THE ADMIXTURE ENGINEERING:
WHAT KIND OF ATOMS WILL HAVE ENCAGE OF FULLERENES

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Introduction

It is know, that a nowadays technological revolution demands of nontraditional energy sources, of global internetization, of development photonics (as a base thecnology for an information transfer). This will have meet needs in newly materials for replacement of mechanical, electrical and electromechanical systems by the nanostructural electronic systems and by the digital apparaturs and devices. Without doubt, that the admixture engineering has been found keys for decision of this problems. It may be done: by means of study of a phase cocristallization and principles of an energy profitable for atomic substitution and stabilization of nanoforms; also by development the electronic state theory for explanation of different properties.

Discussion of results

It is necessary to underline that a cluster principle of nanostructural organization *is foundation*, but participation of admixture (halogens, hydrogen, nitrogen, oxydgen) elements for stabilization nano-forms on the base of a transitioin metals is essential condition.

At present day, the first principles theoretical investigation for reweal of micromechanism formation for the manycomponent nanostructures is absolute nonrealistic.

This because, that the manycomponents of the real systems makes theoretical task very complicated. On it intricates big number of the independent variables, biggest than a number equations from a mathematical system for resolving of task. However, application of the Quantitative Atomic-Isomorphic Mutual-Substitu-tition Theory (QAIMST) gives chance to the prognosis analyse of role an admixture components in modification of structure and properties of nanomaterial. This approach enables the easily prognosis of the most possible micromechanism of the atom replacing, especially for the andohedral and the carbon cage structures (Fig. 1, 2, [1-4]). So far as endohedral metallofullerenes (which can encage a variety of the transition *d*-, *f*-metal atoms in fullerene cages), that a reweal of the controlling principles is very important science and a practical tasks.

This report deals with the results of the theoretical investigation of micromechanisms for substitution of (1H-:-94Pu) elements (as a function of their donor/acceptor microgear principle).

The competitebility of admixture elements has been analyzed by authors. It has been also discussed a phenomenon of the compensatory atomic isomorphism (by Shcherbina) and the phe-nomenon of the Fersman`s compensation valency.
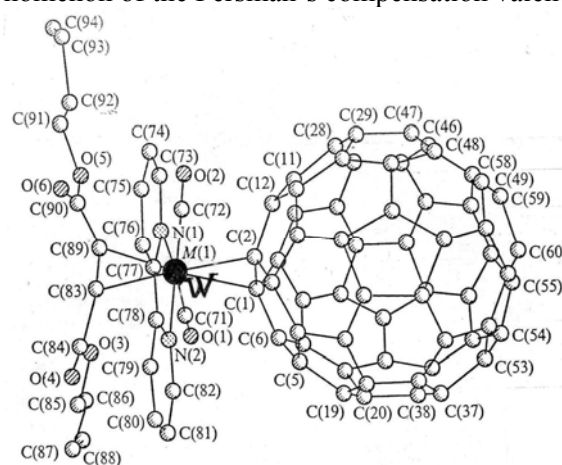

Fig 1. Fullerene C_{94} (W $[N_x, O_{x+2}]_2$).

The analysis of theoretical results shows that the controlling principle of substitution microgear (for a stable solide state nanoform) are two derivatives: the first derivative dE_n/dR from electronegativity $-E_n$ to radius R (as analog of chemical potential μ, which regulations of free energy G of a particle system); other the first derivative $dK_E/d\Omega$ from energodynamical potential K_E to volume Ω per atom (which regulations of an energy compatibilities of components). It was shown, that the *type of micromecha-nism* for substitution of base carbon atoms by other (from 1H-:-94Pu elements) *is depending on* microgear principles (as a function of their donor/acceptor properties).

It has been established, that the signes of the relation electronochemical E_n and energodymamical K_E com-patibilities (first signs) are controlling process in depend on dimensional factors (second signs): [− on (−)], [+ on (+)], [− on (+)], [+ on (−)].

The model view $Sc_3@C_{82}$ and the charge state for the encaged Sc-trimer (with hydrogen atom in center) are shown on Fig. 2, a, b. The distribution of charge state for the encaged Sc-trimer (and Sc-Sc distance ~ 0,23 *nm* against the know 0,3254 nm from other papers) was founded by [4] from the Maximum Entropy Method. As we known, scandium is very valuable metal, because we shall have a problems: what kind of the cheapest chemical elements may have to encage in the fullerene volume; what from ones may will have subs-tituted in position of an element-catalyst.
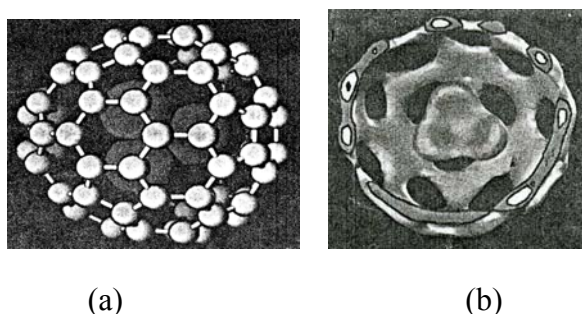

(a)   (b)

Fig. 2. Scandiun in cage of $Sc_3@C_{82}$ fullerene.

Analysis of the signes and auxiliary microscopical parameters of a mutual electrono-chemical compatibilies dE_n/dR for components of system "*carbon–scandium–and centred hydrogen atom*" shown, that as hydrogen, as scandium evences to the basic carbon atoms the donor microgears after the type [+ on (+)] (see table 1).

Table 1.

System	dE_n/dR	$dK_E/d\Omega$
H→(C)	**+0,256(+)**	**–0,280(+)**
H→(Sc)	–5,037(+)	–1,789(+)
H→(Ti)	–2,039(+)	–0,832(+)
H→(Cr)	–0,760(+)	–0,443(+)

After analysis by signes and auxiliary microscopical parameters $dK_E/d\Omega$ of a mutual energo-dynamical profitable of components conclusion was made: hydrogen atom to carbon (as to scandium) plays role of the energy decreasing factor. This give rise to the most phase stability of the fullerene structure.

Intrinsically, the majority of *d-* and *f*-transition metals are having inclination to the donor microgear in according to dE_n/dR [+ on (+)]. Thus, (after **Sc [+1,258(+)]**) donor

microgear is justis for (Ti 1,810), (Cu 2,911), (Fe 3,390), (Cr 3,502). However, it must be realized with principle of energy decreasing of fullerene state in according to $K_E/d\Omega$ **Sc [–0,480 (+)]** (see table 2).

Table 2.

System	dE_n/dR	$dK_E/d\Omega$
Y→(C)	+0,209(+)	–0,331(+)
Zr→(C)	+1,339(+)	–0,546(+)
Hf→(C)	+1,396(+)	–0,582(+)
Ag→(C)	+1,751(+)	–0,933(+)
Nb→(C)	+1,965(+)	–0,816(+)
W→(C)	+2,035(+)	–1,063(+)
Mo→(C)	+2,286(+)	–1,084(+)
Tc→(C)	+2,608(+)	–1,318(+)

Conclusions

1. The competitebility of an substitute atoms depends on the parameters their microgear.
2. For parameters of the Sc-substituting an metal atoms <u>inside cage</u> of fullerene must be justis conditions:

$0 < [+ dE_n/dR (+)] < 2$

$0 < [– dK_E/d\Omega (+)] < 1$

3. For of the catalyst-substituting atoms <u>outward cage</u> of fullerene must be justis this conditions:

$[+ dE_n/dR (+)] > 2$

$[– dK_E/d\Omega (+)] > 1$

4. Most probabilies atoms-substituting of Sc *inside* fullerene *cage* will have *yttrium, zirconium, hafnium, silver* and other ones with analogous parameters.

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