

REACTION MECHANISM GRAPHS*

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The concept of reaction mechanism graphs has been introduced. These graphs describe the decomposition of an arbitrary organic reaction into its most elementary mechanistic steps representing heterolytic or homolytic dissociation and association processes, *etc.* A clustering method of reaction mechanism graphs with the same number of elementary steps is specified. The suggested formalism was successfully used in our preliminary computer analysis of reaction mechanism.

In our recent communications¹⁻³ we have introduced the graph-theory approach for mathematical model of organic chemistry. This model covers both static and dynamic aspects of organic chemistry. In particular, the third communication³ of this series is devoted to the so-called reaction graphs which formally represent the change of a molecular graph into another in the course of a chemical transformation process. The reaction graph reflects overall changes in the educt molecular graph, its decomposition into elementary mechanistic steps always running over a pair of atoms and choosing their relative ordering, provides the concept of reaction mechanism graphs. In general, the reaction mechanism graph is a graph, the edges of which are evaluated by ordered 4-tuples specifying more deeply elementary mechanistic steps. We believe that a systematic application of reaction mechanism graphs to the formal analysis of feasible mechanisms⁴⁻⁷ provides the effective tool how to classify and rationalize organic reactions from the standpoint of their mechanistic realization⁸.

Molecular Graphs and Reaction Graphs

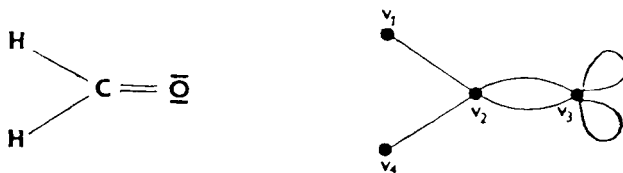
The molecular graph¹ G is defined as an ordered 5-tuple

$$G = (V, E, L, \varphi, \mathcal{B}). \quad (1)$$

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Using the usual graph-theory terminology¹, we say that the molecular graph is a graph, its vertices are evaluated by symbols (in general, alphanumeric strings) belonging to the vocabulary \mathcal{B} . The introduced concept of molecular graph determines abstractly structural formulae of chemistry. Atoms, bonds and electron lone pairs are identified to vertices, edges and loops, respectively, the multiplicity of an edge is the same as the multiplicity of the corresponding bond. The mapping φ evaluates vertices of the molecular graph G by symbols specifying their chemical nature.

Example: The molecular graph of the formaldehyde molecule looks like this



$$V = \{v_1, v_2, v_3, v_4\}, E = \{e_1 = [1, 2], e_2 = [2, 3], e_3 = [2, 3], e_4 = [2, 4]\},$$

$$L = \{l_1 = [3,3], l_2 = [3,3]\}, \text{ the mapping } \varphi \text{ evaluates the vertices by atomic symbols,}$$

$$\varphi(v_1) = \text{H}, \varphi(v_2) = \text{C}, \varphi(v_3) = \text{O}, \varphi(v_4) = \text{H}, \text{ the vocabulary } \mathcal{B} = \{\text{H}, \text{C}, \text{O}\}. \quad (2)$$

Let us have a pair of isomeric¹ molecular graphs $G_1 = (V, E_1, L_1, \varphi, \mathcal{B})$ and $G_2 = (V, E_2, L_2, \varphi, \mathcal{B})$. Formally, postulate that the molecular graph $G_1(G_2)$ corresponds to an educt (product) molecular system. Then, these graphs may be mutually related by the following chemical transformation process

$$G_1 \Rightarrow G_2. \quad (3)$$

Applying the concept of reaction graphs³, the transformation (3) is "algebraized" as follows

$$G_1 + G_R = G_2, \quad (4)$$

where the reaction graph G_R is determined as an ordered 5-tuple

$$G_R = (\tilde{V}, \tilde{E}, \tilde{L}, \Psi, \{-1, +1\}). \quad (5)$$

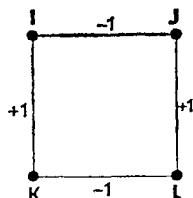
The individual entries of (5) are determined by $\tilde{E} = E_1 + E_2$, $\tilde{L} = L_1 + L_2$, where the binary operation '+' is the "disjunctive sum" of two sets (Appendix in ref.³), $\tilde{V} \subset V$ is composed of those vertices that are incident with edges/loops from \tilde{E} and \tilde{L} , respectively. The mapping Ψ evaluates edges and loops of G_R by integers +1, -1,

$$\Psi(e) = \begin{cases} -1 & (\text{if } e \in E_1) \\ +1 & (\text{if } e \in E_2) \end{cases} \quad (6)$$

$$\Psi(l) = \begin{cases} -1 & (\text{if } l \in L_1) \\ +1 & (\text{if } l \in L_2) \end{cases} \quad (7)$$

This has been done in accordance with the usual convention³, an edge/loop annihilated (created) in a course of process (3) is evaluated by the integer -1 ($+1$). Many examples of reaction graphs covering almost all known organic reactions are listed in our recent communication³.

Example: The reaction graph of the E1 reaction.



Reaction Mechanism Graphs

Following our assumptions⁹, reaction mechanism is understood as a sequence of elementary steps of reorganization of valence electrons (this very important idea was initially introduced to systematize reaction mechanisms by Ingold¹⁰). Each elementary step is running for a pair of atoms; it may be formally represented by a directed edge, its orientation expresses the direction of electron flow. For homolytic processes, where the electron flow should not be specified, the corresponding elementary step is represented by the undirected edge. Furthermore, every edge will be evaluated by an ordered 4-tuple (x_1, x_2, x_3, x_4) with the following meaning of entries:

Entry x_1 – determines the sequential number of the elementary step, $x_1 \in \{1, 2, \dots, n\}$, where n is the total number of elementary mechanistic steps. This may involve some formal difficulties for concerted reactions, see forthcoming sections. Entry x_2 – is equal to a symbol of $\{D, A, \text{Red}_1, \text{Red}_2, D_R, A_R\}$. Hence, an edge corresponds to the heterolytic dissociation or association (if $x_2 = D$ or $x_2 = A$), one- or two-electron redox process (if $x_2 = \text{Red}_1$ or $x_2 = \text{Red}_2$), and homolytic dissociation or association (if $x_2 = D_R$ or $x_2 = A_R$), respectively. Entry x_3 – determines the multiplicity of the broken (dissociation) or formed (association) bond. For redox processes this entry is *a priori* zero ($x_3 = 0$). Then $x_3 \in \{0, 1, 2, 3\}$. Entry x_4 – if $x_4 = 0$ ($x_4 = 1$), then both vertices of the given edge belong to the same component (different components) of educt molecular graph, $x_4 \in \{0, 1\}$. In other words, this entry specifies whether elementary mechanistic step courses for a pair of atoms from the same substrate ($x_4 = 0$) or an atom is from the substrate and another from the reagent ($x_4 = 1$).

Let

$$\mathcal{C} = \{[v, d] \mid v \in \tilde{V} \text{ and } d \in \{0, 1\}\} \quad (8)$$

be a set of ordered pairs $[v, d]$, where the first entry is an arbitrary vertex of \tilde{V} and the second entry is the integer 0 or 1. The mapping

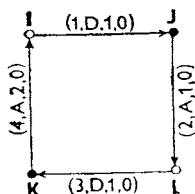
$$\Gamma : \tilde{V} \rightarrow \mathcal{C}' \subset \mathcal{C} \quad (9)$$

assign to every vertex of \tilde{V} a subset of \mathcal{C} ; if $[y, 1] \in \Gamma(x)$, then the ordered pair $[x, y]$ is called the directed edge and represents either heterolytic or redox process, the flow of electrons is determined by the orientation of $[x, y]$, that is from x to y . If $[y, 0] \in \Gamma(x)$, then the pair $[x, y]$ is called the undirected edge and represents the homolytic process. Formally, the reaction mechanism graph is defined as an ordered 6-tuple

$$G_{\text{RM}} = (\tilde{V}, \Gamma, \varphi_1, \mathcal{L}, \varphi, \mathcal{B}), \quad (10)$$

where φ_1 is a mapping of edges (directed and/or undirected) into the set $\mathcal{L} = \{(x_1, x_2, x_3, x_4)\}$ and φ, \mathcal{B} are defined by (1).

Example: The reaction mechanism graph of the second example in the previous section (E1 reaction) looks as follows:



Summarizing, the reaction mechanism graph G_{RM} is composed of those vertices that are originally used for its counterpart G_{R} , the edges are directed as well as undirected. Each edge is evaluated by the ordered 4-tuple (x_1, x_2, x_3, x_4) specifying the sequential number, type, etc. of the given elementary mechanistic step. From the reaction mechanism graph G_{RM} we know all the necessary information how to construct the corresponding reaction graph G_{R} , but from the given G_{R} we are able to construct many different reaction mechanism graphs. The concept of reaction mechanism graphs have been initially introduced in a rudimentary form⁴⁻⁷.

The works of Sinanoglu⁴ and Nemes and coworkers⁵ are mainly devoted to the formal aspects of reaction mechanisms, in particular, to enumerate all the possible reaction mechanisms of an over-all reaction and their mutual independency. Roberts⁶ and Hass and coworkers⁷ have formulated a graphical approach closely related

to our idea of reaction graphs³, the breakdown of the reaction graph ascribed to an over-all reaction on its more elemental ordered sub-units (which is necessary to affect reaction mechanisms) was not done.

String Representation of Reaction Mechanism Graphs

The edges of G_{RM} can be straightforwardly indexed by the first entry of the assigned 4-tuple. In particular, let e_i be an edge, then $i = x_1^{(i)}$. This fact permits the representation of G_{RM} via four alphanumeric strings S_1, S_2, S_3, S_4 (called ANCOD). Formally,

$$\text{ANCOD} : G_{RM} \rightarrow S_1 S_2 S_3 S_4, \quad (11)$$

where the used strings are of the following meaning: String S_1 , the concatenation of second entries of 4-tuples, specifies the type (dissociation, association, etc.) of elementary mechanistic steps, $S_1 = x_2^{(1)} x_2^{(2)} \dots x_2^{(n)}$. In the case that a part of juxtaposed elementary steps belongs to a concerted process, the corresponding symbols may be placed inside of parentheses. String S_2 , the concatenation of third entries of 4-tuples, specifies the multiplicity of bonds, $S_2 = x_3^{(1)} x_3^{(2)} \dots x_3^{(n)}$. String S_3 specifies the topology of G_{RM} , it is formed of successive concatenation of substrings (I_i, J_i) which characterizes the edge e_i incident with the vertices labeled by I_i and J_i . For heterolytic processes the first label is identified with the label of atom which lost a lone electron pair by association ($\bar{I} + J \rightarrow I - J$) or gained a lone electron pair by heterolysis ($\bar{I} - J \rightarrow \bar{I} + J$). For homolytic processes the order of labels I_i and J_i is not distinguished, and finally, for redox processes the first label I_i is identified with the label of that atom which loses electrons (i.e. this atom is oxidized). String S_4 , the concatenation of fourth entries of 4-tuples, specifies whether the given elementary mechanistic step courses or not for two vertices from the same component of educt molecular graph, $S_4 = x_4^{(1)} x_4^{(2)} \dots x_4^{(n)}$.

Example: The ANCOD of reaction mechanism graph for graph presented in the previous section is $\underbrace{\text{DADA}}_{S_1} \underbrace{1112}_{S_2} \underbrace{(J, I)(J, L)(K, L)(K, I)}_{S_3} \underbrace{0000}_{S_4}$

Distance Vector for Reaction Mechanism Graphs

Let us consider two reaction mechanism graphs $G_{RM} = (\tilde{V}, \Gamma, \varphi_1, \mathcal{L}, \varphi, \mathcal{B})$ and $G'_{RM} = (\tilde{V}', \Gamma', \varphi'_1, \mathcal{L}', \varphi', \mathcal{B}')$ with the same number of elementary steps and with strings $x_2^{(1)} x_2^{(2)} \dots x_2^{(n)} x_3^{(1)} x_3^{(2)} \dots x_3^{(n)} (I_1, J_1) (I_2, J_2) \dots (I_n, J_n) x_4^{(1)} x_4^{(2)} \dots x_4^{(n)}$ and $x_2'^{(1)} x_2'^{(2)} \dots x_2'^{(n)} x_3'^{(1)} x_3'^{(2)} \dots x_3'^{(n)} (I'_1, J'_1) (I'_2, J'_2) \dots (I'_n, J'_n) x_4'^{(1)} x_4'^{(2)} x_4'^{(3)} \dots x_4'^{(n)}$.

The distance vector between these two graphs is formally determined as an ordered 4-tuple

$$d(G_{\text{RM}}, G'_{\text{RM}}) = (d_1, d_2, d_3, d_4), \quad (12)$$

where d_1, d_2, d_3, d_4 are non-negative integers specified below. First, we have to define the so-called δ -function

$$\delta(x, x') = \begin{cases} 1 & (\text{if } x \neq x'), \\ 0 & (\text{if } x = x'), \end{cases} \quad (13)$$

where x, x' are either integers or alphanumeric chars¹¹.

Entry d_1 :

$$d_1 = \sum_{i=1}^n \delta(x_2^{(i)}, x'_2{}^{(i)}). \quad (14a)$$

Entry d_2 :

$$d_2 = \sum_{i=1}^n \delta(x_3^{(i)}, x'_3{}^{(i)}). \quad (14b)$$

Entry d_3 : Its determination is not so simple as for d_1 and d_2 , it reflects a "topology" similarity between G_{RM} and G'_{RM} . In order to keep our consideration as simple as possible, we will define the entry d_3 by making use of strings S_3 and S'_3 ; in particular, the value of $d_3 \in \{0, 1, 2, 3\}$ will depend on the type of mapping of S_3 into S'_3 (or reversely S'_3 into S_3). We have to define the F and F' functions:

$$\begin{aligned} F(I_j) &= I'_j, F(J_j) = J'_j \\ F'(I'_j) &= I_j, F'(J'_j) = J_j \quad (j = 1, 2, \dots, n) \end{aligned}$$

The following four different cases should be separately treated:

1) $d_3 = 0$ – there F is identity; 2) $d_3 = 1$ – there F is a one-to-one correspondence (but not identity); 3) $d_3 = 2$ – there F or F' is surjection (but not bijection); 4) $d_3 = 3$ – other possibilities.

Entry d_4 :

$$d_4 = \sum_{i=1}^n \delta(x_4^{(i)}, x'_4{}^{(i)}). \quad (14c)$$

From this determination of the distance vector $d(G_{\text{RM}}, G'_{\text{RM}})$ between an arbitrary pair of reaction mechanism graphs with the same number of edges (elementary mechanistic steps) immediately follows its very important symmetry property

$$d(G_{\text{RM}}, G'_{\text{RM}}) = d(G'_{\text{RM}}, G_{\text{RM}}). \quad (15)$$

Example: We have three reactions determined by ANCOD strings

1)	E1	DADA 1112	(J, I) (J, L) (K, L) (K, I)	0000
2)	E1 ^(B)	DADA 1112	(J, I) (B, L) (K, L) (K, I)	0100
3)	E2	ADAD 1121	(B, L) (K, L) (K, I) (J, I)	1000

Distance vectors are then determined by

$$\begin{aligned}d(G_{\text{RM}}^{(1)}, G_{\text{RM}}^{(2)}) &= d(G_{\text{RM}}^{(2)}, G_{\text{RM}}^{(1)}) = (0, 0, 2, 1) \\d(G_{\text{RM}}^{(1)}, G_{\text{RM}}^{(3)}) &= d(G_{\text{RM}}^{(3)}, G_{\text{RM}}^{(1)}) = (4, 2, 3, 1) \\d(G_{\text{RM}}^{(2)}, G_{\text{RM}}^{(3)}) &= d(G_{\text{RM}}^{(3)}, G_{\text{RM}}^{(2)}) = (4, 3, 2, 2).\end{aligned}$$

Clusters of Reaction Mechanism Graphs

The present formal approach of the reaction mechanisms is very useful for computer analysis. It is based on the similarity of ascribed graphs G_{RM} and strings ANCOD, respectively. In the previous section we have introduced the concept of distance vectors, they quantify by a proper manner the above mentioned similarity between graphs G_{RM} . The purpose of this section is demonstrate a way of the processing of distance vectors and an application of this process will be done. The used method is nothing else than a process of successive comparison (which clusters different reaction mechanisms represented by reaction-mechanism graphs or ANCOD strings) of distance vectors; for different sets of weight coefficients affecting the proposed importance of individual entries of distance vectors we obtain different clustering of studied class of reaction mechanisms.

Let us have a set $\mathcal{G} = \{G_{\text{RM}}^{(1)}, G_{\text{RM}}^{(2)}, \dots, G_{\text{RM}}^{(p)}\}$ of p reaction mechanism graphs with the same number, n , of elementary mechanistic steps. We introduce for distance vectors the abbreviated notation, $d(i, j) = d(j, i) = d(G_{\text{RM}}^{(i)}, G_{\text{RM}}^{(j)})$, where $G_{\text{RM}}^{(i)}, G_{\text{RM}}^{(j)} \in \mathcal{G}$; these entities form a set $\mathcal{D} = \{d(i, j); i < j = 2, 3, \dots, p\}$, $|\mathcal{D}| \leq p(p-1)/2$. The elements of \mathcal{D} may be lexicographically ordered, this ordering depends on a permutation

$$\pi = (\pi_1, \pi_2, \pi_3, \pi_4) = \begin{pmatrix} 1 & 2 & 3 & 4 \\ \pi_1 & \pi_2 & \pi_3 & \pi_4 \end{pmatrix} \quad (16)$$

of entries from the distance vectors. In particular, selecting the permutation π in the form (16) to achieve the lexicographical ordering of distance vectors (d_1, d_2, d_3, d_4) , the first entry to be compared is d_{π_1} , the second d_{π_2} , and so on. Hence, the set \mathcal{D} may be lexicographically ordered by $4! = 24$ different ways by making use of 24 different permutations π of four objects (indices 1, 2, 3, 4). We denote this lexicographical ordering related to the permutation π by \mathcal{O}_π .

After these specification of ordering of \mathcal{D} , we turn our attention to the problem how to cluster the elements of \mathcal{G} with respect to the ordering \mathcal{O}_π . We use the Johnson's method¹² known in the theory and practice of artificial intelligence. Its modification is shortly described. In the first step (initialization) choose the smallest distance vector $d(i, j)$ of \mathcal{D} (with respect to the ordering \mathcal{O}_π). If there exist a few distance vectors classified as smallest, choose an arbitrary of them. Form a cluster $C = \{G_{\text{RM}}^{(i)}, G_{\text{RM}}^{(j)}\}$ and denote these reaction mechanism graphs by the label "clustered" and the remaining ones by the label "unclustered". Unclustered reaction mechanism graphs and the formed clusters (composed of clustered graphs) will be in our forthcoming considerations treated as single graphs. Therefore we have again to recalculate all distance vectors and form a new set \mathcal{D}' , where $|\mathcal{D}'| < |\mathcal{D}|$. The distance vector between two clusters C and C' is determined by

$$d(C, C') = \min \{(i, j) \mid G_{\text{RM}}^{(i)} \in C \text{ and } G_{\text{RM}}^{(j)} \in C'\} \quad (17a)$$

or

$$d(C, C') = \max \{d(i, j) \mid G_{\text{RM}}^{(i)} \in C \text{ and } G_{\text{RM}}^{(j)} \in C'\}. \quad (17b)$$

This formula may be automatically used also for the recalculation of the distance vector between the cluster C and the unclustered graph G_{RM} , the cluster C' is then composed of the graph G_{RM} . The elements of \mathcal{D}' are lexicographically ordered by making use of the same permutation π . In the second step choose the smallest distance vector $d(k, l)$ which was not considered in this step (if there exist more than one, choose an arbitrary of them). The following four different possibilities should be separately treated:

1) The graphs $G_{\text{RM}}^{(k)}, G_{\text{RM}}^{(l)}$ are labeled by "clustered" and belong to the same cluster, the clusters remain without a modification. 2) The graphs $G_{\text{RM}}^{(k)}, G_{\text{RM}}^{(l)}$ are labeled by "clustered" and belong to different clusters, then these clusters are joined together into a bigger new cluster. 3) The graphs $G_{\text{RM}}^{(k)}, G_{\text{RM}}^{(l)}$ are labeled by "clustered" and "unclustered", respectively, and $G_{\text{RM}}^{(k)}$ belongs to a cluster, then the graph $G_{\text{RM}}^{(l)}$ is added to the mentioned cluster and is relabeled by "clustered". 4) The graphs $G_{\text{RM}}^{(k)}, G_{\text{RM}}^{(l)}$ are labeled by "unclustered", then a new cluster composed of them is formed, both graphs are relabeled by "clustered".

Similarly as in the first step, we recalculate distance vectors between clusters and still unclustered graphs (the clusters are treated as single graphs), the resulting vectors are lexicographically ordered with respect to the permutation π . The second step is repeated until all graphs are labeled by "clustered". The formed clusters C_1, C_2, \dots represent a decomposition of the set \mathcal{G} into disjoint subsets

$$\mathcal{G} = C_1 \cup C_2 \cup \dots, \quad (18)$$

where $C_i \cap C_j = \emptyset$ for $i \neq j$. The decomposition (18) must be related to the fixed lexicographical ordering \mathcal{O}_π of \mathcal{D} , for different \mathcal{O}_π we get another decomposition of \mathcal{S} into disjoint clusters. This observation implies very important role of the permutation π , therefore in our forthcoming considerations will be called the classification key.

Illustration of Clustering

Example 1: Let us study the following twelve reaction mechanisms specified by ANCOD strings:

1)	E1	DADA 1112	(J, I) (J, N) (M, N) (M, I)	0000
2)	E1cB	ADDA 1112	(B, N) (M, N) (J, I) (M, I)	1000
3)	E2	ADAD 1121	(B, N) (M, N) (M, I) (J, I)	1000
4)	E2 ⁺	DAAD 1121	(J, I) (B, N) (M, I) (M, N)	0100
5)	Ad _N	DADA 2111	(M, I), (J, I) (J, N) (B, N)	0101
6)	Ad _E 2	ADAD 1211	(I, K) (I, J) (L, J) (L, K)	1010
7)	Ad _E 2	ADDA 1211	(I, K) (I, J) (L, K) (L, J)	1001*
8)	Ad _N (Gr)	ADDA 1211	(M, N) (M, I) (J, M) (J, I)	1001**
9)	S _N 1	DADA 1111	(J, I), (K, I) (K, L) (J, L)	0101
10)	S _N 2	ADAD 1111	(K, I) (J, I) (J, L) (K, L)	1010
11)	S _E 2	ADAD 1111	(I, K) (I, J) (L, J) (L, K)	1010
12)	S _N 2(C ⁺)	DAAD 1111	(J, I) (K, I) (J, L) (K, L)	0110

All different distance vectors are listed and their lexicographical ordering for four different permutations π (Table I). We arrive at four different clustering with classification keys $\pi_1 = (1, 4, 2, 3)$; $\pi_2 = (2, 1, 4, 3)$; $\pi_3 = (4, 1, 2, 3)$; $\pi_4 = (3, 1, 4, 2)$. The results are presented in Table II.

The clustering with respect to the classification key π_1 prefers the sequence of elementary steps (D, A). At the first step, mechanisms Ad_E2 and Ad_N are clustered together, this cluster is enlarged at the seventh step by the mechanism E1cB, denoted by the letter *a*. The common feature of these reactions is that the reaction coordinate runs through the top left corner of More O'Ferrall (MOF) plot¹⁴ with an anionic intermediate. All these reactions contain the same fourth elementary step, association, which essentially determines the rate of formation of product. Starting at the second clustering step the classification key π_1 clusters bimolecular mechanisms with $S_1 = ADAD$, their transition states are located at the centre of MOF plot, *i.e.* S_N2 and S_E2 mechanisms. This cluster is enlarged at the fourth clustering step by E₂ mechanism and at the fifth step by Ad_E, all these mechanisms are denoted by letter *b*. At the third clustering step the classification key starts to form two-element cluster composed of Ad_N and S_N1 mechanisms with the same string $S_1 = DADA$, at the eighth clustering step it is enlarged by E1 mechanism. Their reaction coordinate runs through bottom right corner of MOF plot. The initial step is a dissociation and an existence of the carbocation intermediate is typical for these three mechanisms. At the sixth clustering step the classification key π_1 clusters reactions E2⁺ (with formation of the carbocation in the initial step and the participation of a base in the next step and S_N2(C⁺) (reaction of triphenylmethyl halogenides with oxygen nucleophile with fast heterolysis of C-Hal bond and forthcoming slow association of a reagent in the second step) with $S_1 = DAAD$.

* Fourth step slow.

** Ad_N of Grignard compounds to $\text{>C}=\ddot{\text{O}}$.

TABLE I
All different distance vectors and their lexicographical ordering for four different permutations π

No	Distance vector	Numbers of ANCOD strings	$\pi = (1, 4, 2, 3)$	$\pi = (2, 1, 4, 3)$	$\pi = (4, 1, 2, 3)$	$\pi = (3, 1, 4, 2)$
1.	(4, 2, 3, 1)	(1, 4)	7. (4, 4, 2, 3)	7. (2, 4, 4, 3)	7. (4, 4, 2, 3)	7. (3, 4, 4, 2)
2.	(4, 2, 3, 2)	(1, 6)(2, 4)	9. (4, 4, 1, 3)	6. (2, 4, 3, 2)	9. (4, 4, 1, 3)	9. (3, 4, 4, 1)
3.	(4, 1, 3, 2)	(1, 10)	8. (4, 4, 1, 1)	2. (2, 4, 2, 3)	8. (4, 4, 1, 1)	11. (3, 4, 4, 0)
4.	(4, 1, 1, 2)	(1, 11)	10. (4, 4, 0, 3)	1. (2, 4, 1, 3)	11. (4, 4, 0, 3)	2. (3, 4, 2, 2)
5.	(4, 1, 2, 3)	(2, 12)(3, 9)	11. (4, 4, 0, 1)	17. (2, 2, 3, 3)	10. (4, 4, 0, 1)	3. (3, 4, 2, 1)
6.	(4, 2, 2, 3)	(3, 5)(4, 7)(4, 8)	6. (4, 3, 2, 2)	14. (2, 2, 2, 3)	17. (3, 4, 2, 3)	1. (3, 4, 1, 2)
7.	(4, 2, 3, 4)	(5, 6)	5. (4, 3, 1, 2)	13. (2, 2, 1, 3)	6. (3, 4, 2, 2)	17. (3, 2, 3, 2)
8.	(4, 1, 1, 4)	(5, 10)	2. (4, 2, 2, 3)	16. (2, 2, 0, 3)	18. (3, 2, 1, 3)	18. (3, 2, 3, 1)
9.	(4, 1, 3, 4)	(5, 11)(6, 9)(7, 12)(8, 12)	3. (4, 2, 1, 3)	21. (2, 0, 2, 3)	5. (3, 2, 1, 2)	14. (3, 2, 2, 2)
10.	(4, 0, 1, 4)	(9, 10)	4. (4, 2, 1, 1)	23. (2, 0, 1, 3)	2. (2, 4, 2, 3)	15. (3, 2, 2, 1)
11.	(4, 0, 3, 4)	(9, 11)	1. (4, 1, 2, 3)	9. (1, 4, 4, 3)	3. (2, 4, 1, 3)	20. (3, 2, 2, 0)
12.	(2, 0, 3, 1)	(1, 2)	17. (2, 3, 2, 3)	8. (1, 4, 4, 1)	4. (2, 4, 1, 1)	13. (3, 2, 1, 2)
13.	(2, 2, 3, 1)	(1, 4)(2, 6)(3, 7)(3, 8)(4, 5)	18. (2, 3, 1, 3)	5. (1, 4, 3, 2)	14. (2, 3, 2, 3)	19. (3, 2, 1, 1)
14.	(2, 2, 3, 2)	(1, 7)(1, 8)(5, 7)(5, 8)	14. (2, 2, 2, 3)	3. (1, 4, 2, 3)	15. (2, 2, 1, 4)	12. (3, 2, 1, 0)
15.	(2, 1, 3, 2)	(1, 12)(5, 12)(6, 12)(7, 9)(8, 9)	15. (2, 2, 1, 3)	4. (1, 4, 2, 1)	20. (2, 2, 0, 3)	16. (3, 2, 0, 2)
16.	(2, 2, 3, 0)	(7, 10)(7, 11)(8, 10)(8, 11)	20. (2, 2, 0, 3)	18. (1, 2, 3, 3)	21. (2, 0, 2, 3)	21. (3, 0, 2, 2)
17.	(2, 2, 3, 3)	(2, 3)	13. (2, 1, 2, 3)	15. (1, 2, 2, 3)	22. (2, 0, 1, 3)	22. (3, 0, 2, 1)
18.	(2, 1, 3, 3)	(2, 5)(4, 6)	19. (2, 1, 1, 3)	19. (1, 2, 1, 3)	1. (1, 4, 2, 3)	23. (3, 0, 1, 2)
19.	(2, 1, 3, 1)	(2, 9)(3, 12)(4, 10)(4, 11)	12. (2, 1, 0, 3)	22. (1, 0, 2, 3)	13. (1, 2, 2, 3)	25. (3, 0, 1, 1)
20.	(2, 0, 3, 2)	(2, 10)(2, 11)(4, 9)	16. (2, 0, 2, 3)	25. (1, 0, 1, 3)	19. (1, 2, 1, 3)	27. (3, 0, 0, 1)
21.	(0, 2, 3, 2)	(3, 4)(6, 7)(6, 8)(9, 12)	21. (0, 2, 2, 3)	24. (1, 0, 1, 2)	12. (1, 2, 0, 3)	29. (3, 0, 0, 0)
22.	(0, 1, 3, 2)	(10, 12)(11, 12)	22. (0, 2, 1, 3)	27. (1, 0, 0, 3)	23. (1, 0, 2, 3)	6. (2, 4, 3, 2)
23.	(0, 2, 3, 1)	(1, 5)	23. (0, 1, 2, 3)	26. (1, 0, 0, 1)	25. (1, 0, 1, 3)	5. (2, 4, 3, 1)
24.	(0, 1, 2, 1)	(1, 9)	25. (0, 1, 1, 3)	11. (0, 4, 4, 3)	24. (1, 0, 1, 2)	24. (2, 0, 1, 1)
25.	(0, 1, 3, 1)	(2, 7)(3, 8)(3, 6)	24. (0, 1, 2, 2)	10. (0, 4, 4, 1)	16. (0, 2, 2, 3)	8. (1, 4, 4, 1)
26.	(0, 1, 1, 0)	(3, 10)	27. (0, 0, 1, 3)	20. (0, 2, 2, 3)	27. (0, 0, 1, 3)	10. (1, 4, 4, 0)
27.	(0, 1, 3, 0)	(3, 11)(4, 12)	26. (0, 0, 1, 2)	12. (0, 2, 1, 3)	26. (0, 0, 1, 1)	4. (1, 4, 2, 1)
28.	(0, 0, 3, 0)	(5, 9)	28. (0, 0, 0, 3)	29. (0, 0, 0, 3)	29. (0, 0, 0, 3)	26. (1, 0, 0, 1)
		(6, 10)(16, 11)				
		(7, 9)(10, 11)				

On the MOF plot these reactions are located between centre and bottom right corner. We may say that the classification key π_1 classifies the studied reaction mechanisms from the standpoint of the position of transition states on the MOF plot.

The clustering of reaction mechanisms with the classification key π_2 , provides very rough classification reflecting changes of hybridization states of atoms at reaction sites. The cluster composed of additions with increasing hybridization of carbon atom ($sp \rightarrow sp^2$ and $sp^2 \rightarrow sp^3$) was formed after five clustering steps, the cluster of substitutions (hybridization is saved) was formed after four clustering steps. The third cluster of elimination (hybridization is decreased) was formed after four clustering steps.

The classification π_3 prefers reactions with similar participation of reagents. In particular, at the first and second clustering steps (letters a and b, respectively) are clustered those reactions for which a participation of another component is very important (reagent, catalytor). At the third step are clustered together S_N1 and Ad_N mechanisms, they are initialized by the dissociation of strategic substrate bond for which a participation of other components is irrelevant (the strings S_4 and S_1 are very important). This cluster is enlarged at the eighth clustering step by the mechanism E1.

TABLE II

Clustering of reaction mechanism graphs. This table contains the process of successive inclusions of individual G_{RM} into different clusters. Its rows are assigned to reaction mechanism graphs, the broad columns represent individual steps of the used clustering, and the narrow columns (placed inside of broad columns) represent different classification keys $\pi_1, \pi_2, \pi_3, \pi_4$. If a pair of graphs $G_{RM}^{(k)}$ and $G_{RM}^{(l)}$ belongs to the cluster (with respect to a fixed classification key π_i), then the same letter is placed in the table for the column π_i and rows k and l . For instance, the clustering with the classification key π_1 may be schematically expressed as follows (the graphs are represented by their indices): (7, 8) \rightarrow (7, 8) (10, 11) \rightarrow (7, 8) (10, 11) (5, 9) \rightarrow (7, 8) (10, 11, 3). (5, 9) \rightarrow (7, 8) (10, 11, 3, 6) (5, 9) \rightarrow (7, 8) (10, 11, 3, 6) (5, 9) (4, 12) \rightarrow (7, 8, 2) (10, 11, 3, 6). (5, 9) (4, 12) \rightarrow (7, 8, 2) (10, 11, 3, 6) (5, 9, 1) (4, 12)

Step No	1				2				3				4				5				6				7				8											
	Key				Key				Key				Key				Key				Key				Key															
Mechanism	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4								
1 E1						b	c	b		c	b	c		b	c	b						b								e	c	c		e						
2 E1cB								c				c			c	d		c	d	c		e	c	a		e	c	a		e	c	e								
3 E2										b	d	a		b	d	d		a	b	d		e	a	b		e	e	b		e	e	e								
4 E2 ⁺											d				d				d			d	d	d		d	d	d		d	d	d								
5 Ad _N						a				a	c	c		a	c	c		a	c	c		b	c	a		c	c	a		c	c	c		e	c	e				
6 Ad _E												a		b				b	a	b		b	e			b	e			b	e	e								
7 Ad _E 2	a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a	
8 Ad _N (Gr)	a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a		a	a	a	
9 S _N 1		a				a				c	c	a		c	b	c		a	c	b		c	a	c		c	a	c		c	e	c		c	e	c				
10 S _N 2					b	b	b		b	b	b	a	b	b	b	a	b	b	b	a	b	b	b	a	b	e	a	b	e	e	b	e	e	e	b	e				
11 S _E 2					b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	e	b	b	e	e	b	e	e	e	b	e				
12 S _N 2(C ⁺)												b						b				c	d			c	d			d	c	d		d	c	d				

The classification key π_4 prefers the topology of assigned reaction mechanism graphs. In order to obtain reasonable results for this classification key, we have to use a unified labeling of atoms (vertices). The obtained clustering of studied reaction mechanisms produces their vague decomposition into different clusters. Likely, this classification key might be of an importance only for rather extensive data base of reaction mechanisms.

Example 2: ANCOD strings for same set of nucleophile reaction mechanisms:

1)	S_N2	ADAD 1111	(K, I) (J, I) (J, L) (K, L)	1010
2)	S_Ni	ADDA 1112	(K, I) (J, I) (K, L) (J, L)	1001
3)	S_N2'	ADDA 1212	(K, N) (M, N) (J, I) (M, I)	1000
4)	$S_N2(\text{Ar})$	ADDA 1212	(K, I) (M, I) (J, I) (M, I)	1000
5)	S_N1	DADA 1111	(J, I) (K, I) (K, L) (J, L)	0101
6)	S_N1'	DADA 1122	(J, I) (K, N) (M, N) (M, I)	0100
7)	$S_N2(\text{C}^+)$	DAAD 1111	(J, I) (K, I) (J, L) (K, L)	0110
8)	$\text{Ad}_N(\text{C}=\text{O})$	ADAD 1211	(J, I) (M, I) (M, N) (J, N)	1010
9)	$\text{Ad}_N(\text{C}=\text{O})$	ADAD 1112	(M, N) (B, N) (J, I) (M, I)	1010
10)	$\text{Ad}_N(\text{C}=\text{Z})$	ADAD 1211	(J, I) (M, I) (M, N) (K, N)	1010
11)	$\text{Ad}_N(\text{C}=\text{O})$	ADDA 1211	(M, N) (M, I) (J, M) (J, I)	1001
12)	$\text{B}_{Ac}2$	ADDA 1212	(J, I) (M, I) (K, I) (M, I)	1000

The results of our clustering procedure are given in Table III. In the following we discuss the obtained clusters of reaction mechanisms globally relating to all classification keys.

a) The mechanisms $S_N2(\text{Ar})$ and $\text{B}_{Ac}2$ are similar in a D_N substituent and the elementary reaction step Ad_N (a π -bond is broken and successively formed). Their graphs are isomorphic (they are different only in a permutation of entries from S_3 strings). At the second clustering step S_N2' is added containing also a broken π -bond, but now instead of its reconstruction there exists a transition of the electron pair to a juxtaposed bond.

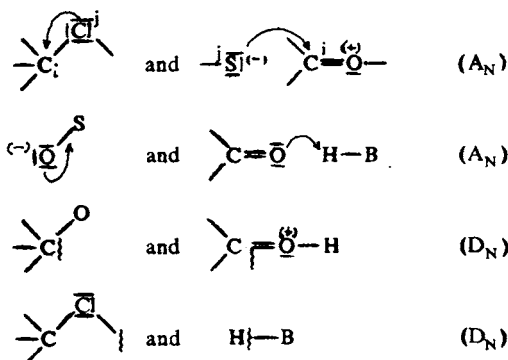
b) $\text{Ad}_N(\text{C}=\text{O})$ and $\text{Ad}_N(\text{C}=\text{Z})$ are mechanisms of nucleophile additions to double bonds, they are different only in an additional reaction step for another atom from the reagent. The mechanism S_N2 is added. We may look for a similarity between steps of the nucleophile association: $\text{Nu} \overset{\curvearrowright}{>}\text{C}-\text{X}$ and $\text{Nu} \overset{\curvearrowright}{>}\text{C}=\text{X}$. For the mechanism S_N2 the graph edge (J, I) corresponds to a dissociation, whereas for the mechanism Ad_N the edge (J, I) is an association. Another similarity there exists in the dissociation steps of $\text{C}\overset{\curvearrowright}{-}\text{X}$ and $\text{C}\overset{\curvearrowright}{=}\text{X}$ bonds, and also in the final reaction step in which an electrophile part of the reagent is connected with anions $\bar{\text{X}}^{(-)}$ and $-\bar{\text{O}}^{(-)}$, respectively. At the end of clustering process the mechanism $\text{Ad}_N(11)$ is added, this is only a small modification of $\text{Ad}_N(8)$, they have different rate of reaction steps corresponding to edges (J, I), (M, N) and (J, N) (J, I).

c) The mechanisms S_N2 , S_N1 , $S_N2(\text{C}^+)$. The mechanisms S_N2 and S_N1 are different in their molecularities, *i.e.* both these mechanisms contain elementary reaction steps D and A, only their order is transposed. The mechanism $S_N2(\text{C}^+)$ is kinetically closely related to the mechanism S_N2 . Formally, it may be treated as a version of S_N1 , they have only differently ordered elementary reaction steps. We say that the mechanism $S_N2(\text{C}^+)$ represent a link between S_N2 and S_N1 . After third clustering step the item (b) is enlarged by S_N1 , it is also a nucleophile substitution, elementary reaction steps are similar, only their mutual ordering is different. After fourth clustering step the item (b) is enlarged by $\text{Ad}_N(\text{C}=\text{O})(9)$ which is the mechanism $\text{Ad}_N(\text{C}=\text{O})(8)$ with added general acid catalysis.

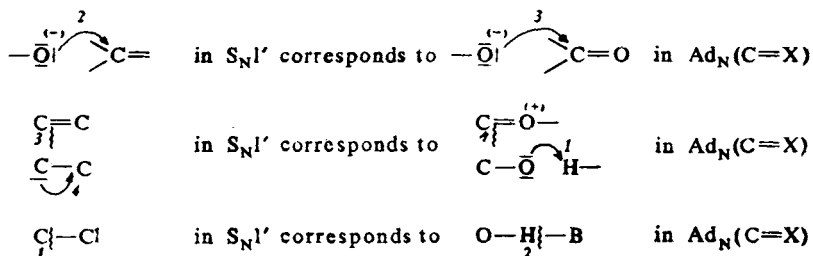
TABLE III
Clustering of reaction mechanism graphs

No	Step		2		3		4		5		6		7		8		9			
	1	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2		
Mechanism	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
1 SN2		b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b
2 SNi			d	d	c	c	c	c	c	c	c	c	c	c	c	c	c	c	c	c
3 SN2'		aaa	aaa	aaa	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a
4 SN2(Ar)	aaaa	aaaa	aaaa	aaaa	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a
5 SNi			c	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b
6 SNi'			c	d																
7 SN2(C ⁺)			c	c	c	c	c	c	c	c	c	c	c	c	c	c	c	c	c	c
8 AdN(C=O)		bbb	bbb	bbb	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b
9 AdN(C=O)			d	d	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b
10 AdN(C=Z)		bbb	bbb	bbb	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b
11 AdN(C=O)		aaaa	aaaa	aaaa	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b	b
12 B _{AC} 2	aaaa	aaaa	aaaa	aaaa	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a

d) The mechanisms S_{N_i} and $Ad_N(C=O)$. Their similarity is based on the assumption that an analogy between elementary reaction steps A and D is accepted.



After fourth clustering step are clustered together S_{N_i} , $Ad_N(9)$ and $S_{N1'}$.



After fourth clustering step the item (c) is enlarged by S_{N_i} : it is known a similarity between A_N step in S_{N2} on C^i and D_N step in S_{N1} on C^i (C^i —O), hence its attachment to the item (c) looks naturally. After fifth clustering step the item (c) is enlarged by $Ad_N(11)$, this is closely related to the same event in the item (b) between S_{N2} , $Ad_N(8)$, $Ad_N(10)$, i.e. this mechanism we may consider as a link with the item (b). After sixth clustering step the item (d) is enlarged by S_{N_i} , $S_{N2'}$, $S_{N2}(Ar)$, $Ad_N(11)$, B_{Ac2} . Their common feature is an attack of a nucleophile with a participation of the π -bond. The mechanism B_{Ac2} is linked through $S_{N2}(Ar)$, their graphs are different only in a permutation of S_3 strings. Similarly, the mechanism $Ad_N(11)$ is linked through S_{N_i} . After seventh clustering step are added S_{N1} and $S_{N1'}$, they have different only S_2 strings. Finally, after eighth clustering step we have obtained two big clusters, the first (second) one is composed of all bimolecular substitutions (nucleophile additions to multiple bonds).

Concerted Processes

Let us consider a reaction mechanism graph G_{RM} , some part of its juxtaposed elementary steps corresponds to a concerted process. If we permute the relative order of these elementary steps by the so-called feasible permutation P we arrive at another reaction mechanism graph formally denoted by PG_{RM} . It expresses the same me-

chanism as the original graph G_{RM} , but now the relative ordering of elementary steps assigned to the concerted process is different with respect to G_{RM} and is unambiguously specified by the feasible permutation P . The distance vector between two graphs $G_{RM}^{(1)}$ and $G_{RM}^{(2)}$ with the same number of elementary steps and juxtaposed steps of concerted processes is determined for a classification key π (specifying the lexicographical ordering θ_π) by

$$d_\pi(G_{RM}^{(1)}, G_{RM}^{(2)}) = \min_{P_1, P_2} \{d(P_1 G_{RM}^{(1)}, P_2 G_{RM}^{(2)})\}_{\theta_\pi}, \quad (19)$$

where the minimum is taken for the given lexicographical ordering θ_π . Employing this enlarged definition of the distance vector for reaction mechanism graphs of concerted processes, the Johnson's clustering method is automatically applicable.

Example: We illustrate the Johnson's clustering method for the following eight reactions (specified by ANCOD in the previous section): (1) E1, (2) E1cB, (3) E2, (4) Ad_N, (5) Ad_E, (6) S_N1, (7) S_N2, and (8) S_E2. Furthermore, let us assume that for reactions 3, 5, 7, and 8 the last three elementary steps are concerted. For two classification keys $\pi = (1, 4, 2, 3)$ and $\pi = (2, 1, 4, 3)$ we get the following clustering:

1) Classification key $\pi = (1, 4, 2, 3)$

$$C_1 = \{2, 3, 5, 7, 8\} = \{S_{N2}, S_{E2}, Ad_E, E1cB, E2\}$$

$$C_2 = \{1, 4, 6\} = \{Ad_N, S_{N1}, E1\}.$$

2) Classification key $\pi = (2, 1, 4, 3)$

$$C_1 = \{4, 6, 7, 8\} = \{S_{N2}, S_{E2}, Ad_N, S_{N1}\}$$

$$C_2 = \{1, 2, 3, 5\} = \{E1cB, E2, E1, Ad_E\}.$$

We have obtained almost the same clustering as for the asynchronous reactions studied in the previous section.

Immersion of Reaction Mechanism Graphs

In order to relate mutually two reaction mechanism graphs $G_{RM} = (\tilde{V}, \Gamma, \varphi_1, \mathcal{L}, \varphi, \mathcal{B})$ and $G'_{RM} = (\tilde{V}', \Gamma', \varphi'_1, \mathcal{L}', \varphi', \mathcal{B}')$. We introduce a concept of the so-called immersion of G'_{RM} into G_{RM} if the following requirements are satisfied:

1) $\tilde{V}' \subset \tilde{V}$, 2) $\Gamma(v) = \Gamma'(v)$ for every $v \in \tilde{V}'$, 3) for every edge e' of G'_{RM} there must exist an edge e of G_{RM} in such a way that their evaluation by 4-tuples (realized by mapping φ_1 and φ'_1 , respectively) saves the second and third entry,

$$\varphi'_1(e') = (x'_1, x'_2, x'_3, x'_4) \Rightarrow \varphi_1(e) = (x_1, x'_2, x'_3, x_4),$$

and the difference $(x_1 - x'_1)$ is a constant integer for all such pairs of e and e' (it

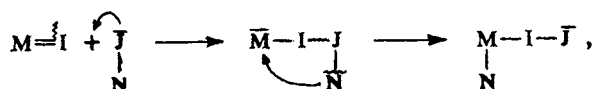
means the serial number of e' is only shifted about a constant integer with respect to the edge e).

The graph G'_{RM} is strongly immersed into the graph G_{RM} if the next two requirements are satisfied too,

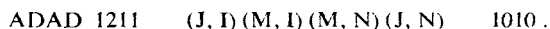
4) $\mathcal{B}' \subset \mathcal{L}$, 5) for every $v \in \tilde{V}'$ we have $\varphi'(v) = \varphi(v)$ (i.e. vertices of G'_{RM} are evaluated by the same symbols as in the graph G_{RM}).

The immersion relation among reaction mechanism graphs leads to the concept of partial ordering of all graphs.

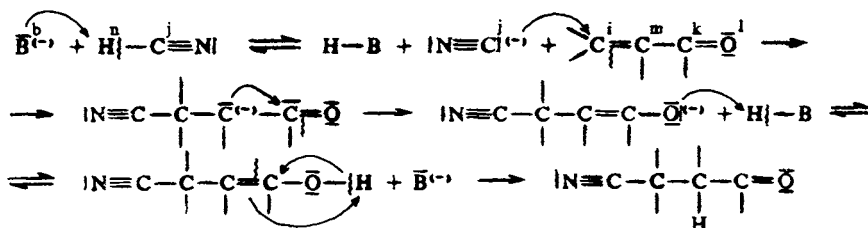
Example: Rearrangement of enols via the nucleophile addition is immersed into the mechanism of the nucleophilic addition to systems $C=C-C=O$. Schematically, the Ad_N reaction (in this case) is



assigned ANCOD is then determined by



For the nucleophilic addition to systems $C=C-C=O$



the corresponding ANCOD is ADADAD AD ADAD 111222 11 1211 (B, N) (J, N) (J, I) (M, I) . (M, K) (L, K) (L, N) (B, N) (L, K) (M, K) (M, N) (L, N) 101000 10 1010.

It is easy to see, that the last four steps of the mechanism of nucleophilic addition to systems $C=C-C=O$ are the mechanism Ad_N .

CONCLUSIONS

Three main targets have been aimed at in this paper. As far as a model is concerned, we have tried to develop formal apparatus for a more exact evaluation of similarities and differences between chemical reactions, in other words, to develop formal apparatus for defining the distance between the graphs G_{RM} . Further, we have aimed at developing formal means for approximately evaluating and predicting reactivity of a certain part of a real chemical system and, last but not least, at utilizing the

apparatus for specifying a limited number of often a repeatedly encountered, so called, typized reaction mechanisms which, by itself or in combinations, lead to mechanisms of other chemical reactions.

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