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Hexadecapole Deformations for Nonaxial Shapes*

ABSTRACT

Axial and nonaxial hexadecapole and quadrupole deformations of Nilsson potential are investigated. Potential energies, quadrupole and hexadecapole electric moments are studied for actinide and transfermium nuclei and compared to old theoretical values.

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1. INTRODUCTION

It is known that the fissioning nuclei acquire the nonaxial shapes along the path to fission [1,2]. Up to now, only the nonaxial quadrupole component of the deformed shape has been investigated [3] and only this component has been taken into account in the study of properties of nuclei.

Recently more general parametrization of the quadrupole and hexadecapole deformations for nonaxial shapes was introduced [4]. The aim of present paper is to examine the new parametrization. In particular we investigate the energy of deformation and quadrupole and hexadecapole electric moments of nuclei. We study the influence of the new hexadecapole degrees of freedom (γ_4, δ_4) on the smooth part (liquid drop) as well as on the total energy.

At the end we compare our results to those obtained with old parametrization [5].

2. HEXADECAPOLE DEFORMATIONS FOR NONAXIAL SHAPES

An expansion of the nuclear radius $R(\theta,\phi)$ in spherical harmonics:

$$R(\theta,\phi) = R\left[1 + \sum_{\lambda\mu} a_{\lambda\mu} Y_{\lambda\mu}(\theta,\phi)\right] , \tag{1}$$

is rotationaly invariant. Here $a_{\lambda\mu}$ are components of the spherical tensor of rank λ. The parametrs $a_{\lambda\mu}$ are not uniquely determined by the surface. They also depend on the designation of the intrinsic axes: x,y,z and on the choice of positive direction for them. There exist 24 different possibilities for designations and directions of the axes. Each of them may be obtained from another by superposition of three basic rotations $R_i (i = 1,2,3)$ ($R_1 = R(\pi,\pi,0)$, $R_2 = R(0,0,\pi/2)$, $R_3 = R(0,\pi/2,\pi/2)$), where the arguments are the Euler angles. The rules of transformations of $a_{2\mu}$ and $a_{4\mu}$ under R_i are rather complicated.

Defining the quadrupole shapes as the quadrupole part ($\lambda = 2$) of the surface (1) and restricting ourselves to the surfaces which are symmetric with respect to reflections in three main planes of the system we obtain:

$$\begin{aligned} a_{\lambda\mu} &= a_{\lambda-\mu} \,, \\ a_{\lambda\mu} &= 0 \qquad \text{for odd } \mu \,, \\ a_{\lambda\mu} &= 0 \qquad \text{for odd } \lambda \,. \end{aligned} \tag{2}$$

In this case the quadrupole part has two free parameters: a_{20} and a_{22}. For the quadrupole ($\lambda = 2$) and hexadecapole ($\lambda = 4$) shapes eq. (1) reads:

$$\begin{aligned} R(\theta,\phi) = \; & R_0 \{1 + [a_{20}Y_{20} + a_{22}(Y_{22} + Y_{2-2})] \\ & + [a_{40}Y_{40} + a_{42}(Y_{42} + Y_{4-2}) + a_{44}(Y_{44} + Y_{4-4})]\} \,. \end{aligned} \tag{3}$$

As it is seen the quadrupole and hexadecapole part has a five free parameters. It is convenient to express $a_{2\mu}$ and $a_{4\mu}$ in terms of parameters which have simpler transformation rules. For the quadrupole deformation one usually introduces the parameters β and γ [2]:

$$a_{20} = \beta\cos\gamma\,, \qquad \sqrt{2}a_{22} = \beta\sin\gamma\,, \tag{4}$$

where $\beta \geq 0$ and $-\pi \leq \gamma \leq \pi$.

The relations (4) may be interpreted as the transformation from the rectangular a_{20}, a_{22} to the polar β, γ coordinates. The parameter β is an invariant of all possible rotations of the coordinate system, in particular of rotations R_i, and thus is uniquely determined by the surface. The parameter γ transforms in the following way under the rotations R_i:

$$R_1:\ \gamma \rightarrow \gamma\,; \quad R_2:\ \gamma \rightarrow -\gamma\,; \quad R_3:\ \gamma \rightarrow \gamma - \frac{2\pi}{3}\,. \tag{5}$$

Due to this, to get uniquness in the determination of γ by the surface, it is sufficient to restrict the variation if γ to the region $0 \leq \gamma \leq \frac{\pi}{3}$.

The hexadecapole part of the surface has been parametrized in a way similar to the quadrupole part. We define the quantities:

$$b_4 = \sqrt{\frac{5}{12}}a_{40} - \sqrt{\frac{7}{6}}a_{44}\,, \qquad c_4 = -\sqrt{2}a_{42}\,, \tag{6}$$

which have the same transformation rules under R_i as coordinates a_{20} and a_{22}. Due to this, we parametrize them in the same way, i.e.

$$b_4 = \rho_4\cos\gamma_4\,, \qquad c_4 = \rho_4\sin\gamma_4\,, \tag{7}$$

where $\rho_4 = \beta_4\sin\delta_4$ and it is invariant under R_i. The γ_4 $(-\pi \leq \gamma_4 \leq \pi)$ has the same transformation rules as γ (see eq.5).

One can prove that the quantity

$$a_4 = \sqrt{\frac{7}{12}}a_{40} + \sqrt{\frac{5}{6}}a_{44} \tag{8}$$

is invariant under R_i and

$$a_4^2 + b_4^2 + c_4^2 \equiv \beta_4^2\,. \tag{9}$$

Eqs. (6-8) define a new set of spherical coordinates $(\beta_4, \delta_4, \gamma_4)$ of a point specified by the rectangular coordinates a_4, b_4 and c_4, i.e.

$$\begin{aligned} a_4 &= \beta_4\cos\delta_4\,, \\ b_4 &= \beta_4\sin\delta_4\cos\gamma_4\,, \\ c_4 &= \beta_4\sin\delta_4\sin\gamma_4\,. \end{aligned} \tag{10}$$

According to the transformation rules (5), it is sufficient to restrict the region of variation γ_4 to $0 < \gamma_4 \leq \frac{\pi}{3}$ in order to get one-to-one correspondence between a surface and the parameters $(\beta_4, \delta_4, \gamma_4)$ describing it. The deformation parameter β_4 is a close analogue of β of the quadrupole deformation and the nonaxiality parameters δ_4 and γ_4 are rather natural generalization of nonaxiality quadrupole deformation γ. More details on the presented parametrization are given in ref. [4].

3. METHOD OF CALCULATIONS

According to the Strutinsky prescription the deformation energy was composed of a shell and a pairing correction parts and the smooth average energy was identified with the energy of the liquid drop model of Myers and Swiatecki [6].

To generate the single-particle spectrum, we used the Nilsson potential. An application of eqs. (3,4,10) to the Nilsson potential leads to the formulae [4]:

$$\begin{aligned} V(\varepsilon, \gamma, \varepsilon_4, \delta_4, \gamma_4) \;=\; & \frac{1}{2}\hbar\omega_0\rho^2 \Bigg\{ 1 - \frac{2}{3}\varepsilon\sqrt{\frac{4\pi}{5}}\left[\cos\gamma\, Y_{20} + \frac{1}{\sqrt{2}}\sin\gamma\,(Y_{22}+Y_{2-2})\right] \\ & + 2\varepsilon_4\sqrt{\frac{4\pi}{5}}\Bigg[\left(\sqrt{\frac{7}{12}}\cos\delta_4 + \sqrt{\frac{5}{12}}\sin\delta_4\cos\gamma_4\right) Y_{40} \\ & - \frac{1}{\sqrt{2}}\sin\delta_4\sin\gamma_4 (Y_{42}+Y_{4-2}) \\ & + \left(\sqrt{\frac{5}{24}}\cos\delta_4 - \sqrt{\frac{7}{24}}\sin\delta_4\cos\gamma_4\right)(Y_{44}+Y_{4-4})\Bigg]\Bigg\}, \end{aligned} \tag{11}$$

where the radius ρ and the angles in the arguments of $Y_{\lambda\mu}$ are given in the stretched coordinate system. Parameters κ and μ of the Nilsson single-particle potential are chosen to be ones called "A=242" parameters [5]. The pairing correlations were included in the BCS model and the pairing strength constant G was equal to that given in [5]. All the calculations were done for even-even nuclei within the region $92 \leq Z \leq 110$ and $140 \leq N \leq 170$.

4. RESULTS

Results obtained in the present study are shown in successive figures in which we plot different characteristics of nuclei. Among them there are energy surfaces $E(\overline{\beta})$ as functions of special sets of deformation parameters, minima of the potential energy and nuclear multipole moments. The important is the deformation energy defined as $E_{def} = E_{min} - E_0$, where E_{min} is the minimum value of $E(\overline{\beta})$ and $E_0 = E(0)$.

In order to obtain these plots for the considered nuclei we studied main effects of new degrees of freedom on the total energy. Fixing some of deformation parameters we looked at the behaviour of $E(\overline{\beta})$. Figure 1 shows the effect of (δ_4, γ_4) on the energy $E(\varepsilon^0, \varepsilon_4^0, \gamma_2^0; \delta_4, \gamma_4)$ for ^{252}Fm, where ε^0, ε_4^0 and γ_2^0 correspond to the approximate minimum of $E(\overline{\beta})$ in the case of $\gamma_4 = 0$, $\delta_4 = \delta_4^0 \approx 40.2^0$ (the old Nilsson potential). From figures like this one can see that the new degree of freedom γ_4, is close to zero in the considered region of nuclei. We have to say here that the axial asymmetry γ_2 is also equal to zero in

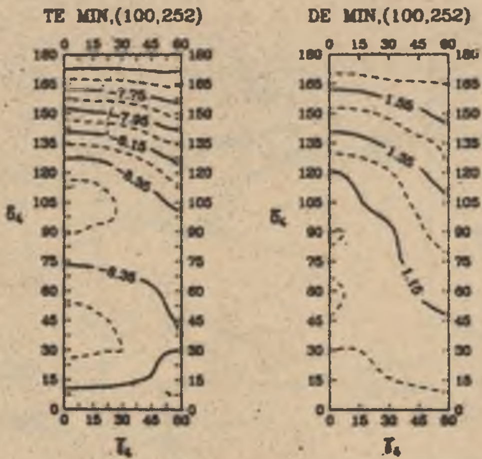


Figure 1 : The energy surface $E(\delta_4, \gamma_4)$ *in the region of the first minimum for* ^{252}Fm. *The left part gives total energy and the right part liquid drop model contribution.*

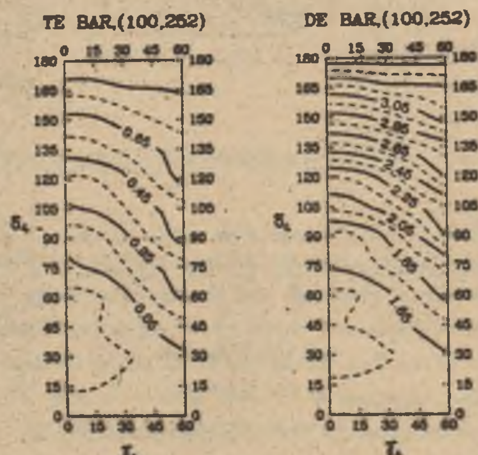


Figure 2 : The same as Fig.1. but for the barrier region.

the minimum of the potential energy E_{min} [1,2]. On the right hand side of figure 1 the macroscopic part of the energy E for the same situation is plotted. We see from it that the nonzero contribution, which "deforms" the nucleus in direction of δ_4 degree of freedom, comes from the microscopic part δE_{shell}. The similar situation is registered in Fig.2. for the same nucleus (^{252}Fm) but at the deformation point corresponding to the vincinity of the first barrier ($\varepsilon^0 = 0.4, \varepsilon_4^0 = 0.0, \delta_4 = \delta_4^0$ and $\gamma_2^0 = 0$). As it was shown in many papers [2] the deformation γ_2 is nonzero in the barrier region and lowers the barrier energy on 1

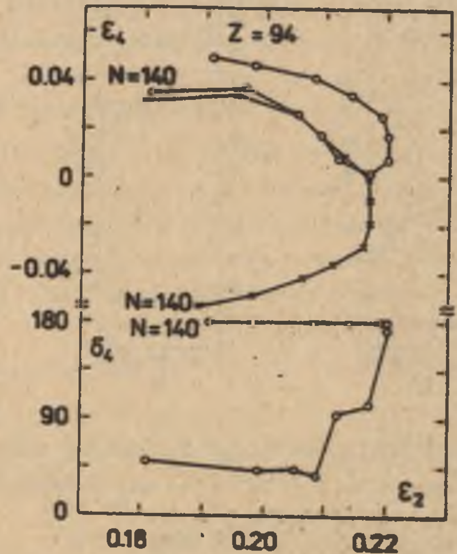


Figure 3 : Minima of potential energy surface for plutonium isotopes (circles). Old results are depicted by crosses.

to 2 MeV for the considered nuclei. Because we look only at the differences between results for old ($\delta_4 = \delta_4^0$) and new potentials and the absolute energy is not important here, then the choice of $\gamma_2 = 0$ dose not matter in our estimates. Looking at Fig.2 we can say that in the region of the first barrier the effect of the hexadecapole γ_4 degree of freedom is like in the first minimum of E, i.e γ_4 is close to zero. The corresponding macroscopic contribution to the potential energy E is shown in Fig.2b.

On the basis of our calculations we can draw the following conclusion: The γ_4 contribution to the potential energy $E(\overline{\beta})$ is negligible and even equal to zero in the case of minimum. At the first fission barrier this statement may not be correct and the tendency of decreasing the barrier on few tens of MeV for nonzero γ_4 is likely.

From Fig.1a one can see that the minimum of E appears at $\delta_4 \approx 100^0$ and $\gamma_4 = 0$. However in the barrier region (Fig.2.) the minimum with respect to δ_4 is close to its Nilsson value $\delta_4 \doteq \delta_4^0 \approx 40.2^0$. The same figure shows the minimum of the macroscopic part of E, for which δ_4 equals to δ_4^0 value as well.

After these introductory tests we can state that in the vicinity of the minimum point one has $\gamma_2 = 0$ and $\gamma_4 = 0$ and the only important deformation parameters are $\varepsilon, \varepsilon_4$ and δ_4.

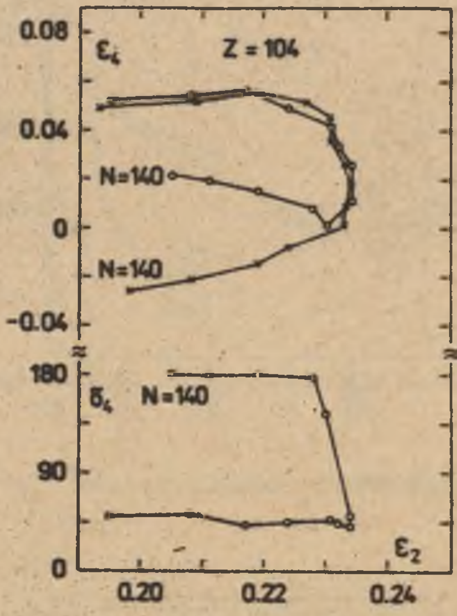


Figure 4 : The same as Fig.3. but for rutherfordium isotopes.

The minimization of the potential energy with respect to these deformation parameters was performed exactly. This minimization was carried out by calculating the $E(\varepsilon, \varepsilon_4, \delta_4)$ in the following points:

$$\begin{aligned} \varepsilon &= 0.15\ (0.05)\ 0.35\,, \\ \varepsilon_4 &= 0\ (0.04)\ 0.12\,, \\ \delta_4 &= 0^0\ (45^0)\ 180^0\,. \end{aligned}$$

The results of the minimization procedure for each nuclei are minima shown in Fig.3 and 4 for the case of isotopes Z=94 and Z=104 and N ranging from 140 to 162. In these figures crosses correspond to the old version of Nilsson parametrization with ε and ε_4 only (negative values of ε_4 are allowed). The new results are represented by open circles. We see that for $\varepsilon_4 > 0$ new results nearly coincide with old ones. Parameters δ_4 minimizing the energy are shown in the lower parts of Fig.3 and 4. Their values are embraced by limits 45 and 180 degrees. The correspondence between the new and the old $\varepsilon_4^0 < 0$ is not the case here because the new parametrization allows only positive values for ε_4. The δ_4 parameter takes care about the sign of $Y_{4\mu}$ terms as well as its value in the single particle potential.

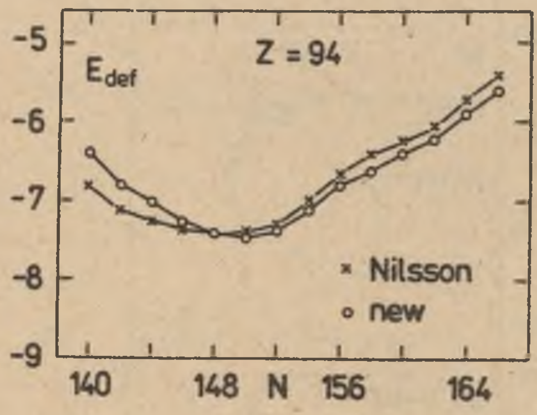


Figure 5 : Deformation energies (in MeV*) for plutonium isotopes.*

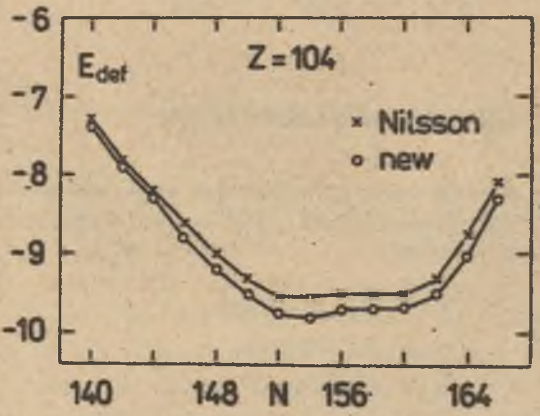


Figure 6 : Deformation energies (in MeV*) for rutherfordium isotopes.*

The new and the old deformation energies E_{def} are shown in Figures 5 and 6 correspondingly. Except of cases of light nuclei (Z=94, N < 148) one sees deepest first minima in the case of new parametrization (circles) as compared to the old ones (crosses). The fact that the potential energy minima of the light nuclei are higher in new parametrization of the single particle potential means that in this case the new degrees of freedom (i.e. γ_4 or/and δ_4) become important and they have to be taken into account accurately in the analysis of the deformation energy.

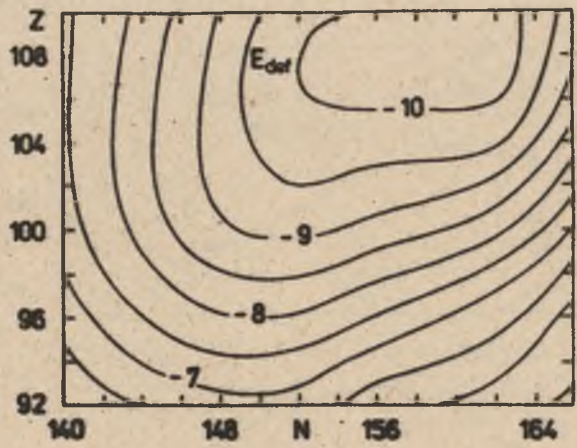


Figure 7 : Deformation energies for the whole actinide and transfermium region (MeV).

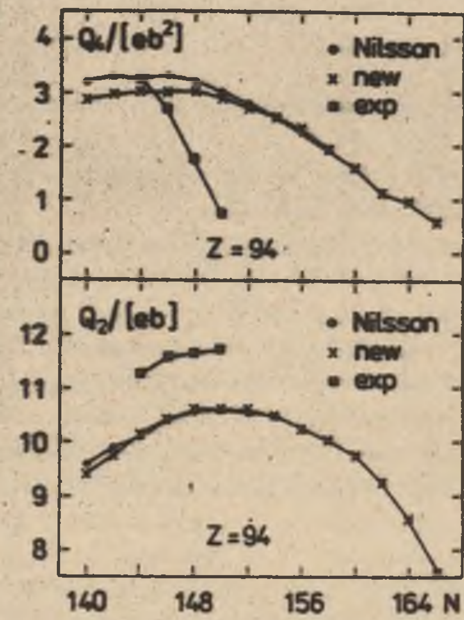


Figure 8 : Electric quadrupole (lower part) and hexadecapole (upper part) moments for plutonium isotopes.

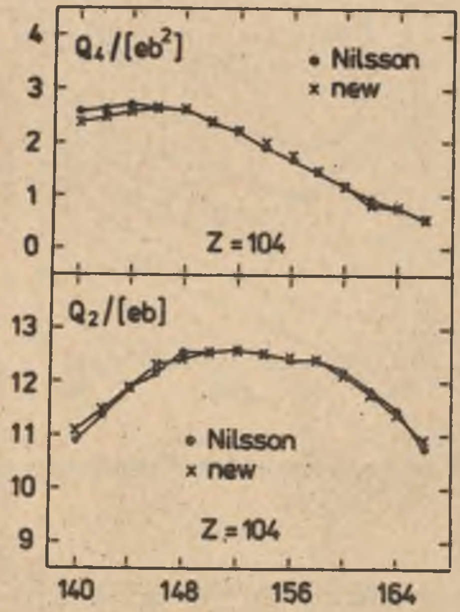


Figure : 9 The same as Fig.8. for rutherfordium isotopes.

For the sake of completeness we show the new deformation energies E_{def} of nuclei from the actinide-transfermium region in Fig.7.

It is a good practice to compare not the deformation parameters (which differs one of another e.g. ε_4^{old} and ε_4^{new} from definition) but more physical nuclear shape characteristics as eg. electric multipole moments of the ground states of nuclei. Figures 8 and 9 show quadrupole and hexadecapole moments respectivelly for the selected Z=94 and Z=104 isotopes. The comparison with the old values is given on the same figures. One observes a small differences in recent quadrupole and hexadecapole moments as compared to the former ones. These differences are however very systematic. From these results we observe that both ways of parametrization of the single particle potential generate nearly the same sequence of the equilibrium nuclear shapes in the region of actinide and transfermium nuclei. For completeness, we present again both quadrupole Q_2 and hexadecapole Q_4 moments for the whole actinide-transfermium region of nuclei in the next Fig.10 and 11.

The general conclusion from presented calculations is the following. Both parametrizations the old and the new one give approximately the same results for the deformation energies (or masses which are directly connected to them) and to the shapes of even-even nuclei (quadrupole and hexadecapole electric moments) in their ground states. However,

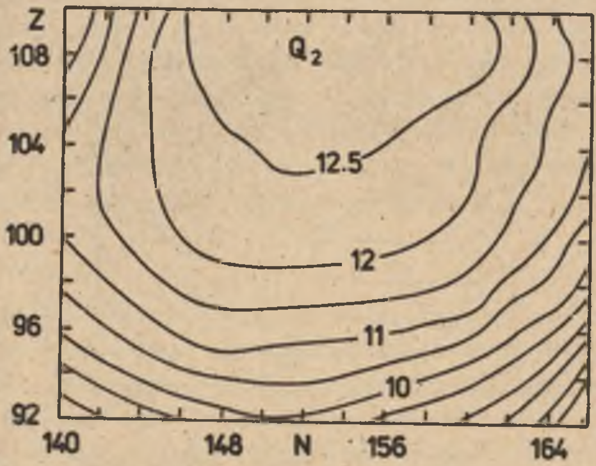


Figure : 10 Quadrupole electric nuclear moments (in eb units) for actinide and transfermium nuclei.

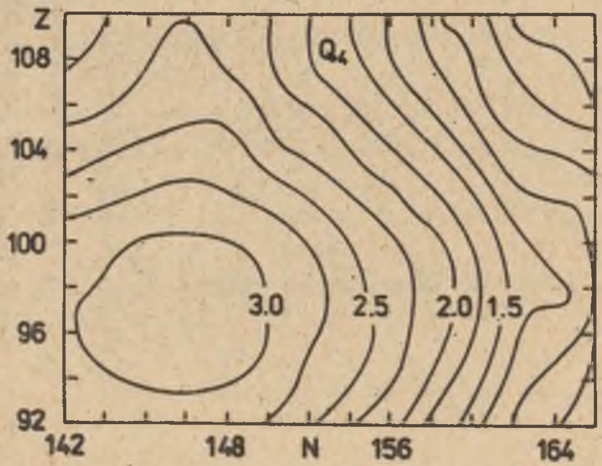
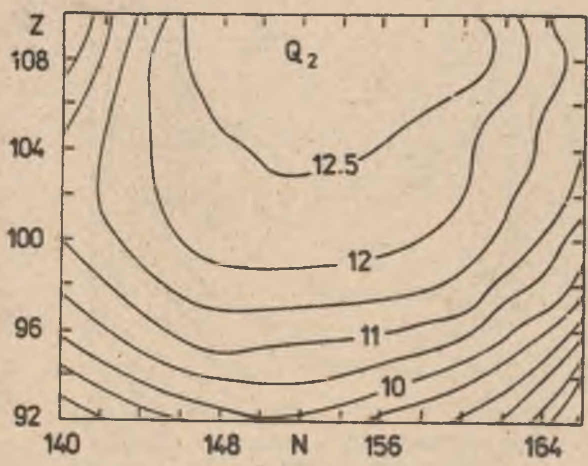


Figure : 11 Hexadecapole electric nuclear moments (in eb^2 units) for actinide and transfermium nuclei.

the present parametrization of the hexadecapole part of the Nilsson potential has a greate advantage which we want to point here. As it is known from early papers on inclusion of *partial* axially asymmetric hexadecapole terms into single particle potential [7], the following problem of discontinuity of the potential energy arises. In the case of zero ϵ_4 degree of freedom, starting at a prolate ($\gamma = 0$) shape and passing the γ-region on the



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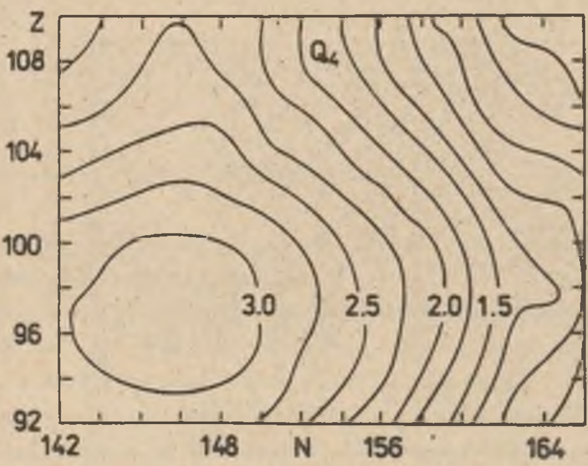

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