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Fractality of Abundance-weighted N,Z -Chart of Isotopes and Systematics of Atomic Weights of Chemical Elements

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We show that stable isotopes display a fractal pattern in the N,Z -chart and abundance-weighted chart of isotopes with the fractal dimension $d_f \approx 1.2$. On this basis a scale invariant power law for atomic and molecular weights can be introduced and applied to systematics of chemical elements and compounds.

Key words: fractality, N,Z -chart of isotopes, systematics of atomic weights, box counting method.

The concept of atomic weights (relative atomic masses) of chemical elements and molecular weights (relative molecular masses) of chemical compounds is fundamental to chemistry and the problem to determine their values has captured attention of chemists for a long time.^{1,2}

On the other hand, fractal ideas of Mandelbrot³ have been extended to studies of various forms in nature on a wide range of length scales, from astronomical to microscopic (such as clusters of galaxies,³ distribution of earthquakes,⁴ structure of coastlines and rivers,^{3,5,6} cracks in sedimentary rocks,⁷ protein surfaces,⁸ *etc.*). Fractal structures occur very often in nature, emerging as a result of evolution of complex interacting systems. A fractal structure can be linked to a certain power-law behavior of an appropriately selected quantity. In some cases fractal properties are »hidden« and can only be perceived if data are studied as function of time or mapped in some spe-

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cial way,⁹ as for example, for heartbeat time series,^{10,11} reactions in heterogeneous chemistry,¹² chromatin texture in benign and malignant breast cells,¹³ long-range correlations in nucleotide sequences,¹⁴ fractal structures in the eye lens of vertebrates,¹⁵ basal metabolic rate in biological organisms,¹⁶ *etc.*

In this letter we address the question whether the fractal concept can be extended to the realm of atomic and molecular weights of chemical elements and compounds. In addition to its fundamental scope, this question is interesting also from another point of view. Namely, it is well known that the presence of fractality hints to some kind of scale invariant power law.^{15,16} Thus, if an evidence for fractality is found for atomic weights of chemical elements, an ensuing power law can provide a new mathematical expression for atomic and molecular weights of the systematics of chemical elements and compounds. In this connection we note that an extension of fractality to general dynamics of the quantum systems has been recently discussed.¹⁷

As an indirect evidence for fractality associated with molecular weights we might interpret also some recent experimental results on the effects of molecular weight on the interactions between polyethylene oxide layers adsorbed to glass surfaces.¹⁸ It was shown that the adsorbed layer thickness scales roughly with the molecular weight through a power law. Having in mind that a power law is associated with a fractality of the system, this result may provide a hint for an underlying fractality.

In our attempt to reveal a hidden fractality, which is relevant for the systematic of atomic weights of chemical elements, let us start from the N, Z -chart of isotopes (Figure 1).^{19,20} Chart of nuclides displays valley of nuclear stability. The solid squares represent the stable nuclei plotted as a

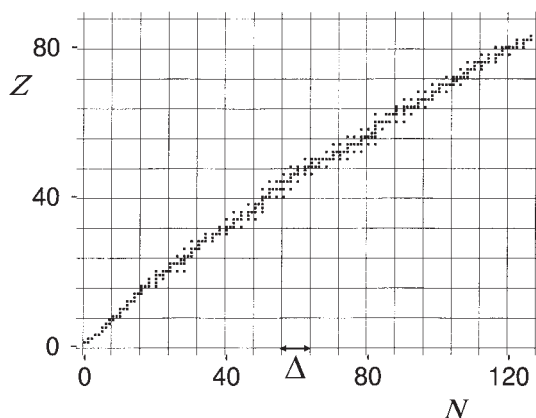


Figure 1. N, Z -chart of stable isotopes. For description see the text.

function of the number of neutrons, N , and number of protons, Z . The numbers along the left-hand side, marking the horizontal rows, represent the atomic number Z (the number of protons in each nucleus of that row). Each horizontal row represents one chemical element; the filled spaces indicate the known stable isotopes of that element. The numbers at the bottom of the vertical columns represent the number of neutrons N in each nucleus of that column. In this way the 283 stable nuclides are classified in the nuclear chart. Data are taken from Refs. 21 and 22.

Already a visual inspection of the geometrical pattern in the N,Z -chart hints to the similarity with a developed coastal line of mainland and islands, which is fractal.^{3,6} This observation is corroborated by a direct calculation of fractal dimension using the box counting method. The box counting method has been successfully used in calculating fractal dimension of various natural objects, with fractality restricted to a certain range.^{3,12}

Here we calculate fractal dimension of the valley of stability in the N,Z -chart of nuclides employing the box counting method for a »granular« structure provided by the N,Z -sites (boxes) in the chart of nuclides. Usually to determine fractal dimension of an object in nature, the photographs of the object are digitized using a grid of pixels.^{3,23} The fractal dimension of digitized pattern is then obtained using the box-counting method. A similar approach, but having a rather small number of pixels, is adopted in our study of the chart of nuclides. We assign one pixel to each site in the chart of nuclides corresponding to a stable nucleus. Then the box counting method is applied to pixels, which correspond to the valley of stability. The chart is overlaid with a grid of square boxes of size $s = \Delta Z = \Delta N$. The number of nonempty boxes N_i of size s_i is plotted on the log-log diagram as a function of s_i (Figure 2.a). An approximate straight-line correlation is obtained in the interval from $s = 2$ to $s = 18$. We note that this range of grid sizes is in accordance with the general requirement that the finest grid size must be larger than the pixel size and that the number of nonempty boxes has to be sizeable. The slope of this line gives the fractal dimension d_f of the valley of stability:

$$d_f = 1.21 \pm 0.03 \tag{1}$$

For comparison, we note that the fractal dimension of the Koch curve,²⁴ which is considered as a prototype of geometrical fractal, is $d_f = 1.26$.

Plotting the χ^2 -fit for the straight line

$$\log N(s_i) = k \log (1/s_i) \tag{2}$$

fitted through the log-log plot for each value of the coefficient k in the interval 1.0–1.4, the minimum of the χ^2 versus k graph is obtained at $k \approx 1.2$

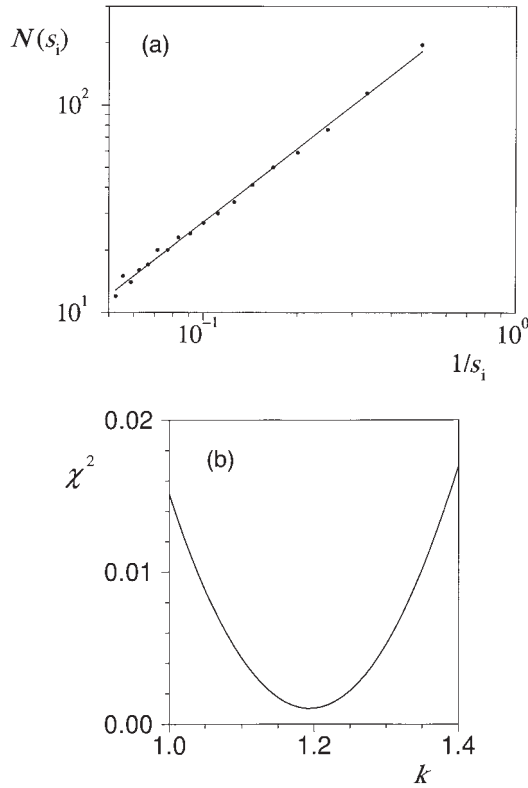


Figure 2. a) Log-log plot for the number of nonempty boxes *vs.* $1/s_i$ (s_i is the size of a grid box) overlaying the abundance-weighted N,Z -chart of stable isotopes in Figure 1 (closed circles). The straight line is fitted through the points calculated for various values of the box size s_i . b) χ^2 -fit of the straight line (2) through the log-log plot in dependence on the coefficient k . The pronounced minimum of the χ^2 *versus* k graph is at $k \approx 1.2$, which is equal to the fractal dimension d_f associated with the valley of stability.

(Figure 2.b). This is just the fractal dimension $d_f(1)$ associated with the valley of stability.

Thus, the valley of stability in nuclear chart appears as a line-area hybrid, a fractal object over roughly a decade in the length scale. This is within the range of fractality found for natural objects; the range of scaling properties for declared fractal objects in nature is centered around one order of magnitude.²⁵ Recently we have investigated the problem of fractal dimension of truncated fractals.^{29,30}

In order to get some insight into the robustness of calculated fractal dimension, we have considered some modifications of the N,Z -chart of isoto-

pes. In this sense, we modify the N,Z -chart of isotopes in such a way that the surface of each black square in the chart of isotopes corresponding to an isotope of chemical element with atomic number Z is proportional to the natural abundance of that isotope (represented as fraction) in the chemical element. We introduce the following rule: a surface of the black square in the N,Z -chart corresponding to an isotope with atomic number Z and neutron number N should be multiplied by a factor $a = \sqrt{\kappa p}$, where p denotes the natural abundance of the isotope (N, Z) in the chemical element with atomic number Z and k is a coefficient of proportionality. For example, a size of the square corresponding to the isotope Ti-48 (with natural isotopic abundance $p = 0.737$) at $\kappa = 2$ is $a = \sqrt{2 \cdot 0.737} = 1.21$ (in units of the surface of each black square in the standard chart of isotopes). (At $\kappa = 2$ each black square can overlap at most with its immediate neighbors in the N,Z -chart.) The size of a square corresponding to the isotope Ti-49 (natural abundance $p = 0.054$) at $\kappa = 2$ is $a = \sqrt{2 \cdot 0.054} = 0.33$. Such modified N,Z -chart, which contains information on isotopic abundances already by its geometrical shape, will be referred to as the abundance-weighted N,Z -chart of stable isotopes. Such chart contains geometric information both on nucleon composition of isotopes and on the natural isotopic abundance of chemical elements.

In Figure 3 the abundance-weighted N,Z -chart is displayed at $\kappa = 2$. The corresponding calculated fractal dimension is:

$$d_f = 1.19 \pm 0.02 \tag{3}$$

The fractal dimension d_f remains at the values $d_f \approx 1.2$ when κ is decreasing below 2. The variation of sizes of squares presenting isotopes has

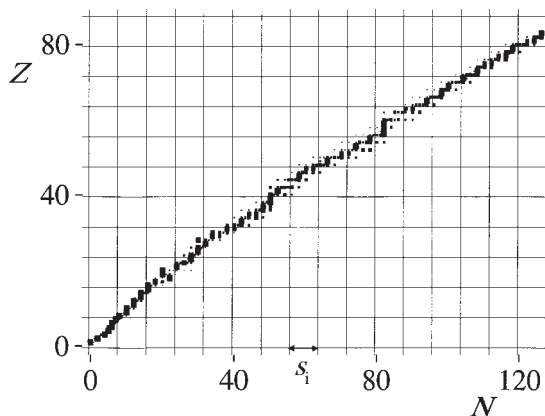


Figure 3. Abundance-weighted N,Z -chart of stable isotopes at $\kappa = 2$. For description see the text.

only a small influence on the calculated fractal dimension. If we take very small κ , for example $\kappa = 10^{-6}$, the log-log plot is the same as in Figure 2.a, *i.e.*, the one corresponding to the N, Z -chart with equal-size boxes, and therefore the fractal dimension has the same value. This corresponds to fractal dimension of a system of pixels. However, it should be noted that the smallest box size included in the analysis of the box counting method should be larger than the distance between the centers of the neighboring N, Z -sites, which is a typical size of the pattern. The smallest box size in the calculation is $s_i = 2$. On the other hand, the upper limit on the box size is determined by the condition that N_i should be larger than ten. In order to have a minimal number of nonempty boxes, in accordance with the box counting method, the origin of the box grid is placed at the position $(-0.5, -0.5)$. The problem of multiple counting could appear if the position of the origin is placed at an integer value of coordinate, which appears at singular position. Otherwise, the results appear stable if the position of the origin is randomly shifted.

We have also tested stability of our result with respect to the geometrical shape associated with each isotope, by taking instead of square a circular area of the same surface. Such a change of the shape has no effect on the calculated fractal dimension, confirming its robustness.

We have shown that the systematics of isotopes presented in the N, Z -chart of isotopes appears as a line-area hybrid, a fractal object over a decade in the »length« scale s_i .

Once the fractality associated with abundance weighted isotope chart was established, we argue for the existence of scale invariant power law involving atomic weights. We note that several convincing examples of relation between fractality and power law have been found for some objects in nature, as for example, the fractal structure of organisms, acting as area-volume hybrids^{9,27} in relation to the power law dependence of basal metabolic rate on the mass of mammals¹⁶ and the fractal dimension of a river network in relation to the power-law distribution of the drainage-basin area.^{5,26}

As the main implication, we note that our finding of fractality in the abundance-weighted N, Z -chart of isotopes is associated with the power law:²⁷

$$A_r = \alpha_c Z^{\beta_c} \quad (4)$$

where

$$\alpha_c = 1.48 \pm 0.02 \quad (5)$$

$$\beta_c = 1.120 \pm 0.004 \quad (6)$$

This law describes well the dependence of atomic weights A_r of stable chemical elements on atomic number Z . The value of the power law exponent (6) is obtained by a fit to data on atomic weights. The power law exponent (6) is close to the value of the fractal dimension (1).

Quite generally, the power law is associated with fractality and the power law exponent β is a specific function of fractal dimension of the object d_f :

$$\beta = f(d_f) \quad (7)$$

where the form of the function f follows from dynamics of the system. For some systems the explicit form of this function was determined, as for example in Ref. 5, while in most cases the values of β and d_f are independently determined numerically. The closeness of the power law exponent of the $A_r(Z)$ dependence and the fractal dimension d_f found numerically reveals that in this particular case the function f is close to unity, but this should be considered as an accidental consequence of complex nuclear dynamics governing the structure of nuclei.

As to the physical meaning of the present result, its origin is related to the role of fractal geometry in quantum physics and quark dynamics which was recently studied in a general framework.¹⁷ The fractal geometry, which shows up in particular observables, is generated by dynamics of the quantum system, the first example of fractal geometry in quantum systems being invoked in describing selfsimilarity of paths occurring in the Feynman path integral method. The velocity-dependent interactions, which are important in the theory of nuclear matter, lead to fractality and moreover the fractal dimension appears for free fermion propagator, which is relevant for the geometry of quark propagation in quantum chromodynamics. This provides a physical framework for the natural appearance of scale invariance at the level of bulk properties of atomic nuclei, and consequently of atomic weights.

Concluding, we note that the investigations of the power law related to atomic weights leads to a pronounced regularity in extension of the power law to molecular weights of chemical compounds in a wide range of chemical systematics,²⁸ as well as towards the superheavy chemical elements.²⁹ In this connection we also note that the problem of applicability of fractality to truncated statistical fractals, which is at the core of present approach, has been recently discussed by introducing models with truncated mathematical fractals.³⁰

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SAŽETAK**Fraktalnost N,Z -karte izotopa sa zastupljenošću izotopa i sistematika atomskih težina kemijskih elemenata**

Vladimir Paar, Nenad Pavin, Antun Rubčić i Jasna Rubčić

Pokazali smo da stabilni isotopi u standardnoj N,Z -karti i N,Z -karti s uključenjem izotopne zastupljenosti predstavljaju fraktalnu strukturu s fraktalnom dimenzijom $d_f \approx 1,2$. Na osnovi te fraktalnosti uvodi se baždarno invarijantni zakon potencija za atomske težine koji se može primijeniti u sistematici kemijskih elemenata i spojeva.