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Calculating Energy Levels in ^{49}Mn/^{49}Cr Mirror Nuclei with OXBASH Code

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Abstract: Coulomb Displacement Energies in mirror nuclei ^{49}Mn and ^{49}Cr have been calculated using shell model code OXBASH and compared with experimental results. The calculations were carried out in the F7PN model space with the F748BPN Hamiltonian. This code which is based on one of the most applicable nuclear models, the shell model, deals with evaluating energy levels in nuclei. A comparison had been made between calculated results and the available experimental data to test theoretical shell model description of nuclear structure in mirror nuclei. The energy states of mirror nuclei are almost identical, except for the small effects due to Coulomb interaction where the symmetry in being broken. The calculated energy spectrum is in good agreement with the available experimental data.

Keywords: Mirror Nuclei, OXBASH Code, Shell Model Structure, Model Space, Energy Levels

1. Introduction

Obtaining the nuclear structure and energy levels of nuclei is one of the criteria to improve investigations of nuclei properties. Nuclear models have the property to help us to better understanding of nuclear structure which contains main physical properties of nuclei, and shell-model is one of the most prominent and successful nuclear models [3-6]. The energy states of mirror nuclei (nuclei with the same mass number and the number of protons in one of them equals the number of neutrons in the other) are almost identical, except for the small effects due to Coulomb interaction where the symmetry in being broken. The study of this symmetry breaking reveals details of the mirror nuclei structure. This shift in mirror symmetry will be observed mostly as a function of spin, where the protons and/or neutrons rearrange themselves in new shell model orbits and hence cause changes in Coulomb energy differences. These effects, known as Coulomb Displacement Energies (CDE), have been the subject of several studies in nuclear structure physics [7-9].

Obtaining the nuclear structure and energy levels of nuclei is one of the criteria to improve investigations of nuclei properties. Nuclear models have the property to help us to better understanding of nuclear structure which contains main physical properties of nuclei, and shell-model is one of the most prominent and successful nuclear models [10]. This model can be compared with the electron shell model for atoms. As atomic behavior and properties can be described with valance electrons which exist out of a closed shell, similarly, valance nucleons (protons or neutrons) in a nucleus which are placed out of close shells (with magic numbers 2, 8, 20, 28, 50, 82 and 126) play important roles in determining nuclear properties. Nuclei with magic numbers are very stable and have completely different properties comparing with their neighbors.

One of the most attractive features of the spherical shell model is its relative simplicity for calculations in a strongly restricted configuration space. If the space is sufficiently truncated (i.e. beyond closed shells), one can perform exact shell model calculations which make the comparison with experiments more transparent and hence more attractive also for experimentalists. However, with any reasonable model space truncation one is always left with the problem of determining an effective residual interaction for the nucleons in the considered orbits, usually assumed to be a two-body force [2]. Clearly, the smaller the number of orbits considered the smaller the number of two-body matrix

elements one has to deal with. Since it is a nontrivial problem to establish the two-body matrix elements for a shell model calculation, the uncertainties might increase with a larger shell mode space, although in principle one should get better agreement with experiment.

It has to be recalled that ^{49}Mn and ^{49}Cr are mirror nuclei in the 1*f*7/2 shell, and that their level schemes should be identical in that configuration space.

For light nuclei, there are several standard effective interactions for the *p* and *SD* shells, respectively [11, 12]. Analysis of neutron-rich SD nuclei has been of high interest in recent years as they present new aspects of nuclear structure. Traditional shell-model studies have recently received a renewed interest through large scale shell-model computing in no-core calculations for light and medium nuclei. It is now therefore fully possible to work to large-scale shell-model data and study the excitation levels for larger systems. In these systems, inert core is assumed and space is determined by considering shell gaps. Figure 1 shows the PF and SD model spaces according to shell model theory.

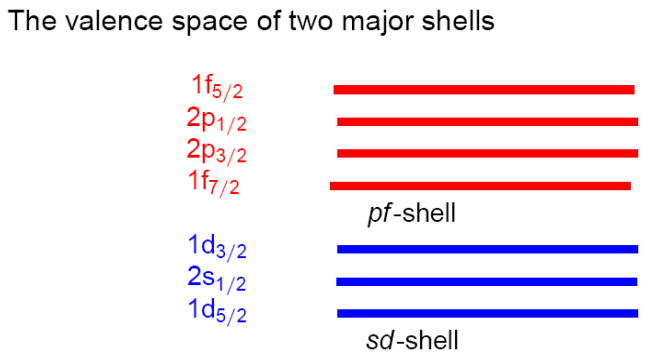

Figure 1. *SD and PF shell model spaces.*

2. Calculations

In order to calculate the nuclear structure properties of both ground and excited states based on the nuclear shell model one needs to have wave functions of those states. These wave functions are obtained by using the shell-model code Oxford- Buenos Aires Shell Model Code, OXBASH [1]. OXBASH code is a computer program that is described with a set of model spaces and interactions to apply in shell model calculations with high dimensions.

Experimental studies on the stability of some nuclei show that nuclei with protons or neutrons numbers (2, 8, 20, 50, 82, etc.) are more numerous and stable. In other words, the existence of these magic numbers suggests shell model structure in nuclear physics similar to atomic physics. In this paper, the energy levels of ^{49}Mn and ^{49}Cr mirror nuclei have been calculated using the code OXBASH. The program includes a set of computational programs which are based on the ability to measure the energy levels by forming ground state matrices with dimensions up to 2000000 and JT matrix with dimensions up to 100,000. The version of this code is 2005-8 which can be installed and used on any Windows operating system without using any other additional software.

In order to use this code one should specify the model space and interaction. In other words after choosing appropriate model space which is chosen considering valance nucleons, this code constructs a set of possible ground states and then makes JT matrix based on linear combination of ground states which give suitable T and J values. Finally by choosing the desirable interaction potential it constructs the Hamiltonian of the problem and carries out the calculations and as a default gives 10 lowest energies. In this paper, the energy levels of ^{49}Mn and ^{49}Cr mirror nuclei have been calculated using the code OXBASH. Considering the number of valence nucleons for these nuclei, F7PN model space is the suitable model for these calculations which assign separate orbitals for protons and neutrons. This model consists of $1f_{7/2}$ valence orbitals. The code OXBASH for Windows has been used to calculate the nuclear structure for the above nuclei by employing the F7PN (depending charges) model space with the F748BPN effective interaction [2].

3. ^{49}Mn/^{49}Cr Mirror Nuclei

Some calculated results concerning ground and excitation energies of the ^{49}Mn/^{49}Cr mirror nuclei are presented here. Table 1 shows data for ^{49}Mn isotope and table 2 shows data for ^{49}Cr isotope. The first column is spin of states, column two the calculated energies by OXBASH code, columns three and four the measured energies and their respective errors [8].

Table 1. *Data for ^{49}Mn. All energies are in keV.*

Spin(J)	E_Mn(OXBASH)	E_Mn(Exp.)	Mn_Error
2.5	0	0	0.00
3.5	236	262	0.800
4.5	1457	1059	0.800
5.5	3000	1542	1.000
6.5	2479	2483	1.100
7.5	3252	3190	1.200
8.5	4083	4250	1.300
9.5	5329	4447	1.400
10.5	5666	-	-
11.5	6828	6058	1.700
12.5	7355	-	-
13.5	9151	8082	2.000
14.5	9889	-	-
15.5	9503	10726	2.200

Table 2. *Data for ^{49}Cr. All energies are in keV.*

Spin(J)	E_Cr(OXBASH)	E_Cr(Exp.)	Cr_Error
2.5	0	0	0.00
3.5	123	272	0.800
4.5	1575	1084	0.800
5.5	1341	1564	1.000
6.5	2600	2503	1.100
7.5	3384	3193	1.100
8.5	4271	4222	1.200
9.5	5475	4370	1.300
10.5	6115	6136	1.400
11.5	6890	5967	1.500
12.5	8954	8880	1.800
13.5	9292	8012	1.900
14.5	10049	10227	2.000
15.5	9662	10706	2.200

Figures 2 shows calculated and measured energies of ^{49}Mn and figure 3 shows calculated and measured energies of ^{49}Cr. Due to very small measured errors, they have not shown here. As it can be seen, there is relatively good agreement between calculations made by OXBASH code and measured energies.

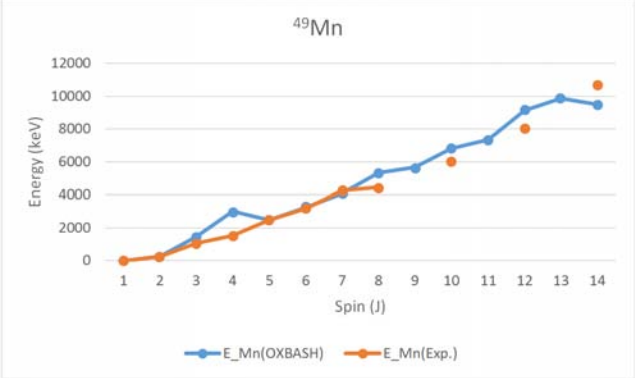

Figure 2. *Calculated and measured energies of ^{49}Mn.*

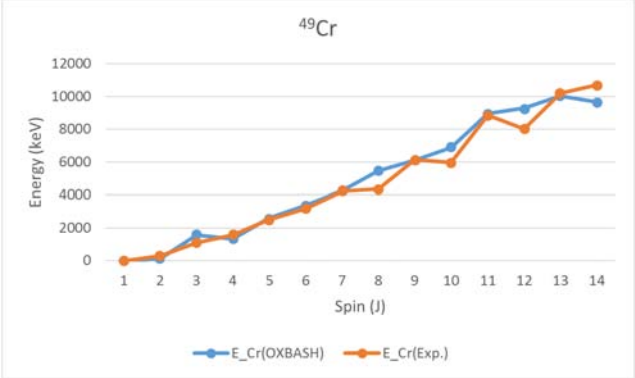

Figure 3. *Calculated and measured energies of ^{49}Cr.*

Figures 4 shows experimental energy differences of ^{49}Mn and ^{49}Cr mirror nuclei and figure 5 shows calculated energy differences of these nuclei. As it can be seen, there is a gradual increase in energy difference with increasing spin in both experimental and calculated results.

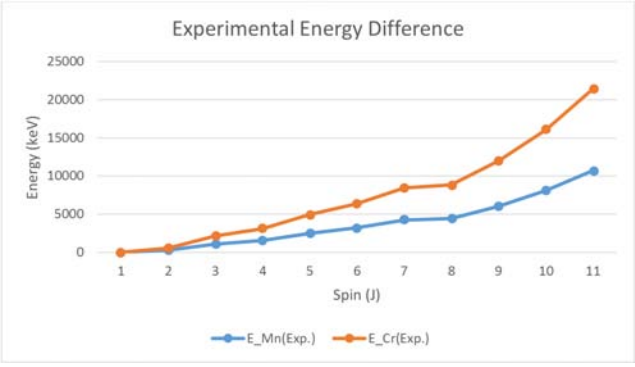

Figure 4. *Experimental energy differences between ^{49}Mn/^{49}Cr mirror nuclei [13].*

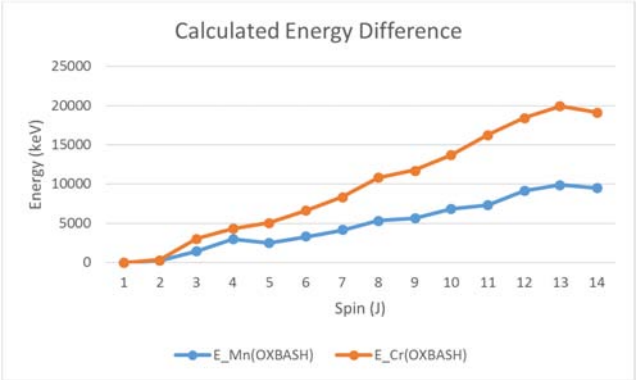

Figure 5. *Calculated energy differences between ^{49}Mn/^{49}Cr mirror nuclei.*

4. Conclusions

Coulomb Displacement Energies in mirror nuclei ^{49}Mn and ^{49}Cr (the Z of the first nucleus must equal the N of the second and thus the N of the first equals the Z of the second) have been calculated using shell model code OXBASH and compared with experimental results. The calculations were carried out in the in the 1*f*7/2 shell of F7PN model space with the F748BPN Hamiltonian. The results show that the CDE of mirror nuclei which is the difference between binding energy of the mirror nuclei is not constant and increases with increasing excitation energy of the nuclei due to rearranging of the nucleons.

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