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Ground State Properties and Shape Transition of Even-Even $_{76}$Os, $_{78}$Pt, $_{80}$Hg and $_{82}$Pb Isotopes in the Framework of Skyrme Hartree-Fock-Bogoliubov Theory

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ABSTRACT

The Hartree-Fock-Bogolyubov (HFB) theory is a good theoretical approximation for describing the nuclear structure of neutron-rich deformed nuclei, it generalized the HF theory with BCS pairing theory. In this work, ground-state properties of even-even $_{76}$Os, $_{78}$Pt, $_{80}$Hg and $_{82}$Pb isotopes from proton drip-line to neutron drip-line have been studied in the framework of the axially deformed Hartree-Fock-Bogoliubov (HFB) method with two Skyrme nucleon-nucleon force HFB9 and UNE1. The numerically calculated results of binding energy, two-neutron separation energy, two-neutron shell gap, quadrupole deformation, neutron pairing gap and charge radius are discussed and compared with the corresponding values obtained in the present experiment, Finite Range Droplet Model (FRDM), Relativistic Mean-Field (RMF) and Hartree-Fock-Bogoliubov based on D1S Gognay force. The energy surface curves are plotted for some isotones of the investigated nuclei, the transition in the shapes was clear with the change in the number of neutrinos. The calculations obtained from this study show good agreements in comparison with other data and results.

1- INTRODUCTION

Scientists are still trying to find a unified model that can predict the shape and properties of nuclei with the same accuracy [1, 2], therefore, the aim of theoretical researches since the discovery of nuclear physics up to today is to understand the reaction properties, structure, and properties of nuclei.

To describe experimental observations many methods and theories are built, starting from direct solutions and conjecture ones then going on to more sophisticated models. For light nuclei (nuclei with mass number A < 50) one can use ab initio calculation based on bare N-N interaction [3, 4]. For nuclei with medium mass numbers, a shell model can be used [5,6]. However,for heavy nuclei (nuclei with mass number A > 60), relativistic [7] and nonrelativistic [8, 9] mean-field (MF) theory can be used. The most popular one among all of these models is the Hartree-Fock (HF) model with adding BCS (HF+BCS), which takes into account the effect of the pairing correlations with mean-field. For nuclei near the line of β-stability HF+BCS give a very good description of the nuclear ground-state properties and structure [10], but for nuclei far from this line, the effect of pairing correlations are increased gradually, so such a model is no longer adequate for studying nuclei near proton and neutron drip-line [11]. Therefore, Hartree-Fock-Bogoliubov (HFB) was introduced to consider both mean-field correlations and pairing correlations self-consistently [12].

Osmium $_{76}$Os with 76 protons, Platinum $_{78}$Pt with 78 protons, and Mercury $_{80}$Hg with 80 protons isotopes have received great attention in the study of nuclear physics [2, 13-15], because they ley beyond proton magic number Z=82 of Pb, it is characterized by a powerful combination between prolate and oblate configuration.

In this work ground-state properties for even-even Os, Pt, Hg, and Pb isotopes were studied, surface energy curves are also calculated for the investigated isotopes from N=108 to 118 to show the difference among

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isotopes and isotones shape transition. Computer code HFBTHO version 3.00 [16] was used in this study with two types of Skyrme interaction (HFB9 and UNE1). This paper is organized as follows: Hartree-Fock-Bogoliubov method briefly presented in section 2, results and discussions are presented in section 3. Finally, in section 4, the conclusion of the study is presented.

2. Hartree-Fock-Bogoliubov Method

A two-body Hamiltonian of many fermion systems can be written in terms of a set of (creation $c^{\dagger}$, annihilation c) operators [17, 18] as follows:

$$H = \sum_{\ell_1\ell_2} t_{\ell_1\ell_2} c^{\dagger}_{\ell_1} c_{\ell_2} + \frac{1}{4} \sum_{\ell_1\ell_2\ell_3\ell_4} \overline{v}_{\ell_1\ell_2\ell_3\ell_4} c^{\dagger}_{\ell_1} c^{\dagger}_{\ell_2} c_{\ell_4} c_{\ell_3} \quad (\mathbf{1})$$

Where the first term represents the kinetic energy and $\overline{v}_{\ell_1\ell_2\ell_3\ell_4} = v_{\ell_1\ell_2\ell_3\ell_4} - v_{\ell_1\ell_2\ell_4\ell_3}$ are anti-symmetrized two-body interaction matrix-element. So, the ground state wave function of HFB method can be defined by quasi-particle operator ($\beta^{\dagger}_a$ and β_a) with a liner Bogoliubov transformation [19]:

$$\beta^{\dagger}_a = \sum_{\ell} U_{\ell a} c^{\dagger}_{\ell} + V_{\ell a} c_{\ell} \qquad \beta_a = \sum_{\ell} U^{*}_{\ell a} c_{\ell} + V^{*}_{\ell a} c^{\dagger}_{\ell} \quad (\mathbf{2})$$

Matrices $U\ and\ V$ should satisfy the relation

$$U^{\dagger}U + V^{\dagger}V = I, \quad UU^{\dagger} + V^{*}V^{T} = I, \quad U^{T}V + V^{T}U = 0, UV^{\dagger} + V^{*}U^{T} = 0 \quad \mathbf{(3)}$$

Single-body density matrix in terms of the normal $\rho\ and\ k$ is defines as:

$$\rho_{\ell\ell'} = \langle \Phi | c^{\dagger}_{\ell'} c_{\ell} | \Phi \rangle, \qquad k_{\ell\ell'} = \langle \Phi | c_{\ell'} c_{\ell} | \Phi \rangle \quad \mathbf{(4)}$$

The energy functional of H (eq. 1) is expressed as:

$$E\,[\rho, k] = \frac{\langle \Phi|H|\Phi\rangle}{\langle \Phi|\Phi\rangle} = Tr\left[t + \tfrac{1}{2}\Gamma\right]\rho - \tfrac{1}{2}Tr[\Delta k^{*}] \quad \mathbf{(5)}$$

Where

$$\Gamma_{\ell_1\ell_3} = \sum_{\ell_2\ell_4} \overline{v}_{\ell_1\ell_2\ell_3\ell_4}\, \rho_{\ell_4\ell_2}, \qquad \Delta_{\ell_1\ell_2} = \sum_{\ell_3\ell_4} \overline{v}_{\ell_1\ell_2\ell_3\ell_4}\, k_{\ell_3\ell_4} \quad (\mathbf{6})$$

The matrix form of the HFB equations is given by:

$$\begin{pmatrix} t + \Gamma - \lambda & \Delta \\ -\Delta^{*} & -(t + \Gamma - \lambda)^{*} \end{pmatrix} \begin{pmatrix} U_a \\ V_a \end{pmatrix} = E_a \begin{pmatrix} U_a \\ V_a \end{pmatrix} \quad (\mathbf{7})$$

Where Δ is pairing potential, and λ is Lagrange multiplier represents fermi energy of the system, more details can be found in [19-23].

3. RESULT AND DISCUSSION

In this section, we present and discuss our result obtained in this study, especially for average binding energy, two-neutron separation energy, two-neutron shell gap, neutron, proton and charge radius, neutron, quadrupole deformation, pairing gap and energy surface curves. The obtained calculations were done using the HFB method with two-Skyrme type interaction (HFB9 and UNE1). Skyrme parameters sets of HFB9 and UNE1 are presented in Table (1).

Table (1): Skyrme parameters sets that has been used in this work

Parameters	HFB9	UNE1
t_0 (MeV.fm^3)	-2043.91	--2078.3
t_1 (MeV.fm^5)	411.59	239.4
t_2 (MeV.fm^5)	-194.18	1575.1
t_3 (MeV.fm^3)	12497.17	14263.6
x_0	0.5149	0.053
x_1	-0.9537	-0.077
x_2	-0.3322	-1.367
x_3	0.8944	-0.162
σ	1.00	1/6

3.1 Binding energy

Binding energy (BE) is important in nuclear physics, it has a direct relation with the stability of nuclei [24]. In Fig.(1), binding energies per nucleon (BE/A) are presented, for the isotopic chain of Os, Pt, Hg, and Pb isotopes. The present calculations with HFB9 and UNE1 functional are compared with FRDM 2012 [25], HFB based on D1S forces [26], and the available experimental data [27]. It can be clearly seen that there is a good agreement between the obtained results and experimental data as well as with all other models. From Fig.(1), one can see that maximum BE/A for Os nuclei appear in the region between $N = 100 - 120$ which is about 7.96 MeV, while for Pt and Hg the maximum values appear in the region between N=100-120 which is about 7.92 and 7.9 MeV, respectively. However, for Pb, it appears in the region between N=110-130 which is about 7.89 MeV. The maximum BE/A values of heavy nuclei decreased with increasing the neutron number. The results of Pt agreed well with those reported by other investigators [2].

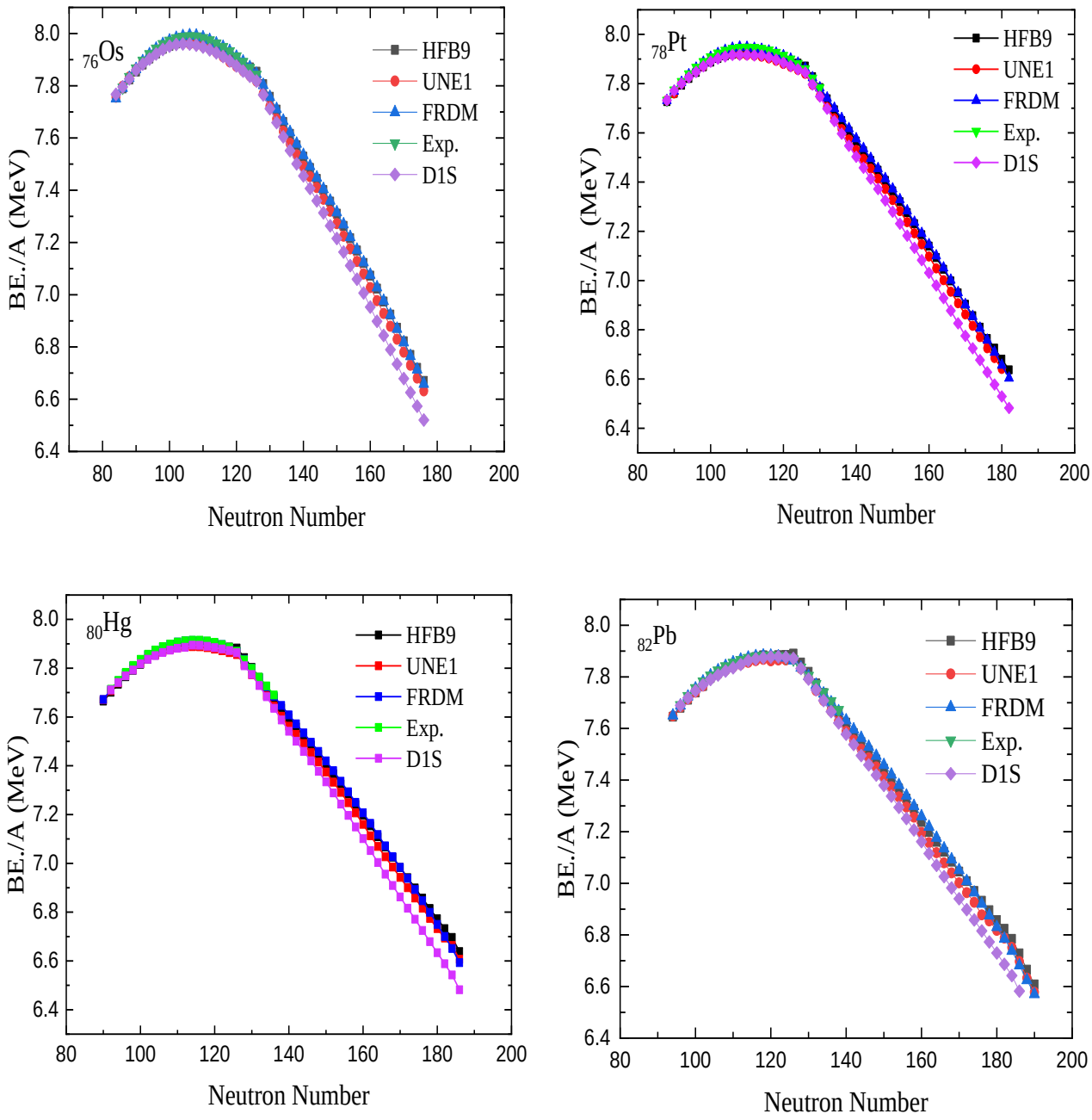

Fig. (1): The binding energy per nucleon (BE/A), for even-even isotopic chains of the Os, Pt, Hg, and Pb nuclei

3.2 Two-neutron separation energy (S_{2n})

The two neutron separation energy **(S_{2n})** is a very important quantity in studying the nuclear structure. The calculated S_{2n} values as a function of neutron number of the investigated isotopes are illustrated in Fig. (2) using two-Skyrme interaction (HFB9 and UNE1), and compared with FRDM 2012 [25], HFB calculation based on D1S forces [26], and with the available experimental data [28]. The S_{2n} values decreased with increasing the neutron number and a sharp decrease appears at the magic number N=126 due to the effect of closed-shell, while for Hg nuclei, a sharp decrease also appears at N=184. This sharp decrease can be seen in the experimental data and in all of the theoretical calculations. There is a good agreement between the present results and experimental data [28] as well as FRDM 2012 [25] and HFB calculation based on D1S forces [26].

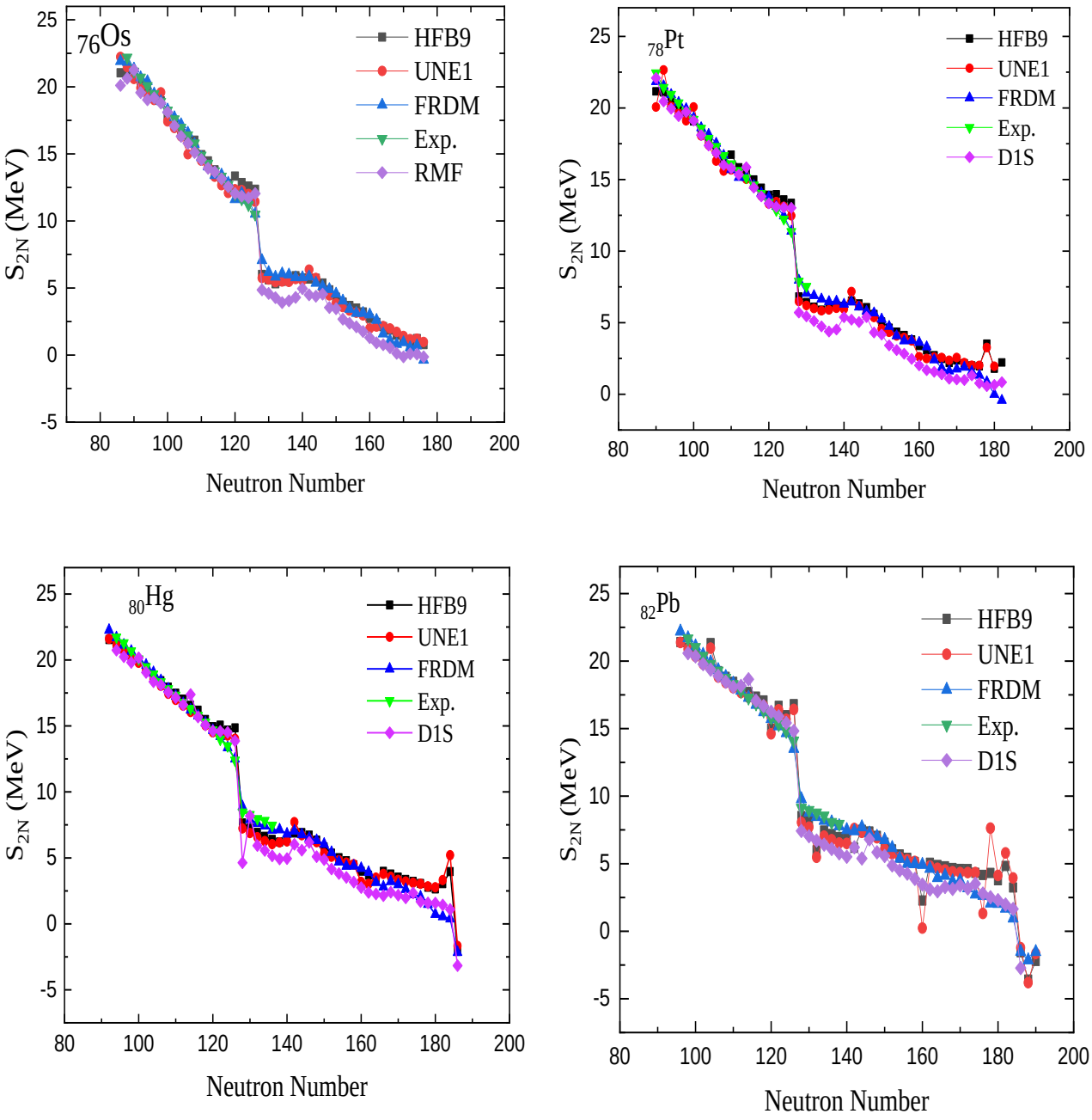

Fig. (2): the same as Fig. (1) for two neutron separation energy S_{2n}

3.3 Two-neutron shell gap (δ_{2n})

In Fig. (3), two-neutron shell gap (δ_{2n}) for isotopic chains of Os, Pt, Hg and Pb nuclei was plotted using (HFB9, UNE1) Skyrme interaction and compared with FRDM [25], HFB calculation based on D1S forces [26], and with the available experimental data [28]. It is shown that the δ_{2n}values are roughly constant for all isotopes except at N=126 for all the investigated nuclei, where some peaks appear. This supports the effect of magic numbers at N=184 for the Hg nucleus. Also, a sharp decrease appears in the same region as that of the S_{2n}.

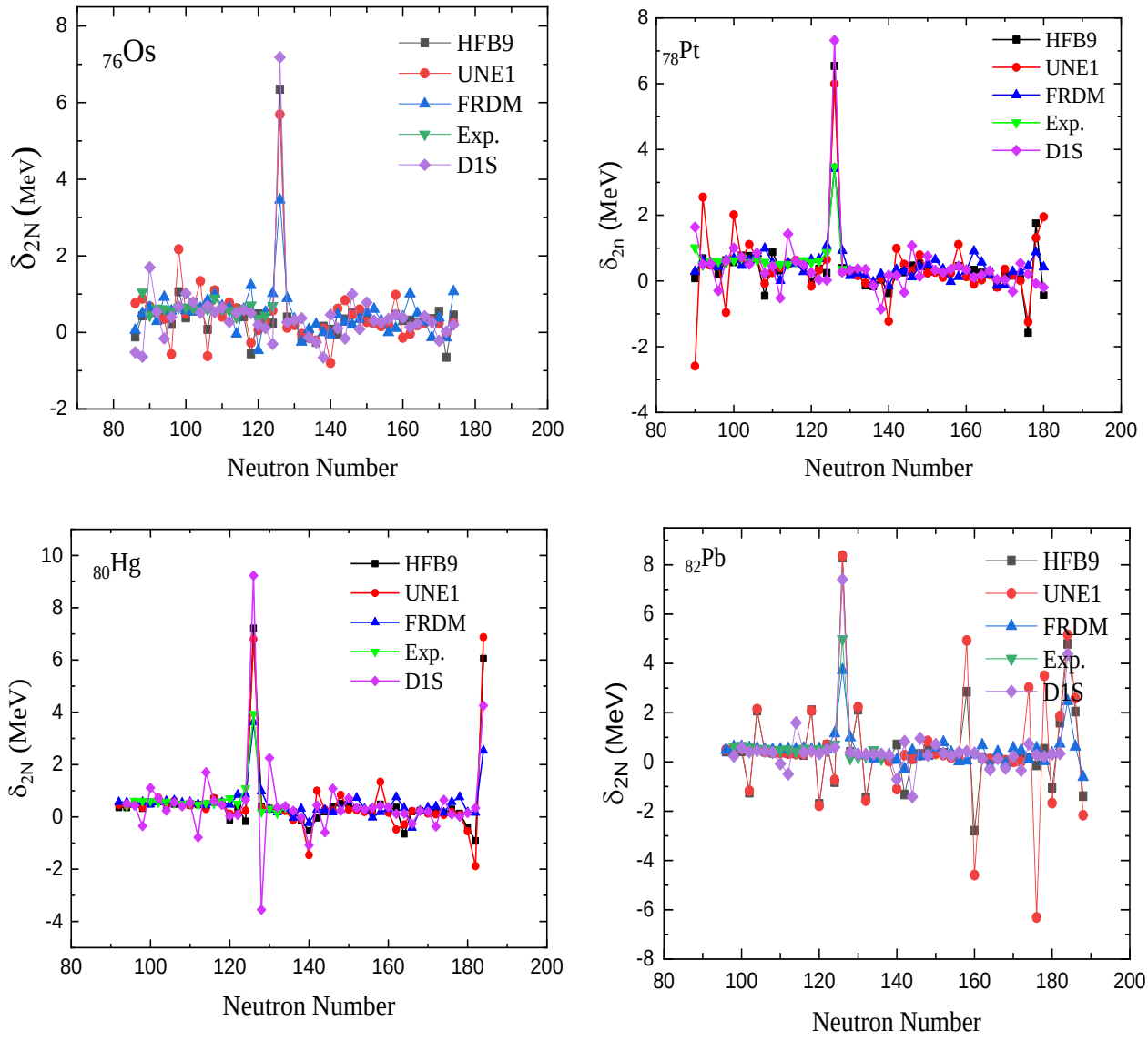

Fig. (3): The same as Fig.(1) for two neutron shell gap δ_{2n}

3-4 Quadrupole Deformation

Quadrupole deformation (β_2) provides a very good picture of the isotopes. In Fig. (4) the calculated β_2 as a function of a neutron number for isotopic chains of Os, Pt, Hg, and Pb nuclei was plotted using two-Skyrme functional (HFB9 and UNE1), where it is compared with FRDM 2012 [25] and RMF [29]. There is a good agreement among all models. Fig.(4) shows that the Os and Pt isotopes appear with small deformation in the oblate side in first isotopes then shift to prolate shape gradually up to $\beta_2 \approx 0.3$ at N=98, 102, then rapidly change to oblate shape at N= 120, 110 for Os and Pt nuclei, respectively up at neutron magic number N=126 which is shown with a spherical shape. This behavior can be seen in all of the comparison models. The Hg isotopes start with an oblate shape and it has a maximum oblate shape at N=112, then translate to spherical shape at neutron magic number, while it has a clear prolate shape at N=140-162. After this region, it rapidly changes to the oblate shape, and at $N = 186$ it appears with a clear spherical shape by the effect of shell closure as that of S_{2n} values. The Pb isotopes start with a spherical shape up to N=140, then rapidly change to prolate shape between N=142-160, after that, the shape gradually changes to spherical one.

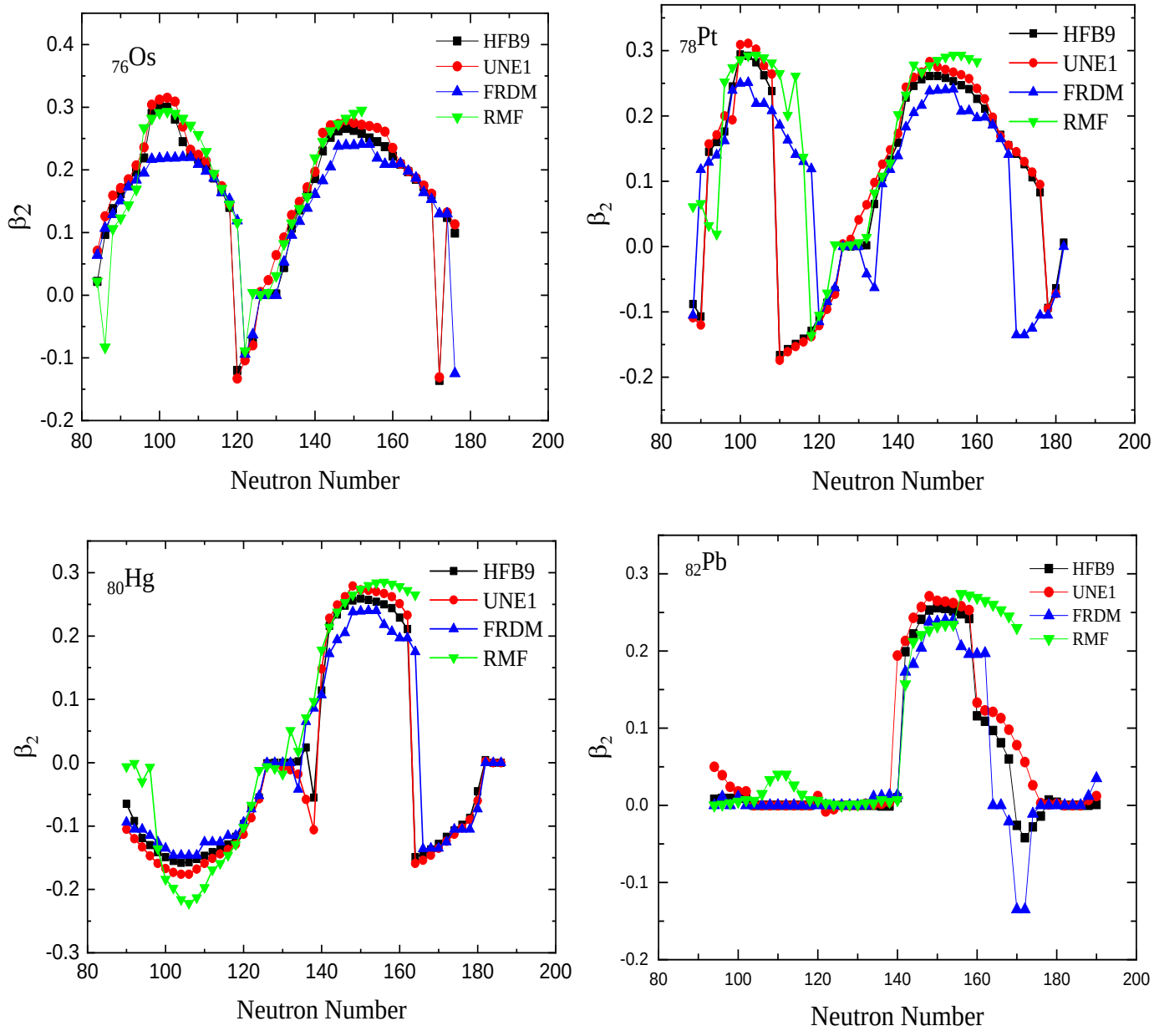

Fig. (4): The same as Fig. (1) for quadrupole deformation β_2

3.5 Pairing Gap

Pairing is very important in open-shell nuclei, especially in deformed nuclei. In Fig.(5) the HFB results of neutron pairing gap for Os, Pt, Hg, and Pb isotopes are presented using HFB9 and UNE1 Skyrme type interaction, in comparison with the FRDM Lipkin-Nogami pairing gap [30]. Our result with HFB9 functional agrees well with FRDM Lipkin-Nogami pairing gap except at the magic neutron number N=126 for all the investigated nuclei and N=184 for Hg and Pb. In the HFB approximation, the pairing correlation has vanished in the case of magic nuclei, i.e. the pairing field becomes zero, this corresponds to the previously reported results [31] for $_{42}$Mo and $_{44}$Ru isotopes.

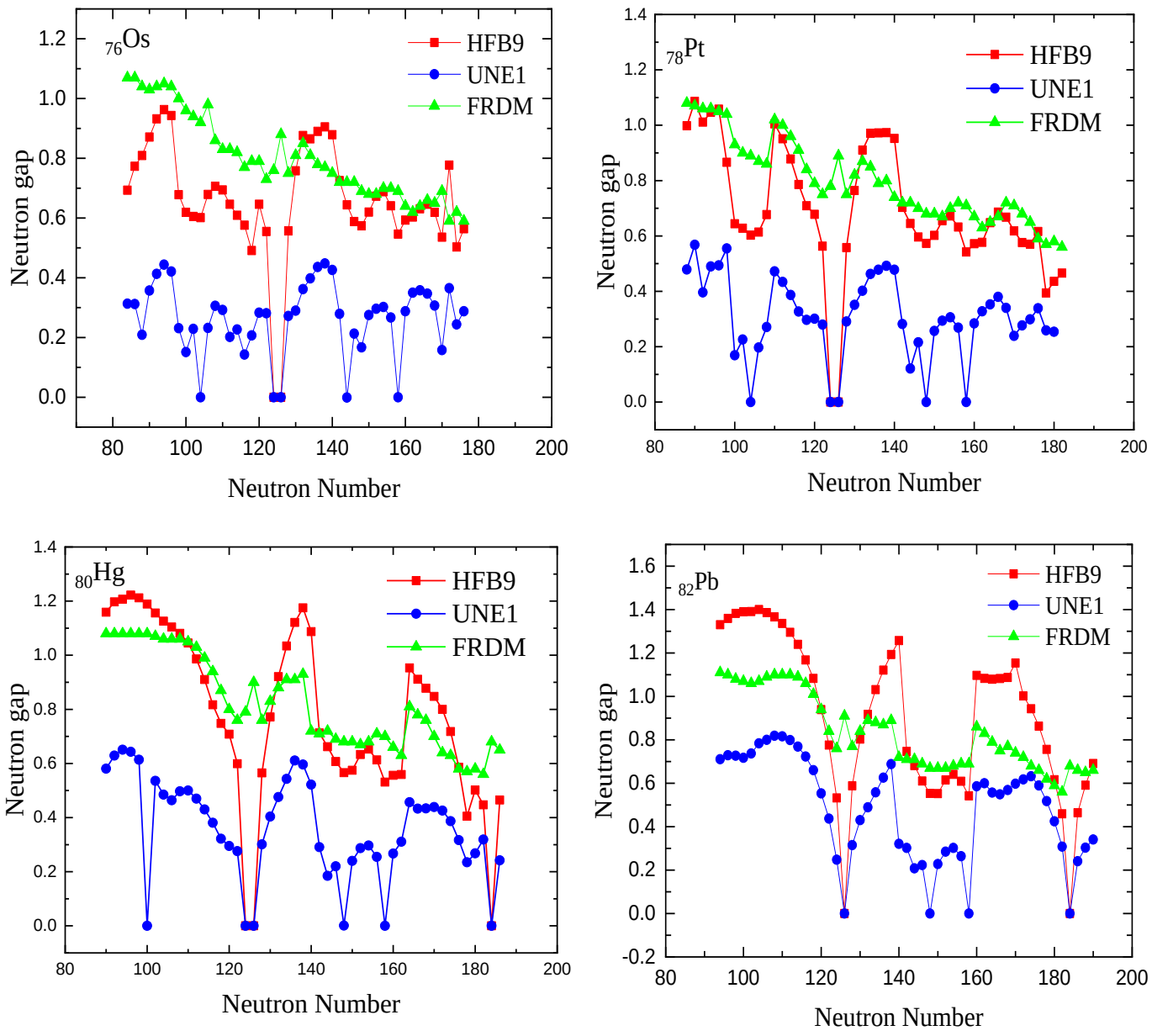

Fig. (5): The same as Fig. (1) for neutron pairing gap

3.6 Charge Radius

The pesent HFB calculations of charge radius by two-Skyrme interaction (HFB9 and UNE1) are presented in Fig. (6), and compared with the values of the RMF [29] and with the experimental data [32]. A good agreement is found between theoretical and experimental data except at the region between N=100 to 110 of *Pt* isotopes, a small difference can be seen due to the effect of the deformation (the shape is changed from prolate to oblate in this region). The charge radius for nuclei increases with increasing the neutron number except at magic number it decreases by the effect of the closed shell.

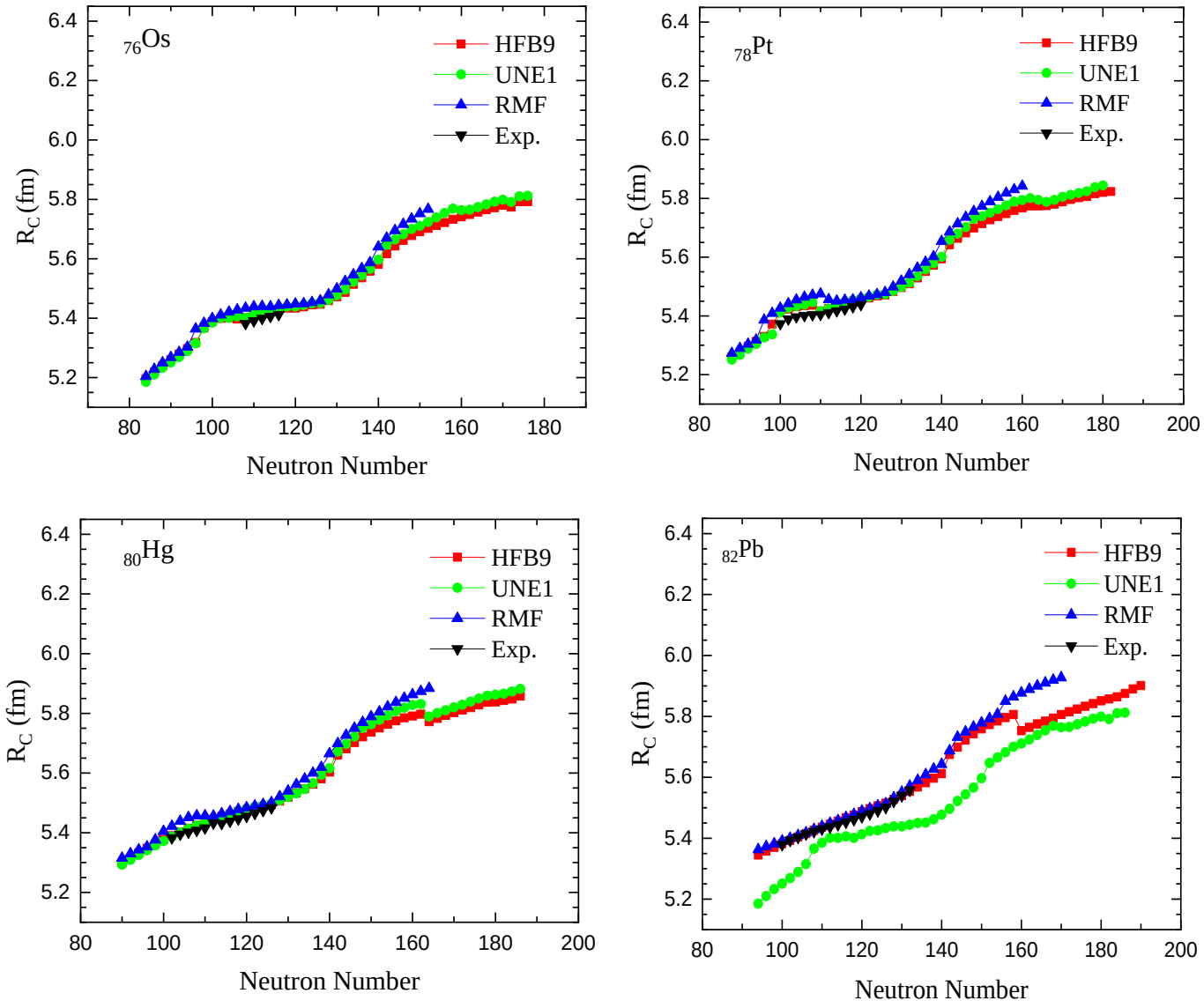

Fig. (6): Same as Fig.1 for Proton charge radius

3.7 Energy Surface Curves

The energy surface curves as a function of quadrupole deformation (β_2) for isotones of Os, Pt, Hg, and Pb nuclei (from N=108 to 118) are depicted in Fig. (7). The calculation was done using the code HFBTHO version 3.00 [16] based on two Skyrme type interaction (HFB9 and UNE1). When the number of protons is increased, the shape is transformed from prolate to oblate for nuclei of N=108, N=110, and N=112, whereas N=114 represents the turning point from prolate to oblate shape for Os nucleus which appears with two minima approximately at the same energy, but nuclei with N=116 and N=118 are transformed from oblate to spherical shape with increasing proton number. The Pt isotopes are started with two minima at the same energy between prolate and oblate shapes then gradually transformed to oblate shape at N=112-118. The shape of the investigated Hg isotopes is oblate. The Pb isotopes start with an oblate shape at N=108 end to be spherical at N≥110.

4. CONCLUSIONS

In this paper, ground state properties of the even-even isotopic chain of Os, Pt, Hg, and Pb have been studied using the HFB calculations with two types of the Skyrme force (HFB9 and UNE1). The present result of BE/A fit well with the experimental data, the maximum value BE/A is for Os nucleus at N=106 which equals 8.154 MeV, while for Pb equals 7.89 MeV at N=126. A sudden drop in the S_{2n} occurred at N=126 for all nuclei, and at N=184 for Hg and Pb nuclei. The charge radius also reproduces the experimental data well except at $N = 100 - 110$ in Pt nuclei, where some differences appear due to the effect of shape transition from prolate to oblate. The proposed energy surface curves of Os, Pt, Hg nuclei illustrate the shape transformation from prolate to oblate shape and the increase in the spherical shape of Pb with N.

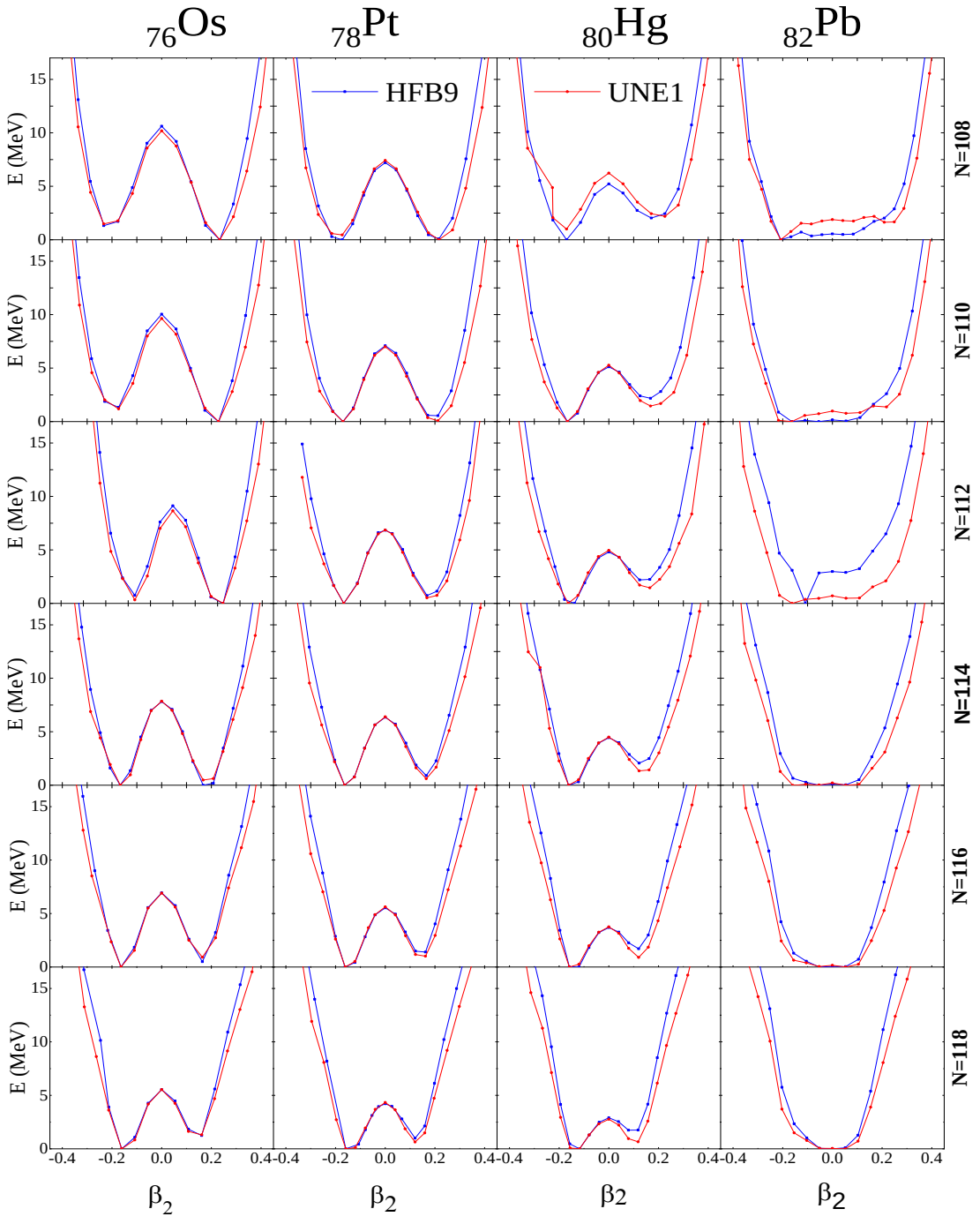

Fig. (7): The energy surface curves, for Os, Pt, Hg, Pb nuclei from $N = 108$ to $N = 118$

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