, $\sum_{n=7}^{40}6s^26pnp$, $\sum_{n=5}^{40}6s^26pnf$. The fs analysis was performed separately for each of configuration parity. The finally obtained eigenvectors were used in hfs parametrization analysis. Due to the insufficient amount of the experimental data, the hfs calculations were performed twice: first, for each configuration parity separately and further within huge base being composed of the configurations from both parities.

For unknown electronic levels predicted values of the level energies and hfs constants are given, which can facilitate further experimental investigations. The value of the electric quadrupole moment of bismuth nucleus was calculated and compared to the literature data.

The research will be completed in near future by data collected in similar analysis performed for the atomic bismuth system.

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