STRUCTURAL MODELS OF RADIATION TRANSFORMATIONS OF BIOORGANIC COMPOUNDS: ETHANOL

V.T. Maslyuk, V.P. Hanulych, N.I. Svatiuk, O.M. Pop
Institute of Electronic Physics of the National Academy of Sciences of Ukraine, Uzhhorod, Ukraine
E-mail: volodymyr.maslyuk@gmail.com

The Ball&Stick model and new color statistics are proposed to explain radiation transformations and ordering of bioorganic compounds (BOCs) under the action of high-energy nuclear particles. It is shown that the nature of BOC destruction, in particular, the disruption of molecular polymer structures and their fragmentation, is determined by the conditions of radiation treatment – the type, energy, and intensity of nuclear particle fluxes. The reverse process of thermodynamic ordering of the array of formed fission fragments is similar to the Lego game, in which the assembly of structural fragments can both restore the initial configuration of the BOS and form new molecular complexes and chemical compounds. In this work, such processes are investigated using the example of molecular ethanol C_2H_6O, for which possible structural models, their configurational entropy, and channels for the synthesis of new chemical compounds have been studied. The obtained results explain the findings of radiation experiments on aqueous ethanol solutions conducted at the M-30 microtron.

INTRODUCTION

Unlike crystalline materials, the theory of radiation transformations, which is a complete science, the radiation physics of polymers, both organic, in particular, bioorganic compounds (BOC), and inorganic, is only at its initial stage. Such materials are non-additive structures, the binding energy of which does not depend on the number of atoms, but is determined by the energy of their bonds. For such structures, there are other algorithms for finding the configurational entropy [1]. This requires the development of a new approach to the thermodynamic conditions ordering of polymeric materials, as well as the introduction of new statistics that take into account the non-equivalence of atoms with different binding energies in the structure. The first stages of such an approach are set out in the works on chalcogenide glasses [2], and BOC [3] and they consist in using the Ball&Stick model to describe the polymer network of materials and color statistics to find the configurational entropy. This work is a continuation of the research presented in the work [4], and ethanol CH_3CH_2OH was used as a model object, whose possible structural configurations formed under the action of ionizing radiation, and their energy and entropy characteristics were studied.

THEORY

The basis of this approach is to take into account the short-range order of the BOC atoms and the conditional allocation of atoms of the C, O, and H types, which have different bond energies in the molecule, by a conditional color. For ethanol, we can consider single bonds x1, x2, x3, which form carbon atoms C: respectively, C-C, C-O, and C-H, y1-bonds O-H, and y2, respectively, O-H. In the general case, for BOC, their numbers satisfy the following system of equations:

$$\begin{aligned} 2x1 + x2 + x3 &= 4N_C, \\ x2 + y2 &= 2N_O, \\ x3 + y1 &= N_H. \end{aligned} \qquad (1)$$

Here N_C, N_O, and N_H mean the number of atoms, respectively, of carbon, oxygen, and hydrogen. For ethanol: $N_C = 2$, $N_O = 1$, $N_H = 6$. The structure of the ethanol molecule and metastable structures that are formed from it during radiation treatment can be described by colored sets (CS) of atoms $\{k_i\}$, which have different bond energies in the structure. The following rules for designating colored atoms are introduced: a capital letter denotes the type of atom in an organic molecule (C, O, H), lowercase letters denote atoms in the immediate vicinity with which single chemical bonds are formed. For example, *Ccchh* describes a carbon atom that has two covalent bonds with neighboring carbon atoms and two hydrogen atoms, *Och* is an oxygen atom bonded to carbon and hydrogen, and others. For each set of homo- and heterobonds that satisfy system (1), several CS $\{k_i\}$ can be implemented, which makes it possible to calculate the configurational entropy according to the rule:

$$S_i = \ln\left(\sum_{j=1}^{n} \omega_i\right) = \ln\left(\sum_{j=1}^{n} \frac{M!}{\prod_{j=1}^{n} k_{j!}^{i}}\right), \qquad (2)$$

$$\sum_{j=1}^{n} k_j^i = \mathrm{M}.$$

Table presents data on possible molecular structures that may form during the radiation-induced destruction of ethanol. As can be seen, such structures are fixed through CS, which determine their configurational entropy and bond energy.

Thus, the obtained results demonstrate the possibilities of using the proposed method for studying radiative transformations of BOC.

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Results of the modelling of molecular configurations that can be formed during the radiation destruction of ethanol. Possible values of specific energy and configurational entropy are given

x1	x2	x3	y2	y3	ccchh	cccoh	cccoo	cchhh	ccohh	cchoo	ccooo	chhhh	cohhh	coohh	hc	hh	ho	occ	och	Overall	Entropy, S/N	Energy, E/N
0	6	2	0	0																		
Dimethyl ether					0	0	0	0	0	0	0	0	2	0	6	0	0	1	0		0.61	
Methane + formaldehyde					0	0	0	0	0	0	0	1	0	1	6	0	0	1	0		0.69	
1	4	2	1	0																1	0.73	4.10
Ethylene oxide + hydrogen					0	0	0	0	2	0	0	0	0	0	4	2	0	1	0		0.91	
Acetaldehyde + hydrogen					0	0	0	1	0	1	0	0	0	0	4	2	0	1	0		0.99	
1	5	1	0	1																2	1.03	4.01
Ethanol					**0**	**0**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**1**	**0**	**1**		**0.89**	
2	**2**	**2**	**2**	**0**																**3**	**0.89**	**4.15**
Oxirene + 2 x hydrogen					0	2	0	0	0	0	0	0	0	0	2	4	0	1	0		0.91	
Ketene + 2 x hydrogen					1	0	1	0	0	0	0	0	0	0	2	4	0	1	0		0.99	
2	3	1	1	1																4	1.03	3.91
Vinyl alcohol + hydrogen					1	1	0	0	0	0	0	0	0	0	3	2	1	0	1		1.14	
2	4	0	0	2																5	1.14	4.05
3	0	2	3	0																		
3	1	1	2	1																		
3	2	0	1	2																		
4	0	0	2	2																		

СТРУКТУРНІ МОДЕЛІ РАДІАЦІЙНИХ ПЕРЕТВОРЕНЬ БІООРГАНІЧНИХ СПОЛУК: ЕТАНОЛ

В.Т. Маслюк, В.П. Гануліч, Н.І. Сватюк, О.М. Поп

Модель Ball&Stick та нова кольорова статистика запропоновано для пояснення радіаційних перетворень та упорядкування біоорганічних сполук (БОС) під дією високоенергетичних ядерних частинок. Показано, що характер деструкції БОС, зокрема, порушення молекулярних полімерних структур та їх фрагментація, визначаються умовами радіаційної обробки – сорту, енергії та інтенсивності потоків ядерних частинок. Зворотній процес термодинамічного упорядкування масиву утворених фрагментів поділу подібний грі Лего, коли складання структурних фрагментів може як відновлювати початкову конфігурацію БОС, так і реалізувати нові молекулярні комплекси та хімічні сполуки. У даній роботі такі процеси досліджуються на прикладі молекулярного етанолу C_2H_6O, для якого вивчено можливі структурні моделі, їх конфігураційна ентропія та канали синтезу нових хімічних сполук. Отримані результати пояснюють результати радіаційних експериментів на водних розчинах етанолу, проведених на мікротроні М-30.