Nuclear Tetrahedral Symmetry: Possibly Present throughout the Periodic Table

J. Dudek,[1] A. Góźdź,[1,2] N. Schunck,[1] and M. Miśkiewicz[2]

[1]Institut de Recherches Subatomiques, IN_2P_3-CNRS/Université Louis Pasteur, F-67037 Strasbourg Cedex 2, France

[2]Katedra Fizyki Teoretycznej, Uniwersytet Marii Curie-Skłodowskiej, PL-20031 Lublin, Poland

(Received 16 November 2001; published 11 June 2002)

More than half a century after the fundamental, spherical shell structure in nuclei had been established, theoretical predictions indicated that the shell gaps comparable or even stronger than those at spherical shapes may exist. Group-theoretical analysis supported by realistic mean-field calculations indicate that the corresponding nuclei are characterized by the T_d^D ("double-tetrahedral") symmetry group. Strong shell-gap structure is enhanced by the existence of the four-dimensional irreducible representations of T_d^D; it can be seen as a *geometrical* effect that does not depend on a particular realization of the mean field. Possibilities of discovering the T_d^D symmetry in experiment are discussed.

DOI: 10.1103/PhysRevLett.88.252502 PACS numbers: 21.10.–k, 21.60.Fw

A possibility that atomic nuclei exhibit tetrahedral symmetry—in quantum physics, it is discussed mainly as a property of certain molecules, metal clusters, or fullerines—has a definite interest for all the related domains of physics. While in the above-mentioned objects the underlying interactions are electromagnetic, the nuclear tetrahedra (pyramidlike nuclei with "rounded edges and corners") are expected to be stabilized primarily by the strong interactions. Within the nuclear mean-field theories, a convenient framework for discussing this phenomenon is provided by the spontaneous symmetry breaking mechanism. It is analogous to the one associated with the existence in nature of numerous deformed nuclei, e.g., ellipsoidal ones. According to such a mechanism, all nuclei are governed by rotationally invariant elementary nucleon-nucleon interactions, yet, for some specific low energy configurations their total energy becomes lower when the corresponding mean fields take nonspherical shapes. The mathematically different but physically analogous mechanism of spontaneous symmetry breaking is related to a discrete symmetry: the inversion. The underlying elementary interactions, although inversion invariant, do not guarantee that all the resulting low energy nuclear configurations lead to stable inversion-invariant shapes, and there is growing experimental evidence of the existence in nature of the octupole deformations, usually pear-shape type, cf., e.g., Ref. [1]. It turns out that the tetrahedral nuclei do break spontaneously both the spherical symmetry and the symmetry by inversion (see below).

In the past, there have been a number of studies published that address the question of the nonaxially symmetric octupole deformations. Using the Strutinsky method and considering a space composed of 2 (quadrupole) + 4 (octupole) + 5 (hexadehapole) + 6 (multipolarity 5) = 17 deformations, the authors of Ref. [2] have suggested that an ensemble of isomeric states of tetrahedral symmetry may exist in the region of light radium nuclei pointing to the importance of the thus far neglected α_{32} deformation. Using the Hartree-Fock approach in their symmetry-unconstrained variant, Takami *et al.*, Ref. [3], obtain in some light $Z = N$ nuclei an α_{32} instability. In Ref. [4] this and other exotic octupole deformations were studied in the ^{32}S nucleus while, in [5], a similar hypothesis has been advanced theoretically for a group of nuclei around $A \sim 70$.

The experimental verification of the discussed phenomenon does not exist thus far. We believe that the mechanism related to α_{32} deformations is just a "visible part of an iceberg": a phenomenon whose physical consequences are much richer than what has been discussed thus far. First of all, the corresponding T_d^D symmetry is nearly unique: Only T_d^D and the octahedral O_h^D point-group symmetries produce in deformed nuclei the nucleonic level degeneracies higher that 2. More precisely, some states must carry twofold and some fourfold degeneracies. The corresponding nuclear Hamiltonians are invariant with respect to the very large number of 48 different symmetry elements (in the case of the O_h^D, this number would be 96). The depth of the nuclear mean-field potential and the number of its bound states depend only very weakly on deformation: The fourfold degeneracy mechanism at nonzero α_{32} implies larger interspacing and helps in producing very large shell gaps that are comparable to or larger than at least some of the gaps at spherical shapes. Moreover, since the argument is geometrical in nature, the predicted strong shell gaps propagate all over the periodic table *in a repetitive fashion* independently of a particular realization of the mean-field approach. This mechanism is far from being an exoticity of a few nuclei here and there. Its presence is predicted in dozens if not hundreds of nuclei. Among unique quantum features, the prediction should be noted that some nucleonic orbitals should have the expectation value of parity *close to zero*—nearly complete disappearance of the quantum characteristic that is otherwise dominating in the microworld of nuclear interactions. Another unique element foreseen concerns the collective (especially low spin) rotation of the quantum tetrahedra:

The corresponding predicted structures of rotational bands will be very different for even (T_d group) and odd (T_d^D group) nuclei since both the number of the irreducible representations (irreps) associated with these groups and the dimensions of the corresponding irreps are very different as well (see e.g., Refs. [6,7]).

The mathematical background of our considerations is well known and can be summarized in a few lines. Consider a nuclear deformed mean-field Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}(\vec{r}, \vec{p}, \vec{s}; \hat{\alpha})$, where $\hat{\alpha}$ represents the ensemble of all the deformations $\{\alpha_{\lambda,\mu}\}$ and a group of symmetry $\mathcal{G}$ with the symmetry operators $\{\hat{\mathcal{O}}_1, \hat{\mathcal{O}}_2, \ldots, \hat{\mathcal{O}}_f\} \Leftrightarrow \mathcal{G}$, so that $[\hat{\mathcal{H}}, \hat{\mathcal{O}}_k] = 0$, for $k = 1, 2, \ldots, f$. Suppose that the group in question has irreducible representations $\{\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_r\}$ with the following dimensions, respectively: $\{d_1, d_2, \ldots, d_r\}$. Then the eigenvalues ε_ν of the problem $\hat{\mathcal{H}}\Psi_\nu = \varepsilon_\nu \Psi_\nu$, $\forall \nu$, appear in multiplets: d_1-fold degenerate, d_2-fold degenerate, ... d_r-fold degenerate. Since the nuclear mean-field Hamiltonians do not depend explicitly on time, it follows that each eigenenergy must be at least twice degenerate (Kramers theorem). In terms of irreducible representations of G, this property manifests itself for the deformed nuclei through the presence of two-dimensional irreducible representations or pairs of *conjugated* one-dimensional ones [7].

The point-group symmetries of the nuclear mean-field Hamiltonian can be very often directly connected to the corresponding deformation parameters: If $\mathcal{R}(\vartheta, \varphi)$ denotes the nuclear surface, expanding it into a series of spherical harmonics $Y_{\lambda\mu}(\vartheta, \varphi)$ with the numerical coefficients $\alpha_{\lambda\mu}$ (deformation parameters) provides a natural classification scheme. Indeed, setting all $\alpha_{\lambda\mu}$ to zero, one obtains a sphere; posing $\alpha_{\lambda=2,\mu=\pm 2,0} \neq 0$ gives the most important example of the "ellipsoidal" D_{2h}^D symmetry, by setting $\alpha_{\lambda=2,3,\mu=0} \neq 0$ we obtain an example of the octupole-axial (C_∞^D) symmetry; many other combinations of the nonzero deformation parameters may lead to more "realistic" realizations of the symmetry groups in nuclei. It can be shown using elementary properties of the spherical harmonics that in the case of the pure octupole deformations the following relations between the nuclear shape and the double point-group symmetries of the fermion Hamiltonians hold: (i) Deformation α_{30} implies the C_∞^D-symmetry group with infinitely many one-dimensional irreps, characterized by the so-called K-quantum numbers; (ii) deformation α_{31} implies the C_{2v}^D symmetry that generates only one two-dimensional irrep; (iii) deformation α_{32} implies the T_d^D symmetry of two two-dimensional and one four-dimensional irreps; (iv) deformation α_{33} implies the D_{3h}^D symmetry, and generates three two-dimensional irreps.

However, the link between the above scheme and the realistic calculations is not always direct—especially when the point groups rich in structure are concerned. Any isomeric minimum is, within the mean-field theory, associated with the presence of energy gaps in the corresponding single particle spectra—usually the larger the gap, the more stable the implied equilibrium deformation.

Within a given symmetry (given irrep) the noncrossing rule implies that the single-particle energies tend towards an equidistant distribution when deformation increases. If a given group admits only one irreducible representation, each level can carry at most two nucleons. When the corresponding irreducible representations have higher dimensionality, e.g., four (the corresponding curves are marked with the double Nilsson labels $[Nn_z\Lambda]\Omega$ in Fig. 1), more particles may reside on one single energy level, leading, in some other place of the energy scale, to effectively diminishing the number of levels and possibly increasing the shell gaps. The features discussed above are followed very

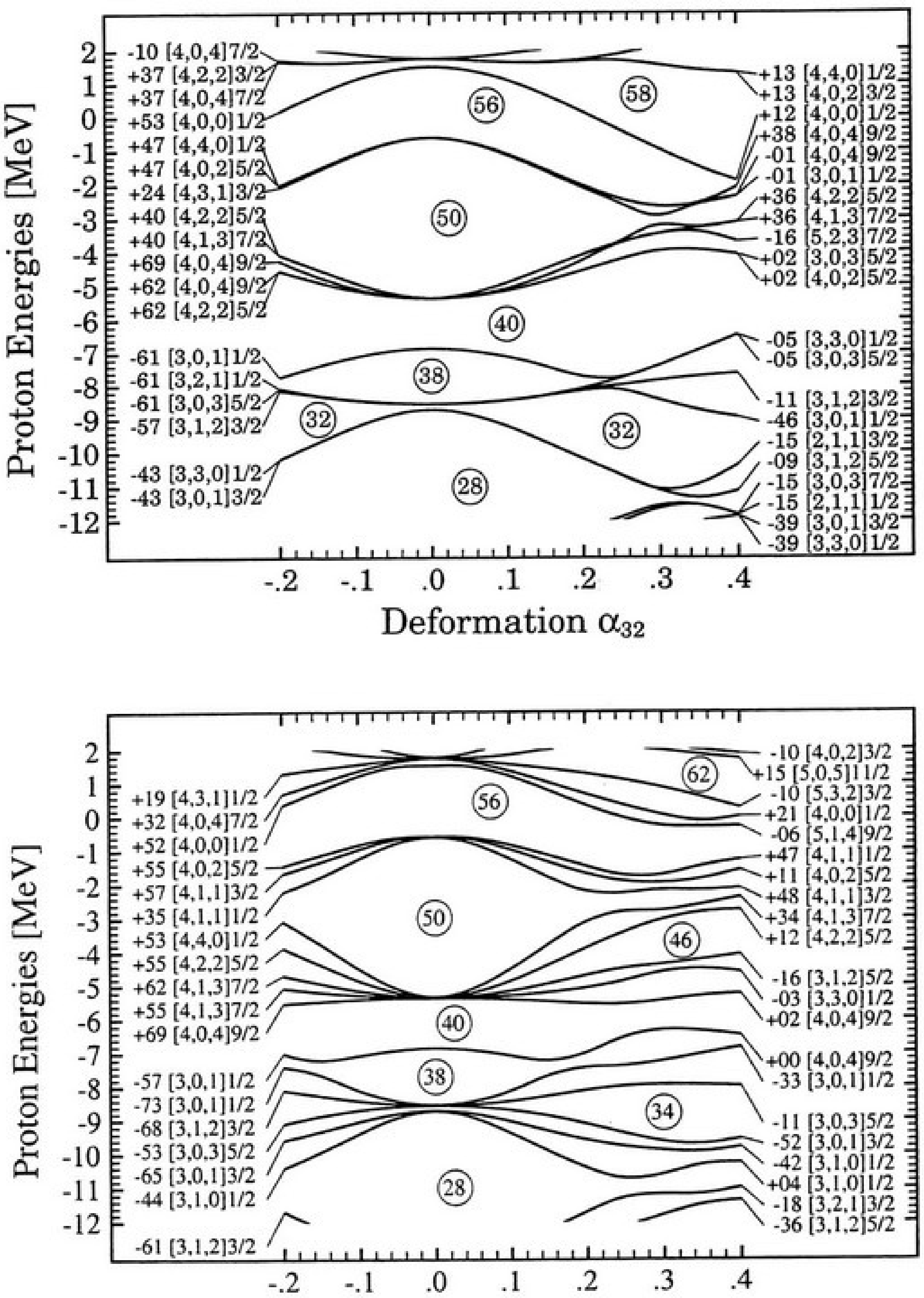

FIG. 1. Results of the realistic calculation of the proton single-particle energies in function of the α_{32} deformation corresponding to the T_d^D symmetry (top) compared to the analogous dependence in function of α_{31} (bottom, C_{2v}^D group). The numbers in front of the Nilsson labels give the expectation values of parity at the extremes of the deformation axes. None of the Nilsson quantum numbers is a good quantum number at tetrahedral deformations: Each label gives the full set of quantum numbers of the strongest basis state. (Results were obtained using a standard deformed Woods-Saxon potential.)

closely by the realistic calculation results of Fig. 1 where, in addition, the extremes on the horizontal axes have been chosen in such a way that, by comparing the labels on the left- and on the right-hand side of the figure, one can read how quickly the parity mixing sets in when the deformation increases (the curves are symmetric with respect to 0). The parity mixing at $|\alpha_{32}| \sim 0.15$ is so strong that the typical calculated parity expectation values are ($\sim \pm 0.5$).

Several observations deserve emphasizing. First of all, there is a qualitative difference in the deformation dependence in the two studied cases as predicted by the considerations based on the point-group symmetries presented above: At $|\alpha_{31}| > 0.15$ the level distribution can already be considered "nearly uniform" except for a relatively small gap at $Z = 56$ that *decreases* slowly with increasing deformation. In contrast, the spectrum in function of α_{32} reveals strongly *increasing* gaps at $Z = 32$, $\Delta E > 2$ MeV, at $Z = 40$ with $\Delta E \sim 3$ MeV, and a huge gap at $Z \rightarrow 56, 58$; the latter can be seen as a $\sim$4 MeV separation in the spectrum "cut across" by a single, usual (i.e., twice degenerate) orbital. These *deformed* gap sizes are comparable to, or larger than, the strongest spherical gaps at $Z = 20$, 28, 40, or even 50, which are known in the medium heavy nuclei; neutron results are similar.

Not all the gaps have an equal impact on the existence (or not) of the well-defined minima on the total energy surfaces. More extended calculations whose results will not be presented here in detail can be summarized as follows: The strongest tetrahedral-symmetry effects appear at proton numbers $Z_t = 16$, 20, 32, 40, 56–58*, 70*, and 90–94*, where the asterisks denote the gaps that are particularly strong (up to $\sim$3 MeV or so). A clear proton-neutron symmetry exists in the calculations leading to the related tetrahedral neutron gaps at $N_t = 16$, 20, 32, 40, 56–58*, 70*, 90–94*, 112, and 136/142.

Typically, tetrahedral minima on the total energy surfaces are accompanied by an oblate- and/or a prolate-symmetry minima. The energy cuts corresponding to the paths from the tetrahedral minima down to the ground state (g.s.) have been calculated in function of increasing β_2 by performing a minimization with respect to the γ deformation as well as, simultaneously, $\{\alpha_{3\mu}; \mu = 0, 1, 2, 3\}$ and $\{\alpha_{4\mu}; \mu = 0, 1, 2, 3, 4\}$, ten-dimensional minimization, using the standard Strutinsky method. These results are presented in Fig. 2 for ${}^{80}_{40}\mathrm{Zr}_{40}$, ${}^{108}_{40}\mathrm{Zr}_{68}$, ${}^{160}_{70}\mathrm{Yb}_{90}$, and ${}^{242}_{100}\mathrm{Fm}_{142}$ nuclei, whose tetrahedral equilibrium deformations are calculated at α_{32} =0.13, 0.13, 0.15, and 0.11, respectively.

The right-hand side minima (Fig. 2) for ^{80}Zr and ^{160}Yb nuclei are at oblate deformations; the corresponding energies visible in the figure are, respectively, at 1.4 MeV and $\sim$0.1 MeV above the prolate g.s. minima, the latter not shown in order not to perturb the legibility of the figure. For the other two nuclei, the right-hand side minima correspond directly to the prolate ground states; in the ^{242}Fm case the tetrahedral minimum lies particularly high (7.1 MeV above the g.s.). One can see from the figure that the calculated barriers are of the order of 1 MeV, similarly to those encountered in the case of the experimentally known prolate/oblate shape coexistence. Unfortunately, lack of information about the collective inertia parameters makes it impossible to speculate about the isomeric half-lives at present.

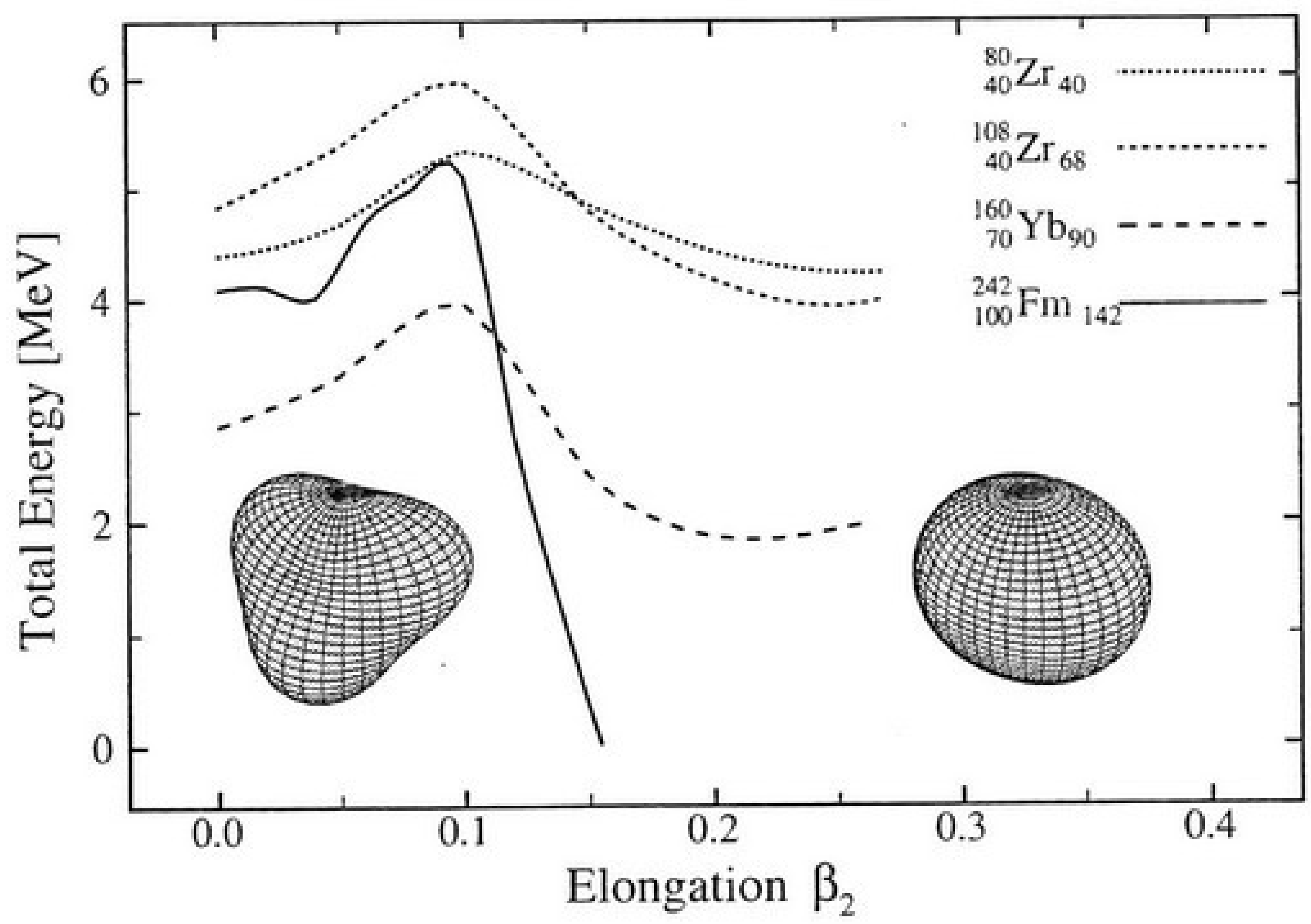

FIG. 2. Results of the multidimensional minimization of the total nuclear energies projected on the quadrupole deformation axis. The gamma deformation as well as all other deformations vary along the β_2 axis following the minimization, for each curve separately. The left-hand side inset shows an exaggerated (for better visibility) view of the tetrahedral shape at $\alpha_{32} = 0.3$, roughly twice the calculated equilibrium deformation. The right-hand side inset shows for comparison an oblate shape surface at $\beta_2 = 0.20$, $\gamma = 60^0$, i.e., roughly at the calculated equilibria.

An experimental identification of proposed T_d^D symmetry may rely on one or a combination of several criteria.

First of all, within the *class of the single-particle excitations,* the presence of the fourfold degeneracies will manifest itself by the presence of a multitude of particle-hole transitions of close-lying energies. For instance, if both the particle and the hole states are associated to the exact-symmetry fourfold degenerate levels, one should expect a *16-fold* exactly degenerate multiplet of transitions. (In realistic situations, the nuclear polarization effects are expected to be, in general, different for various $1p$-$1h$ excitations and the predicted 16-fold degeneracy in the associated decay lines will be only approximate) If the reference configuration was the tetrahedral 0^+ state, the corresponding 16 particle-hole excitations will decay to it. If as a reference configuration an arbitrary particle-hole excited state built on the tetrahedral minimum was taken, for example, of a given spin-parity I^π, a family of $2p$-$2h$ states can be constructed using similar considerations with the resulting 16 close-energy transitions feeding this I^π state. It thus becomes clear that the noncollective decay spectra associated with the tetrahedral minima might contain abundantly the approximate 16-plets of transitions. Although populating and observing such multiplets experimentally is by far a nontrivial task, the good news is that the discussed

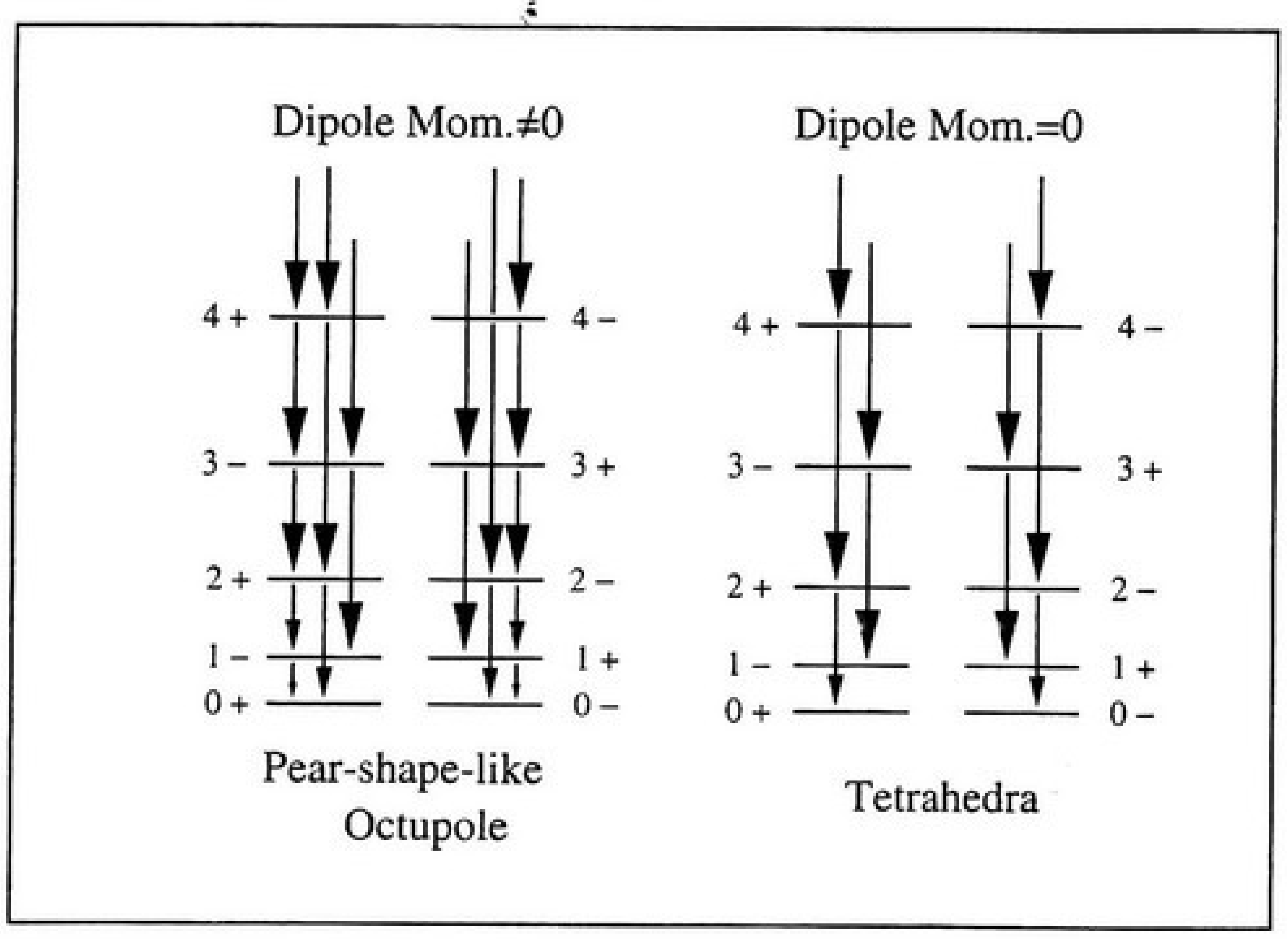

FIG. 3. Qualitative comparison of the electromagnetic transitions in a "pear-shape" nucleus, left, and a tetrahedral nucleus, right. In the former case, the static dipole moments are often strong, thus implying a presence of the collective interband $E1$ transitions in addition to the $E2$ ones. Tetrahedral nuclei generate no static dipole moments and, thus the $E1$ transitions should be absent in this case.

criterion is a "yes/no" condition—a well-defined effect to seek.

Within the class of the *low-lying collective rotational excitations,* not much is known at present as far as *nuclear* tetrahedral quantum rotor behavior is concerned. In a formal treatment of the rotational spectra of the tetrahedral symmetry *molecules* [8], the corresponding rotor Hamiltonians are expanded in terms of tensor operators that are constructed out of $\{\hat{I}_x, \hat{I}_y, \hat{I}_z\}$ angular momentum operators. The *nuclear* rotor Hamiltonians can be constructed analogously: We have performed the corresponding calculations, and the preliminary results indicate characteristic degeneracies of the rotor levels clearly different than those of the "traditional" ellipsoidal rotors.

Fortunately, qualitative criteria of the yes/no type can be formulated that are related to the rotational decay of the tetrahedral nuclei, and this in a nearly model-independent way. The starting point in the considerations is the so-called *simplex invariance,* i.e., the invariance of the Hamiltonian with respect to the product of parity, $\hat{\pi}$ and $\hat{\mathcal{R}}_y$, a 180° rotation about, for example, the $\mathcal{O}_y$ axis: $\hat{S} = \hat{\pi} \cdot \hat{\mathcal{R}}_y$. This invariance implies, as discussed in more detail in Ref. [9], that the rotational energies form two parity-doublet sequences (four parity-doublet $E2$ bands) as illustrated schematically in Fig. 3. Both the "usual" axial-octupole shape nuclei and the tetrahedral nuclei obey the simplex symmetry and thus must produce the parity-doublet bands. However, the tetrahedral nuclei, in contrast to the usual octupole-type ones, are *not* expected to produce the $E1$ interband transitions since the nuclear pyramids, due to their high symmetry, will not have any significant dipole moments.

A particularly appealing, "academic case" possibility corresponds to a pure tetrahedral symmetry with no other multipole deformations present. In such an ideal case, the dipole and quadrupole moments are expected to be zero and the first nonvanishing moments will have $\lambda = 3$. In such a case, the parity-doublet *energies* at the right-hand side of Fig. 3 would be connected by pure $E3$ transitions rather than $E2$ transitions.

In summary, we suggest that the tetrahedral symmetry in nuclei should be present among many isomeric states throughout the periodic table. We predict the proton and neutron numbers for which this effect should be the strongest. The fourfold T_d^D degeneracy of related deformed nucleonic orbitals is a unique feature—only the inversion-conserving octahedral O_h^D symmetry may provide in deformed nuclei the degeneracies higher than two (more precisely, fourfold).

This work has been partly supported by the Program of Scientific Exchange between the IN_2P_3, France, and Polish Nuclear Research Institutions, and by a grant from POLONIUM.

[1] P. A. Butler and W. Nazarewicz, Rev. Mod. Phys. **68**, 349 (1996).
[2] X. Li and J. Dudek, Phys. Rev. C **94**, R1250 (1994).
[3] S. Takami, K. Yabana, and M. Matsuo, Phys. Lett. B **431**, 242 (1998).
[4] M. Yamagami and K. Matsuyanagi, Nucl. Phys. **A672**, 123 (2000).
[5] M. Yamagami, K. Matsuyanagi, and M. Matsuo, Nucl. Phys. **A693**, 579 (2001).
[6] J. F. Cornwell, *Group Theory in Physics* (Academic, New York, 1984).
[7] G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups* (MIT Press, Cambridge, Massachusetts, 1963).
[8] W. G. Harter, *Principles of Symmetry, Dynamics and Spectroscopy* (Wiley, New York, 1993).
[9] A. Bohr and B. R. Mottelson, *Nuclear Structure* (Benjamin, New York, 1975), Vol. II.