Formation of Carbon Nanostructures and Spatial-Energy Stabilization Criterion

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ABSTRACT: A spatial-energy criterion of structure stabilization is obtained. The computational results for 100 binary systems correspond to the experimental data. The basic regularity of organic cyclic compound formation is given and its application for carbon nanostructures is shown. © 2007 Wiley Periodicals, Inc. J Appl Polym Sci 107: 3541–3547, 2008

Key words: spatial-energy parameter; compound stabilization; carbon nanostructures

INTRODUCTION

The problem of an *a priori* assessment of stable structure formation is one of the main problems of chemical physics and material science. Its solution, in turn, is directly linked with the regularities of isomorphism, solubility, and phase formation in general. Surely, such problems can be cardinally solved only based on fundamental principles defining the system of physical and chemical criteria of a substance. Quantum-mechanical concepts of physics and chemistry of a solid suit it.

However, many computations of phase formation based on the application of pseudopotential, quantum-mechanical techniques, and statistical-thermodynamic theories have been carried out only for a comparatively small number of systems.[1–3] Numerous works have been dedicated to the phenomenon of isomorphic replacement, arrangement of an adequate model of solids, and energy theories of solid solutions.[4–7] However, for the majority of actual systems, many problems of theoretical and prognostic assessment of phase formation, solubility, and stable phase formation are still unsolved.

This article develops a method in which complex initial characteristics of an atom are used as a criterion of structure stabilization.

EXPERIMENTAL

Spatial-energy (*p*) parameter

The introduction of the *P* parameter as a criterion of structural interactions is based on the assumption that

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the resulting energy in the system (orbital nucleus), which is immediately responsible for interatomic interactions, can be calculated based on the principle of adding the reverse values of some primary atom characteristics in the initial state.[8] In this model the P_0 parameter is a tabulated constant spatial-energy characteristic of each orbital of an atom.

The criterion $P_E = (P_0/r_i)$ has a physical sense of some averaged energy of valence electrons in the atom at a distance r_i from the nucleus.

The reliability of the initial equations and regulations was proved with numerous calculations and comparisons. In particular, it was shown[8] that the P_E parameter numerically equals the energy of valence electrons in a statistical atom model and is a direct characteristic of electron density in the atom at the given distance from the nucleus.

Spatial-energy principles of isomorphic replacement were found:

1. complete (100%) isomorphic replacement at approximate equality of P parameters of valence orbitals of interchangeable atoms: $P'_E \approx P''_E$ and
2. the P parameters of the atom valence orbital with the least value determine the orbital that is mainly responsible for isomorphism and structural interactions.

However, isomorphism is a particular case of phase formation. Therefore, when we take its ratios as a basis and take coordination into account it can be assumed that the following condition has to be performed for atoms of a stable homogeneous crystalline structure:

$$\frac{P_E'}{K_1} \approx \frac{P_E''}{K_2} \qquad (1)$$

TABLE I
P Parameters of Atoms Calculated Via Ionization Energy

Atom	Valence orbitals	E (eV)	r_i (Å)	q^2 (eV/Å)	P_0 (eV/Å)	P_0 (eV/Å)	$P_i = \dfrac{\sum P_0}{r_i}$ (eV/Å)	r_i (Å)	$P_i = \dfrac{\sum P_0}{(Å^{r_i})}$ (eVÅ)	Note (eV)
H	$1s^1$	13.595	0.5295	14.394	4.7985	4.7985	9.0624	1.36	3.528	For H⁻
C	$2p^1$	11.260	0.596	35.395	5.641					
	$2p^1$	24.383	0.596	35.395	10.302					
	$2s^1$	47.860	0.620	37.243	16.515					
	$2s^1$	64.480	0.620	37.243	19.281	51.739	86.810	2.60	19.900	For C⁴⁻
								0.20	258.7	For C⁴⁺
N	$2p^1$	14.54	0.488	52.912	6.257	6.257	12.822			
	$2p^1$	29.60	0.487	52.912	11.329	17.586	36.111			
	$2p^1$	47.426	0.487	52.912	16.078	33.664	68.984	1.48	22.746	For N³⁻
	$2s^1$	77.472	0.521	53.283	22.966	56.63	108.69			
	$2s^1$	97.89	0.521	53.283	26.012	82.642	158.62	0.15	550.9	For N⁵⁺
O	$2p^1$	13.618	0.414	71.380	5.225	5.225	12.621	1.36	3.8419	For O⁻
	$2p^1$	35.118	0.414	71.380	12.079	17.304	41.797	1.36	12.724	For O²⁻
F	$2p^1$	17.423	0.360	94.641	5.882	5.882	16.389	1.345	4.3774	
Cl	$3p^1$	12.268	0.728	59.842	8.125	8.125	11.161	1.81	4.4890	
Br	$4p^1$	11.84	0.851	73.346	8.859	8.859	10.410	1.96	4.5199	
I	$5p^1$	10.451	1.044	77.65	9.567	9.567	9.1638	2.20	4.3486	
Na	$3s^1$	5.138	1.713	10.058	4.694	4.694	2.7402	0.98	4.7898	
Al	$3p^1$	5.986	1.311	26.44	6.055	31.624	23.939			
	$3s^1$	18.829	1.044	27.119	11.396					
	$3s^1$	28.440	1.044	27.119	14.173					
Fe(II)	$4s^1$	7.893	1.227	26.57	7.098	18.462	15.046			
	$4s^1$	16.183	1.227	26.57	11.369					
Fe(III)	$3d^1$	30.64	0.365	199.95	10.564	29.026	23.656			

or

$$\left(\frac{P_0 N}{Kr}\right)_1 \approx \left(\frac{P_0 N}{Kr}\right)_2; \quad P_1' \approx P_2 \quad (2)$$

where $P_E = (P_0 N / r)$, K is the coordination number of atoms, r is the dimensional bond characteristic of the given atom, and N is the number of homogeneous atoms in the compound formula.

Based on the physical sense of the P_E parameter, the given condition (2) is the condition of equality of the effective values of the structure atom orbitals (in the assumption of paired interatom interaction). In a more complicated case when the central atom (A_1) has heterogeneous surroundings consisting of atoms (A_2, B, C) at different internuclear distances, the condition of stable structure formation looks like the following:

$$\frac{P_0 N}{Kr} = \frac{P_0' N_1}{K_1 r_1} + \frac{P_0'' N_2}{K_2 r_2} + \frac{P_0''' N_3}{K_3 r_3} + \cdots \quad (3)$$

Here, the left-hand part of the equation refers to the central atom and the right-hand part of the equation refers to the atoms surrounding it.

Let us apply correlations (2) and (3) to some types of crystalline structures using tabulated values of P_0 parameters calculated and given previously.[8] At the same time, for structures with basic ionic and metallic bonds, the values of the P_0 parameters calculated via the atom ionization energy (E) were used (Table I).

Crystals with basic ionic bond

Equation (2) contains the value of the actual dimensional bond characteristic of the given atom in the structure. In crystals with a basic ionic bond, the ion radius can be applied as such a dimensional bond characteristic (with a certain approximation). That is, the stabilization condition for such structures is as follows:

$$\frac{N_1 P_0'}{K_1 r_K} \approx \frac{N_2 P_0''}{K_2 r_a}; \quad \left(\frac{P_E}{K}\right)_1 \approx \left(\frac{P_E}{K}\right)_2; \quad P_1 \approx P_2 \quad (4)$$

where r_k is the cation radius and r_a is the anion radius.

Table II contains the results of some calculations following eq. (4) for several structures, such as NaCl. In all calculations mainly the ion radii by Belov–Bokiy (first line) and partly by Goldschmidt–Poling (second line) were used. Comparisons of such calculative parameters (P_E / K) of structure atoms (seventh and eighth columns) prove the equality of these values with a precision of up to 25%.

To determine the structure type from eq. (4) it is necessary to calculate the ratio of the coordination number of the cation and anion (K_1 / K_2). Taking into

TABLE II
Spatial-Energy Criterion of Stable Phase Formation in Structures of Na-Cl Type

Atom	Structure	Orbital	P_0 (eV/Å)	K	r_i (Å)	$P_{E/K1}'$	$P_{E/K2}'$
F	M'F	$2p^1$	5.882	6	1.33	0.737	0.798–0.617
		$2s^1$	6.432	6	1.33	0.806	
					1.36	0.786	
Cl	*M'Cl*	$3p^1$	8.125	6	1.81	0.748	
Br	M'Br	$4p^1$	8.859	6	1.96	0.753	
J	M'J	$5p^1$	9.567	6	2.20	0.725	
					2.16	0.740	
Li	LiΓ	$2s^1$	3.487	6	0.68	0.855	−0.806–0.725
					0.78	0.740	
Na	NaΓ	$3s^1$	4.694	6	0.98	0.798	
K	KΓ	$4s^1$	5.06	6	1.65	0.634	
Rb	RbΓ	$5s^1$	5.728	6	1.49	0.641	
Cs	CsF	$6s^1$	6.106	6	1.05	0.617	0.788
H	M'H	$1s^1$	4.794	6	1.36	0.588	0.798–0.617
O	SrO, BaO	$2P^2$	17.304	6	1.36	2.121	2.195
					1.32	2.185	2.412
	MgO, CaO	$2p^2 + 2p^2$	22.653	6	1.36	2.776	2.533
					1.32	2.860	3.298
Ba	BaO, BaS	$6s^2$	16.172	6	1.38	2.190	2.120
							1.894
Sr	SrO	$5s^2$	17.367	6	1.20	2.412	2.185
Ca	CaO	$4s^2$	15.803	6	1.04	2.033	2.776
	CaS				1.06	2.485	2.664
Mg	MgO	$3s^2$	15.436	6	0.74	3.477	2.860
	MgS				0.78	3.298	2.78
S	BaS	$3p^2$	20.682	6	1.82	1.894	2.195
					1.74	1.981	2.195
	MgS	$3p^2 + 3p^2$	29.092	6	1.82	2.664	3.298
	CaS				1.74	2.78	2.485
	SrS				1.82	2.664	2.412
Eu	EuO	$6s^2$	18.978	6	1.24	2.551	2.776
Ti	TiO	$3d^2$	9.483	6	0.78	2.026	2.121

M', metal of 1st group (Li, Na, K, Rb, Cs); Γ, halogen; M", metal of 2nd group (Mg, Ca, Sr, Ba).

consideration the ratio of the cation and anion radii values (in the model of rigid spheres), the structure itself can be determined.

Crystals with ionic–covalent and metallic bonds: intermetallides

Numerous and various structures belong to these classes of compounds, and a lot of them are practicable. Compounds of metals with each other belong to intermetallic compounds in the narrow sense. However, the distinct border between them cannot be made because there is no such border between metals and nonmetals and their properties frequently change considerably, depending on the composition and temperature; that is, the rational theory of phrase stability has to be the same for different types of structures.

When we applied the initial model to double compounds with ionic–covalent and metallic bonds, the calculations were made based on eq. (2) for 45 binary structures with the assumption of paired interatomic interaction. Some of the results are given in Table III.

Analogous calculations were made for dozens of crystalline structures of penetration, metal carbides and hydrocarbides, some of which are given in Table IV. In all these cases the relative difference of the values of the P parameters of interacting systems can be considered as the stability criterion (coefficient α) based on the following equation:

$$\alpha_E = \frac{P_2 - P_1}{(P_2 + P_1)/2} \times 100\% \qquad (5)$$

From the results of all these calculations it can be concluded that stable structures are formed if $\alpha_{ST} < 25–30\%$.

Formation of carbon nanostructures

After different allotropic modifications of carbon nanostructures (fullerenes, tubules) were discovered, a number of investigations of such materials[9–15] were

TABLE III
Spatial-Energy Criterion of Stabilization of Crystalline Structures

Atom 1	Structures 2	Structure type 3	Orbitals 4	ΣP_0 (eV Å) 5	K 6	R_H' (Å) 7	R' (Å) 8	P' (eV) 9	P'' (eV) 10
As	As₂Fe	FeS₂	$4S^2$	8.210	3		1.48	3.698	3.846
Fe	As₂Fe	FeS₂		18.462	6	0.8		3.846	3.698
Ag(I)	AgSb					1.13		0.529	0.452
	AgAs	Mg	$5S^1$	7.108	12				0.462
	AgCd						1.44	0.411	0.446
As(I)	AgAs	Mg	$4P^1$	8.210	12		1.48	0.462	0.524
									0.411
Ag	Ag₂S	Cu₂O	$5S^1$	7.108	2		1.44	4.936	3.996
	Ag₂O								4.164
Ag(I)	Ag₃Pt	Cu	$5S^1$	7.108	12	1.13		1.572	1.452
Pt(II)	Ag₃Pt	Cu	$6S^2$	24.043	12		1.38	1.452	1.572
Sb(I)	AuSb	Mg							0.516
	AgSb		$5P^1$	8.742	12		1.61	0.452	0.411
As(III)	AlAs	ZnS	$4P^3$	37.448	4	0.69		14.282	13.87
Al(III)	AlAu₄	W	$3S^2 + 3P^1$	31.624	8		1.49	2.764	3.092
Au(I)	AlAu₄	W	$6S^1$	8.909	8		1.44	3.092	2.764
Al(I)	Al₂Pt	CaF₂	$3P^1$	6.055	4		1.43	2.180	2.178
Pt(II)	Al₂Pt	CaF₂	$6S^2$	24.043	8		1.38	2.178	2.180
Al(III)	Al₂Se₃	ZnS	$3S^2 + 3P^1$	31.624	4		1.43	11.057	10.608
Se(II)	Al₂Se₃	ZnS	$4P^2$	22.614	4		1.6	10.609	11.057
As(III)	AsJn	ZnS	$4P^3$	39.448	4		1.48	6.663	6.137
	AsGa								6.776
Zn(III)	AsSn	NaCl	$4P^3$	40.749	4		1.66	6.137	6.617
									6.663
Au	AuCd	Mg	$6S^1$	8.909	12		1.44	0.516	0.446
	AuSb	Cu							0.452
Au	Au₂Pb	Mg	$6S^1$	8.909	12		1.44	1.032	1.045
K	Bi₂K	Cu₂Mg	$4S^1$	5.060	12	1.33		0.634	0.594
Bi	Bi₂K	Cu₂Mg	$6P^1$	12.971	12		1.28	0.594	0.634
Cd(I)	CuCd₃	Mg	$5S^1$	8.349	12		1.56	1.338	1.221
	AgCd₃	Mg							1.266
Ag(II)	AgZn₃	Mg	$5S^2 + 4d^9$	36.965	12		1.44	2.139	2.302
Ni(II)	NiMo	Mg	$4S^2$	18.838	12		1.24	1.266	1.252
Mo(II)	NiMo		$5S^2$	20.872	12		1.39	1.252	1.266
Li	LiAg	W	$2S^1$	3.487	8	0.68		0.641	0.617
Ag(I)	LiAg	W	$5S^1$	7.108	8		1.44	0.617	0.641
Cd(II)	CdSe								2.929
	CdS	ZnS	$5S^1 + 4d^2$	16.671	4		1.56	2.672	2.840
	CdTe								2.915
Pt(VI)	PtGa₂	CaF₂	$6S^2 + 5d^4$	136.65	8		1.38	12.377	13.554
Ni(II)	SnNi₃	SnNi₃	$4S^2$	18.838	12		1.24	3.798	3.666
Sn(IV)	SnNi₃	SnNi₃	$5P^2 + 5S^2$	69.505	12		1.58	3.666	3.798
Ti(IV)	TiCu₃		$4S^2 + 3d^1$	46.839	12		1.46	2.673	2.571
Cu(I)	TiCu₃		$4S^1$	13.165	12		1.28	2.571	2.673
Pt(V)	PtMg₇		$6S^2 + 5d^3$	96.496	12		1.38	5.827	5.628
Mg	PtMg₇		$3S^2$	15.436	12		1.60	5.628	5.827
Sb(III)	Sb₃Cu₁₀		$5P^3$	41.870	12		1.61	6.502	6.02
Cu(I)	Sb₃Cu₁₀		$4S^1$	7.081	12			6.02	6.502
Ga(III)	Ga₂S₃		$4S^2 + 4P^1$	37.678	4		1.39	13.456	12.783
S(II)	Ga₂S₃		$3P^2$	20.682	2.667	1.82		12.783	13.456
Ge(IV)	GeS₂		$4P^2 + 4S^2$	61.176	4		1.39	11.003	11.364
S(II)	GeS₂		$3P^2$	20.682	2	1.82		11.364	11.003
Ni(II)	Ni₂Al₃		$4S^2 + 3d^2$	28.765	8		1.24	5.799	5.529
Al	Ni₂Al₃		$3S^2 + 3P^1$	31.624	12		1.43	5.529	5.799
Se(II)	Cu₃Se₂		$4P^2$	22.614	6	1.93		3.906	3.857
Cu(I)	Cu₃Se₂		$4S^1$	13.165	8		1.28	3.857	3.906

published, which were determined by the perspectives of their vast applications in different fields of material science.

However, a strictly defined model of such system formations does not currently exist. To further study the problem of nanostructure phase formation, the

TABLE IV
Spatial-Energy Criterion of Carbide and Hydride Formation

Atom	Structure	Orbitals	P_0 (eV/Å)	K	R_i (Å)	$[(N/P_0)/(KR_i)]_1$	$[(N/P_0)/(KR_i)]_2$
C	Carbides	$2P^2 + 2P^2$	51.739	6	2.6	3.317	
α-Fe	FeC cementite	$4S^2$	18.462	6	0.6	3.846	3.317
α-Fe	FeC	$4S^2$	18.462	6	0.6	2.885	3.317
Ti(II)	TiC	$4S^2$	17.026	6	0.76	3.639	3.317
V(II)	VC	$4S^2$	17.162	6	0.72	3.973	3.317
Cr(II)	CrC	$4S^2$	18.869	6	0.83	3.769	3.317
Zr(II)	ZrC	$5S^2$	18.547	6	0.925	3.342	3.317
Hf(II)	HfO	$6S^2$	19.826	6	0.963	3.432	3.317
W(II)	WC	$6S^2$	23.344	8	0.956	3.052	3.317
Ce(II)	CeC	$6S^2$	23.4778	6	1.125	3.478	3.317
Nb(II)	NbC	$5S^1 + 4d^1$	16.669	6	0.62	3.429	3.317
SC(II)	ScC	$4S^2$	16.599	6	0.912	3.033	3.317
Mn(II)	MnC	$4S^2$	18.025	6	0.91	3.301	3.317
Ti(I)	TiH	$4S^1$	6.795	14	0.841	0.578	0.588
Ti(II)	TiH$_2$	$4S^1$	17.026	12	0.76	1.819	1.613
H	TiH$_2$	$1S^1$	4.794	4	1.36	1.763	1.619
Li	LiH	$2S^1$	3.487	6	0.66	0.655	0.882
H	LiH	$1S^1$	4.794	6	1.36	0.682	0.655

methodology of the P parameter is applied in this article.

The main conditions of stability of these structures that were formulated based on modeling the compositions of over 30 carbon clusters are the following[9]:

1. stable carbon clusters look like polyhedrons where each carbon atom is three coordinated;
2. more stable carbopolyhedrons containing only five- and six-term cycles;
3. five-term cycles in polyhedrons, isolated;
4. the carbopolyhedron shape is similar to a sphere; and
5. in polyhedrons, an even number of apexes, 12 pentagons, and any number of hexagons.

Let us show some possible explanations of such experimental data based on the application of spatial-energy concepts. As previously, we consider the approximate equality of the effective energies of interacting subsystems as the main condition for the formation of stable structure based on the following equation:

$$\left(\frac{P_0}{KR}\right)_1 \approx \left(\frac{P_0}{KR}\right)_2; \quad P_1 \approx P_2 \tag{2a}$$

where K is the coordination number, R is the bond dimensional characteristic, and N is the number of homogeneous atoms in the structure.

At the same time, the phase-formation stability criterion (coefficient α) is the relative difference of parameters P_1 and P_2 that is calculated following eq. (5) and is agr;$_{ST}$ < 20–25%.

During the interactions of similar orbitals of homogeneous atoms, $P'_0 = P''_0$. When $N_1 = N_2$,

$$K_1R_1 \approx K_2R_2 \tag{6}$$

Let us consider these initial notions as applicable to certain allotropic carbon modifications using dimensional characteristics and values of P parameters that are given by Korablev[8] and Table I:

1. diamond: a modification of structure where $K_1 = 4$, $K_2 = 4$; $P'_0 = P''_0$, $R_1 = R_2$, $P_1 = P_2$, and $\alpha = 0$, which is absolute bond stability;
2. non-diamond carbon modification for which $P'_0 = P''_0$, $K_1 = 1$; $R_1 = 0.77$ Å; $K_2 = 4$; $R_2^{4+} = 0.2$ Å, and $\alpha = 3.82\%$, which is absolute stability due to the ionic–covalent bond;
3. graphite: $P'_0 = D''_0$, $K_1 = K_2 = 3$, $R_1 = R_2$, $\alpha = 0$, absolute bond stability;
4. chains of hydrocarbon atoms consisting of the series of homogeneous fragments with similar P parameter values; and
5. cyclic organic compounds as a basic variant of carbon nanostructures. Apparently, not only the inner atom hybridization of valence orbitals of the carbon atom takes place in cyclic structures, but also total hybridization of all cycle atoms.

The basic dimensional characteristics are both the distance between the nearest similar atoms by bond length (d) and the distance to the geometric center of cycle interacting atoms (D) as the geometric center of the total electron density of all hybridized cycle atoms.

Then, the basic stabilization equation for each cycle atom will take into account the average energy of hybridized cycle atoms:

$$\left(\frac{\sum P_0}{Kd}\right)_i' \approx \left(\frac{\sum P_0}{KD}\right)_i''; \quad P' \approx P'' \tag{7}$$

where $\sum P_0 = P_0 N$, N is the number of homogeneous atoms, P_0 is the parameter of a one-cycle atom, and K is the coordination number relative to the geometric center of cycle atoms. Because in these cases $K = N$, the following simple correlation appears:

$$\frac{P_0'}{d} \approx \frac{P_0''}{D}; \quad P_E' \approx P_E'' \tag{8}$$

During the interactions of similar orbitals of homogeneous atoms $P'_0 \approx P''_0$, then

$$d \approx D \tag{8a}$$

Equation (8) reflects a simple regularity of the stabilization of cyclic structures: *in cyclic structures the main condition of their stability is an approximate equality of the effective interaction energies of atoms along all bond directions.*

The corresponding geometric comparison of cyclic structures consisting of three, four, five, and six atoms results in the conclusion that the bond length (d) equals the length to the geometric center of atoms (D) only in the six-term cycle (hexagon).

$$d = D$$

Such a calculation of α following the equation analogous to eq. (5) gives for the hexagon $\alpha = 0$ and absolute bond stability. For the pentagon $d \approx 1.17D$ and $\alpha = 16\%$; that is, this is the relative stability of the structure being formed. For the other cases in which $\alpha > 25\%$, the structures are not stable. Therefore, hexagons play the main role in nanostructure formation and pentagons are additional substructures, which are spatially limited with hexagons. Based on the stabilization equation, hexagons can be arranged into symmetrically located conglomerates consisting only of three or seven hexahedrons.

A conglomerate of three hexagons contains 1 central atom and 12 atoms around it. A conglomerate of seven hexahedrons comprises 12 external and 12 internal (common) atoms. In these two cases the geometric centers of the hybridized molecular orbitals of each hexahedron are equidistant from the nearest centers of a conglomerate. This apparently explains the experimental fact that polyhedrons of carbon clusters represent an icosahedron: a 12-apex crystalline structure in which each apex is connected to 5 other apexes.

Following such a model, for instance, cluster C_{60} can be formed of two structures with three hexagons in each and two structures with seven hexagons in each ($2 \times 3 + 2 \times 7 = 20$) plus 12 pentagons between them located separately and acting as a binding formation.

It is assumed[12] that defectless carbon nanotubes (NTs) are formed as a result of rolling the bands of a flat atomic graphite net. The graphite has a lamellar structure, with each layer composed of hexagonal cells. Under the center of the hexagon of one layer there is an apex of the hexagon of the next layer. Such a transition from the graphite plane to an NT should be accompanied by the change of coordination numbers of the carbon atoms. The coordination numbers are 3 and 12 for some atoms and 3 and 2 for other atoms. All this can be found in accordance with the stabilization formula based on the given pattern. Examples of this are the following: from eq. (2a) we have

$$\frac{K_1}{K_2} \approx \frac{R_2}{R_1}$$

Then, for graphite we find

$$\frac{K_1}{K_2} = \frac{R_2}{R_1} \approx \frac{1.675 \text{ Å}}{0.77 \text{ Å}} \approx 2:1$$

For an ionic–covalent bond we have

$$\frac{K_H}{K_K} = \frac{R_K}{R_H} = \frac{0.77 \text{ Å}}{0.2 \text{ Å}} \approx 4:1$$

and for an ionic–ionic bond we find

$$\frac{K_H^{4+}}{K_H^{4-}} \approx \frac{R_H^{4-}}{R_H^{4+}} = \frac{2.60 \text{ Å}}{0.2 \text{ Å}} \approx 13:1$$

These are 13 hexagon atoms, the central atom of which has the coordination of 12 atoms. The process of rolling flat carbon systems into NTs is apparently determined by the polarizing effects of cation–anion interactions, resulting in statistic polarization of bonds in a molecule and shifting of the electron density of orbitals in the direction of more electronegative atoms.

Thus, the spatial-energy notions given here allow the general characterization of the directedness of the process of carbon nanosystem formation.

CONCLUSIONS

The introduction of a spatial-energy criterion of structure stabilization is substantiated. The application of this criterion to cyclic systems was shown

with the example of the formation of a carbon nano-structure.

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