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(27) A ring structure wherein p ITS bonds have complex bond numbers of $a + b = 0$ and all other ITS bonds have (a b) of $a + b \neq 0$ and $a \neq 0$ is called a bridge of ring opening of order p (BO_p). The presence of BO_p corresponds to cleavage of p bonds.
(28) A ring structure in which p ITS bonds have complex bond numbers (a b) of $a = 0$ and all other ITS bonds have (a b) of $a + b \neq 0$ and $a \neq 0$ is called a bridge of ring closure of order p (BC_p).
(29) A ring structure that has one ITS bond of $a + b = 0$, another ITS bond of $a = 0$, and other bonds all of $a + b \neq 0$ and $a \neq 0$ is defined as a bridge of rearrangement (BR).
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Description of Organic Reactions Based on Imaginary Transition Structures. 7. Classification and Enumeration of Two-String Reactions with Two or More Common Nodes

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Two-string reactions that have two reaction strings with two or more common nodes are classified by their reaction graphs. Several representative two-string reaction graphs are enumerated by Polya's theorem. Matrix representations of reaction graphs and their canonical forms are discussed.

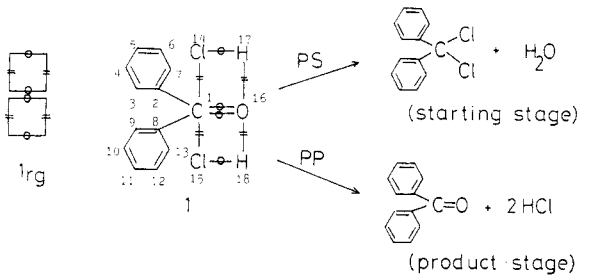
Name reactions have formed an important part of synthetic organic chemistry. However, manipulation of their information has troubled organic and information chemists because many of them contain multistep reactions. For example, the Claisen–Schmidt reaction, the Knoevenagel reaction, aldol condensation, and so on have been retrieved only in terms of their names, since there have been no effective methods for describing structural changes during the reactions.

An imaginary transition structure (ITS) proposed previously is a kind of structural formula with three colored bonds (out-, in-, and par-bonds).[1,2] This novel formulation has afforded versatile methodology in the manipulation of organic reactions, even if these contain multiple steps. Reaction strings, which are extracted from an ITS as graphs with alternate out- and in-bonds, are indicators for the classification of organic reactions, especially of name reactions.[3] Rings involved in ITS's are indices for recognition of ring opening and ring closure and of rearrangement reactions.

As a continuation of the preceding paper,[1] which gives several rules for selection of two or more reaction strings from an ITS, the present paper will discuss their application to further types of organic reactions.

CONNECTION TABLES OF ITS'S, OF RC GRAPHS, AND OF REACTION STRINGS

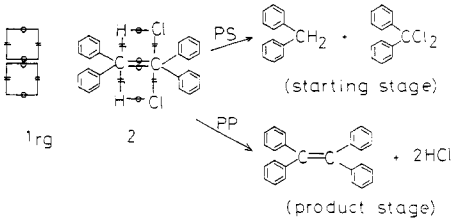
Formation of benzophenone from 1,1-dichloro-1,1-diphenylmethane is represented by ITS **1**.[3,4] The ITS is stored and manipulated by a computer in the form of a connection table of ITS's (Table I). The graph of reaction centers of level 1 (RC graph (1)) is a set of nodes that are incident to in- and out-bonds and the imaginary bonds between them. The corresponding reaction graph, in which values of nodes are ignored in a more abstract sense, is expressed by the formula $\mathbf{1}_{rg}$. The RC graph (1) corresponds to a connection table as shown in Table II.



Two reaction strings, 1–14+17–16+1 and 1–15+18–16+1, are abstracted graphically and represented by a connection table as shown in Table III.

EXAMPLES AND ENUMERATION OF TWO-STRING REACTIONS IN WHICH THE TWO TETRAGONAL REACTION STRINGS SHARE TWO NODES AND ONE ITS BOND

The condensation of diphenylmethane and dichlorodiphenylmethane[5] is represented by ITS **2**. The corresponding



reaction graph $\mathbf{1}_{rg}$ has two tetragonal reaction strings, which fuse at one edge. The reaction strings are extracted as 1–14+29–16+1 and 1–15+30–16+1, wherein – and + represent out- and in-bonds, respectively.

Formation of a ketone from a *gem*-dichloride[6] provides ITS **3** of two strings. The two tetragonal reaction strings share

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Table I. Connection Table of ITS **1**

node	atom or group	coordinate x	coordinate y	neighbor 1 node	neighbor 1 (a b)	neighbor 2 node	neighbor 2 (a b)	neighbor 3 node	neighbor 3 (a b)	neighbor 4 node	neighbor 4 (a b)	neighbor 5 node	neighbor 5 (a b)
1	C	0	0	2	(1+0)	8	(1+0)	14	(1-1)	15	(1-1)	16	(0+2)
2	C	-100	50	1	(1+0)	3	(1+0)	7	(2+0)				
3	CH	-200	50	2	(1+0)	4	(2+0)						
4	CH	-250	100	3	(1+0)	5	(1+0)						
5	CH	-200	150	4	(1+0)	6	(2+0)						
6	CH	-100	150	5	(2+0)	7	(1+0)						
7	CH	-50	100	2	(2+0)	6	(1+0)						
8	C	-100	-50	1	(1+0)	9	(1+0)	13	(2+0)				
9	CH	-200	-50	8	(1+0)	10	(2+0)						
10	CH	-250	-100	9	(2+0)	11	(1+0)						
11	CH	-200	-150	10	(1+0)	12	(2+0)						
12	CH	-100	-150	11	(2+0)	13	(1+0)						
13	CH	-50	-100	8	(2+0)	12	(1+0)						
14	Cl	0	100	1	(1-1)	17	(0+1)						
15	Cl	0	-100	1	(1-1)	18	(0+1)						
16	O	100	0	1	(0+2)	17	(1-1)	18	(1-1)				
17	H	100	100	14	(0+1)	16	(1-1)						
18	H	100	-100	15	(0+1)	16	(1-1)						

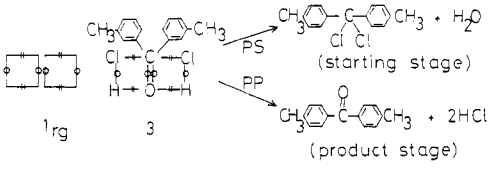
Table II. Connection Table for RC Graph (1) for Reaction of Entry 1

node	atom	neighbor 1 node	neighbor 1 (a b)	neighbor 2 node	neighbor 2 (a b)	neighbor 3 node	neighbor 3 (a b)
1	C	14	(1-1)	15	(1-1)	16	(0+2)
14	Cl	1	(1-1)	17	(0+1)		
15	Cl	1	(1-1)	18	(0+1)		
16	O	1	(0+2)	17	(1-1)		
17	H	14	(0+1)	16	(1-1)		
18	H	15	(0+1)	16	(1-1)		

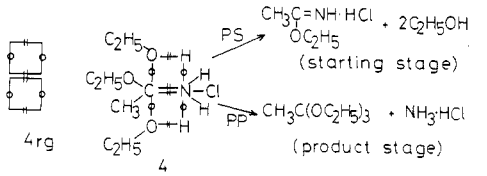
Table III. Connection Table of the Reaction Strings for Reaction of Entry 1

node	atom	bond (a b)	neighbor 1 node	neighbor 1 (a b)	neighbor 2 node	neighbor 2 (a b)
			String 1			
1	C	(1-1)	C	(1+0)	C	(1+0)
14	Cl	(0+1)				
17	H	(1-1)				
16	O	(0+2)				
1	C					
			String 2			
1	C	(1-1)	C	(1+0)	C	(1+0)
15	Cl	(0+1)				
18	H	(1-1)				
16	O	(0+2)				
1	C					

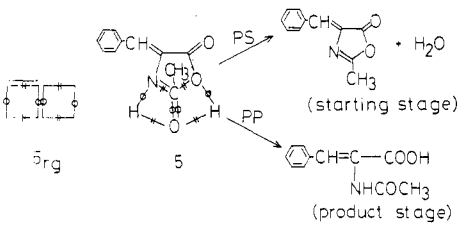
two adjacent nodes. The reaction graph of this reaction is the same as that of reaction of entry **2**.



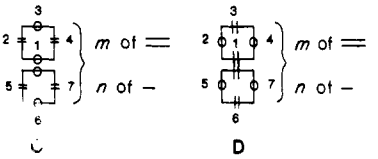
Formation of ethyl orthoacetate from ethyl iminoacetate hydrochloride[7] has ITS **4** of two-strings. The abstracted reaction graph $\mathbf{4}_{rg}$ contains two tetragonal reaction strings, which share two adjacent nodes.



Hydrolysis of an azlactone[8] is represented by ITS **5**, which has two tetragonal reaction strings fusing at an edge. This reaction needs neither acid nor base catalysis. The reaction graph $\mathbf{5}_{rg}$ is modified by a single par-bond.



The reaction graphs of this type are enumerated by use of Polya's theorem.[9] The cycle index $Z(\mathbf{D}_2)$ for enumeration of reaction graphs based on the basic graph **C**, which can be



superposed on itself by four permutation operations, i.e., (1)(2)...(7), (1)(2 7)(4 5)(3 6), (1)(2 5)(4 7)(3 6), and (1)(2 4)(5 7)(3)(6), is shown in eq 1. When each variable s_k in

$$Z(\mathbf{D}_2) = (1/4)(s_1 + 2s_1s_2^3 + s_1^3s_2^2) \quad (1)$$

$$s_k = 1 + x^k + y^k \quad (2)$$

$$G(x,y) = 1 + 3x + 3y + 8x^2 + 12xy + 8y^2 + 12x^3 + \ldots \quad (3)$$

eq 1 is substituted by a figure-containing series (eq 2), the resulting polynomial series ($G(x,y)$ of eq 3) gives the numbers of reaction graphs as the coefficients of the terms $x^m y^n$.

The basic graph **C** is converted into the corresponding reverse reaction graph **D** by transformation of reverse reaction. As a result, each graph based on **C** is transferred to the counterpart based on **D**. Each pair of such graphs constructs a reaction pair. Table IV collects the lower members of reaction graphs based on **C**. Reaction graphs based on **D** can be obtained by transformation to reverse reaction, i.e., exchange of all in-bonds and out-bonds with each other.

EXAMPLES AND ENUMERATION OF TWO-STRING REACTIONS IN WHICH THE TWO HEXAGONAL REACTION STRINGS SHARE TWO NODES AND ONE ITS BOND

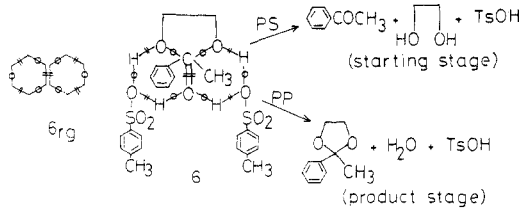
The acetalization (ITS **2**) described in the preceding paper

Table IV. Reaction Graphs Based on the Graph C ($m = 0$, $n = 0$–4)[a]

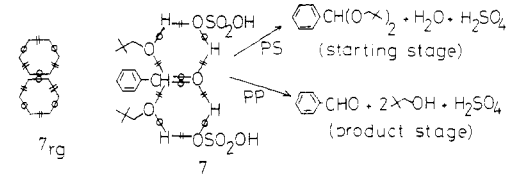
m	n	no. of reacn graphs[b]	reaction graphs
0	0	1	
0	1	3	
0	2	8	
0	3	12	
0	4	12	

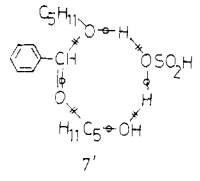
[a] The counterpart based on graph **D** can be obtained by transformation of each reaction graph collected above to reverse reaction. [b] The numbers of reaction graphs are the coefficients of $x^m y^n$ in $G(x,y)$ (eq 3).

is an example of this type. The following example is formation of a cyclic acetal (1,3-dioxolane).[10]

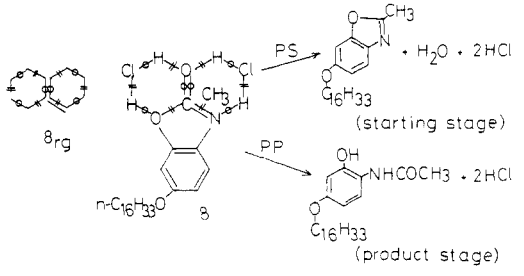


Hydrolysis of dineopentyl acetal of benzaldehyde has been reported to result in the recovery of neopentyl alcohol. No rearranged products were observed.[11] This fact indicates that the hydrolysis of the acetal corresponds to ITS **7** and not to ITS **7′**.

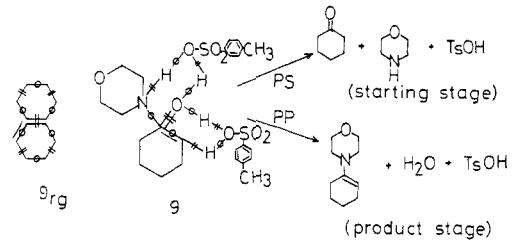




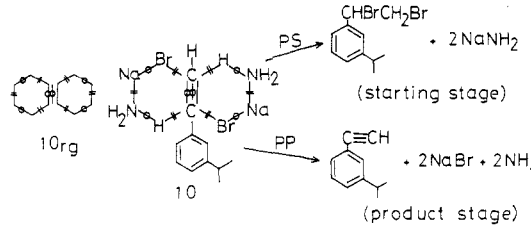
Hydrolysis of a benzoxazole[12] is represented by ITS **8**, which is characterized by a reaction graph of two strings ($\mathbf{8}_{rg}$).



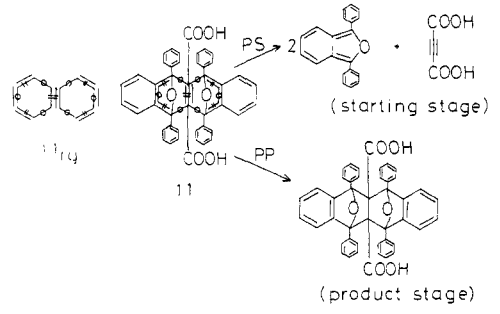
Enamine formation[13] yields ITS **9**, from which fused reaction graph $\mathbf{9}_{rg}$ can be abstracted. The reaction graph is modified by a single par-bond.



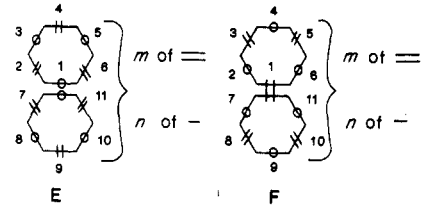
Formation of an acetylene via a vicinal dibromide[14] is represented by ITS **10**. The corresponding two-string reaction graph $\mathbf{10}_{rg}$ is modified by a single par-bond at the fused edge, which is denoted by ITS bond (1+2).



A further complex example is the double Diels–Alder addition,[15] which is characterized by ITS **11**. The reaction graph $\mathbf{11}_{rg}$ has seven modifying single par-bonds.



The basic graph **E** or **F** is invariant with respect to four permutational operations, i.e., (1)(2)...(11), (1)(2 11)(3 10)(4 9)(5 8)(6 7), (1)(2 7)(3 8)(4 9)(5 10)(6 11), and (1)(2 6)(3 5)(4)(7 11)(8 10)(9), when the edges are numbered as shown.



$$Z(\mathbf{D}_2) = (1/4)(s_1^{11} + 2s_1s_2^5 + s_1^3s_2^4) \quad (4)$$

$$G(x,y) = 1 + 4x + 4y + 18x^2 + 29xy + 18y^2 + 47x^3 + 130x^2y + 130xy^2 + 47y^3 + 92x^4 + \ldots \quad (5)$$

Hence, the cycle index $Z(\mathbf{D}_2)$ and the graph-counting polynomial series $G(x,y)$ are as follows. The coefficients of $x^m y^n$ in $G(x,y)$ (eq 5) are the numbers of the reaction graphs based on **E** (or **F**) that have m double par-bonds and n single par-bonds.

The list of lower members counted by eq 5 is found in Table V, which shows only the graphs based on **E**. The reaction graphs based on **F** can be easily obtained by transformation of the corresponding graphs of Table V into the reverse reaction graphs.

Table V. Reaction Graphs Based on Graph **E** (m = 0, n = 0–3)[a]

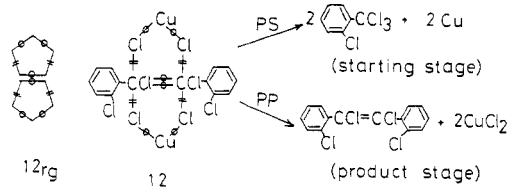
m	n	no. of reacn graphs[b]	reaction graphs
0	0	1	
0	1	4	
0	2	18	
0	3	47	

[a] The counterpart based on graph **F** can be obtained by transformation of each reaction graph collected above to reverse reaction. [b] The numbers of reaction graphs are the coefficients of $x^m y^n$ in $G(x,y)$ (eq 5).

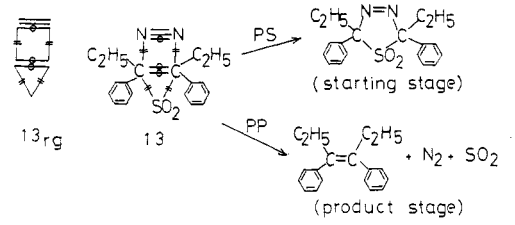
OTHER TYPES OF TWO-STRING REACTIONS IN WHICH THE TWO REACTION STRINGS SHARE TWO NODES AND ONE ITS BOND

Further examples that have two reaction strings sharing two adjacent nodes will be mentioned here:

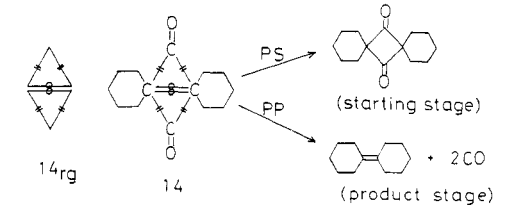
Olefin formation via coupling[16]



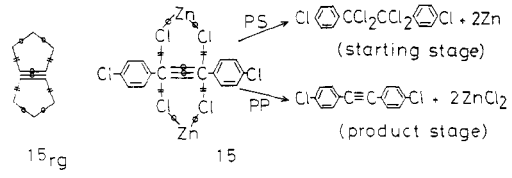
Staudinger–Pfenninger elimination[17]



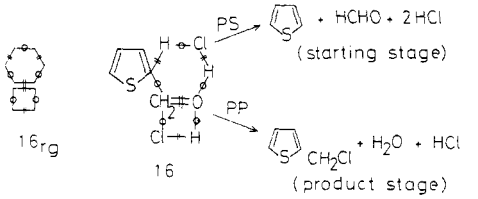
Olefin from 1,3-cyclobutanones[18]



Reductive formation of an acetylene[19]

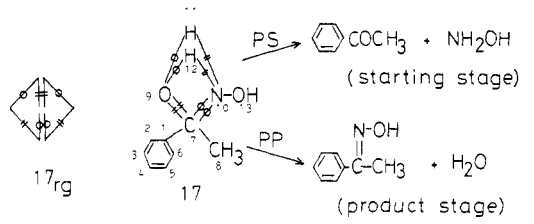


Chloromethylation of thiophene[20]



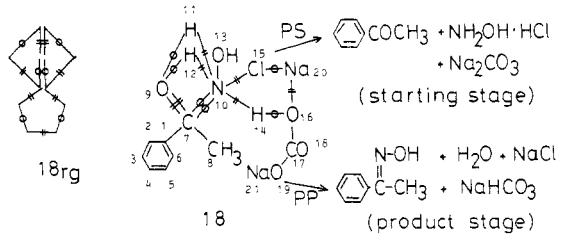
EXAMPLES AND ENUMERATION OF TWO-STRING REACTIONS IN WHICH THE TWO REACTION STRINGS SHARE THREE NODES AND TWO ITS BONDS

Oximation of acetophenone[21] is a two-string reaction that yields ITS **17**, if free hydroxylamine is considered to participate



the reaction. ITS **17** contains two tetragonal reaction strings that have three nodes and two ITS bonds in common.

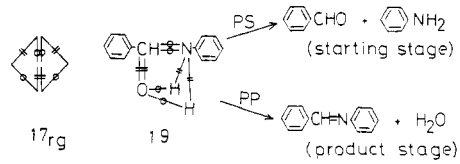
When one considers the preceding reaction of hydroxylamine and sodium carbonate giving free hydroxylamine, the corresponding ITS (**18**) is three string. Abstraction of the three



reaction strings, 10+7–9+11–10, 10+7–9+12–10, and 10–14+16–20+15–10, is easy from the viewpoint of chemistry. However, it is noted that there is some ambiguity in this procedure, since a single reaction string such as 10–11+9–7+10–14+16–20+15–10+7–9+12–10 is possible to be selected. In order to avoid such selection, we decide another criterion that *if in-bonds and out-bonds incident to the same node are different in number, abstraction of odd-membered cyclic reaction string(s) such as 10–14+16–20+15–10 should be preferred.*

Condensation of ketones with amines or hydrazines yields the same reaction graph (**17**$_{rg}$):

Formation of a Schiff base[22]



Formation of dimethylhydrazones[23]

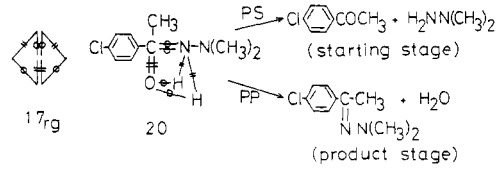
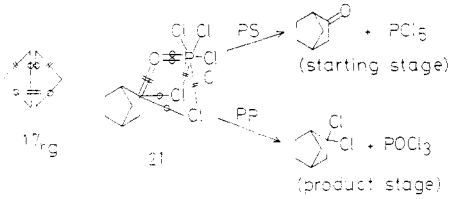


Table VI. Reaction Graphs Based on Graph G (m = 0, n = 0–2)

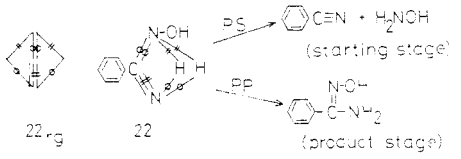
m	n	no. of reacn graphs[a]	no. of reacn pairs[b]	reaction graphs[c]
0	0	1	1	
0	1	4	2	
0	2	9	6	

[a] The numbers of reaction graphs are the coefficients of $x^m y^n$ in $G(x,y)$ (eq 7). [b] The numbers of reaction pairs are the coefficients of $x^m y^n$ in $P(x,y)$ (eq 9). [c] Each couple of reaction graphs linked with a bracket is a reaction pair.

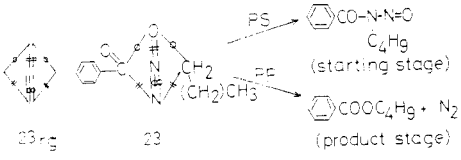
Formation of a geminal dichloride from a ketone[24] yields ITS **21**, which has two tetragonal reaction strings sharing three nodes and two ITS bonds.



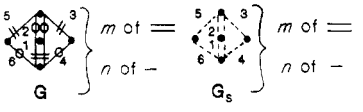
Par-bond modification is illustrated in the following examples:
Formation of amidoximes[25]



Deamination of *N*-alkyl-*N*-nitrosoamide[26]



Enumeration of reaction graphs based on basic graph **G** can be conducted in a similar way. The cycle index $Z(\mathbf{C}_2)$ and a graph-containing series $G(x,y)$ are obtained as follows (eq 6 and 7, respectively). Since basic graph **G** forms a self-reaction pair, several reaction graphs, if modified appropriately by par-bonds, construct self-reaction pairs also. Enumeration of reaction pairs is translated to counting isomeric reactions based on the corresponding par-bond skeleton ($\mathbf{G}_s$). The cycle index $Z(\mathbf{D}_2)$ and a pair-counting series $P(x,y)$ are represented by eq 8 and 9, respectively. The coefficients of $x^m y^n$ in $G(x,y)$ (eq 7) and in $P(x,y)$ (eq 9) indicate the numbers of reaction graphs and reaction pairs, respectively. The list of reaction graphs based on **G** (m = 0, n = 0–2) is found in Table VI.



$$Z(\mathbf{C}_2) = (1/2)(s_1^6 + s_1^2 s_2^2) \quad (6)$$

$$G(x,y) = 1 + 4x + 4y + 9x^2 + 16xy + 9y^2 + 12x^3 + 32x^2y + 32xy^2 + 12y^3 + 9x^4 + \ldots \quad (7)$$

$$Z(\mathbf{D}_2) = (1/4)(s_1^6 + s_1^2 s_2^2 + 2s_2^3) \quad (8)$$

$$P(x,y) = 1 + 2x + 2y + 6x^2 + 8xy + 6y^2 + 6x^3 + 16x^2y + 16xy^2 + 6y^3 + 6x^4 + \ldots \quad (9)$$

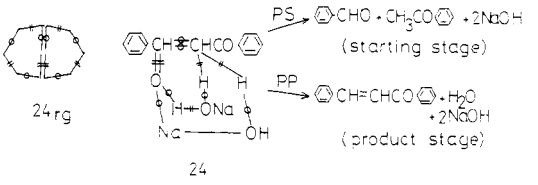
Table VII. Reaction Graphs Based on Graph H (m = 0, n = 0–2)

m	n	no. of reacn graphs[a]	no. of reacn pairs[b]	reaction graphs[c]
0	0	1	1	
0	1	6	3	
0	2	25	15	

[a] The numbers of reaction graphs are the coefficients of $x^m y^n$ in $G(x,y)$ (eq 11). [b] The numbers of reaction pairs are the coefficients of $x^m y^n$ in $P(x,y)$ (eq 13). [c] Each couple of reaction graphs linked with a bracket is a reaction pair.

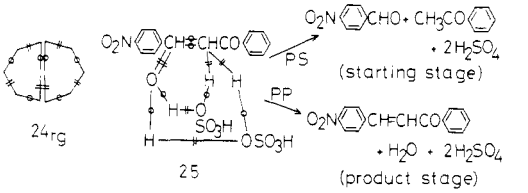
EXAMPLES AND ENUMERATION OF TWO-STRING REACTIONS IN WHICH THE TWO HEXAGONAL REACTION STRINGS SHARE THREE NODES AND TWO ITS BONDS

This category contains many synthetically useful reactions. The Claisen–Schmidt reaction[27] yields ITS **24** of this category.

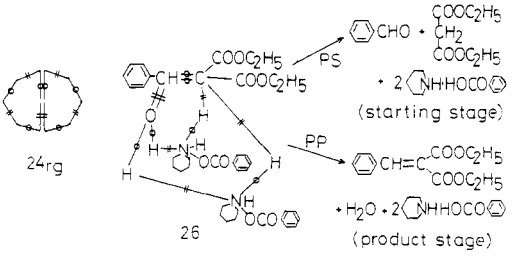


It is noted that participation of sodium hydroxide is different in the two reaction strings.

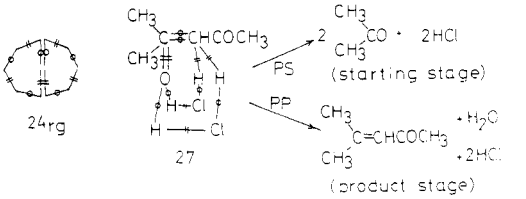
Condensation of aldehydes at the methyl group of methyl alkyl ketones is accomplished with acid catalysis.[28] The process is represented by ITS **25**, which has two reaction strings sharing three adjacent nodes.



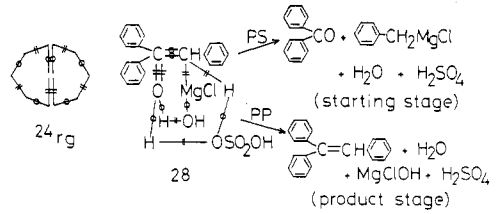
The Knoevenagel reaction,[29] aldol condensation followed by dehydration,[30] and Grignard addition followed by dehydration[31] provide ITS's of this category:
Knoevenagel reaction:



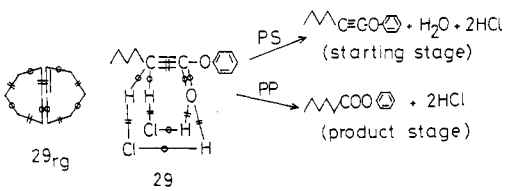
Aldol condensation–dehydration:



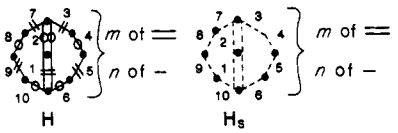
Grignard addition–dehydration:



Acid-catalyzed hydration of an acetylene[32] is represented by ITS **29**. The reaction graph $\mathbf{29}_{rg}$ contains two reaction strings sharing three adjacent nodes and having a single modifying par-bond.



Enumeration of reaction graphs based on basic graph **H** is accomplished in a similar way. The cycle index $Z(\mathbf{C}_2)$ and



$$Z(\mathbf{C}_2) = (1/2)(s_1^{10} + s_1^2 s_2^4) \quad (10)$$

$$G(x,y) = 1 + 6x + 6y + 25x^2 + 46xy + 25y^2 + 64x^3 + 184x^2y + 184xy^2 + 64y^3 + 110x^4 + \ldots \quad (11)$$

$$Z(\mathbf{D}_2) = (1/4)(s_1^{10} + s_1^2 s_2^4 + 2s_2^5) \quad (12)$$

$$P(x,y) = 1 + 3x + 3y + 15x^2 + 23xy + 15y^2 + 32x^3 + 92x^2y + 92xy^2 + 32y^3 + 60x^4 + \ldots \quad (13)$$

a graph-counting polynomial series $G(x,y)$ are represented by eq 10 and 11, respectively. The cycle index $Z(\mathbf{D}_2)$ for the corresponding par-bond skeleton ($\mathbf{H}_s$) is eq 12, from which a pair-counting polynomial series $P(x,y)$ (eq 13) is obtained.

MATRIX REPRESENTATIONS OF REACTION GRAPHS

ITS's are stored as connection tables which have information of bonds in terms of complex bond numbers (a b) (see Table I). They can also be represented by various types of matrices. For example, ITS **1** is represented by the corresponding matrix, $M_1 = ((a_{ij}\ b_{ij}))$, in which each intersection element of the ith row and jth column is (a_{ij} b_{ij}), corresponding to an imaginary bond between the ith and jth atoms. This matrix representation is a unitary representation embracing Ugi's B, E, and R matrices without considering diagonal elements. When only a_{ij}'s are collected, one can easily obtain Ugi's B matrix. The matrix ($a_{ij} + b_{ij}$) corresponds to Ugi's E matrix,[33] and one can obtain Ugi's R matrix when b_{ij}'s are collected.

When one takes up elements of $b_{ij} \neq 0$ from the matrix M_1, the matrix representation (M_{lrg}) of the reaction graph is obtained. This matrix (M_{lrg}) corresponds to the representation of Table II.

$$M_{lrg} = \begin{array}{c} \\ 1 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \end{array} \begin{array}{c} \begin{array}{cccccc} 1 & 14 & 15 & 16 & 17 & 18 \end{array} \\ \begin{bmatrix} & 1\text{-}1 & 1\text{-}1 & 0\text{+}2 & & \\ 1\text{-}1 & & & & 0\text{+}1 & \\ 1\text{-}1 & & & & & 0\text{+}1 \\ 0\text{+}2 & & & & 1\text{-}1 & 1\text{-}1 \\ & 0\text{+}1 & & 1\text{-}1 & & \\ & & 0\text{+}1 & 1\text{-}1 & & \end{bmatrix} \end{array}$$

Brandt and von Scholley[34] have indicated the importance of canonical representation of reaction matrix. The present concept of reaction strings is versatile to obtain a newly defined canonical representation of an R matrix. We select now a canonical matrix in which b_{ij}'s of off-diagonal elements have values +1 and −1 alternately.

The matrix representation of the two-string reaction described above can be divided into two pairs of canonical matrices, which correspond to the two reaction strings. The pair S_{11} and S_{12} corresponds to the first reaction string, 1–2+6–7+1, and the pair T_{11} and T_{12} to the second one, 1–5+8–9+1, wherein only b_{ij} are collected for simplicity. This

$$\begin{array}{c} \begin{array}{cccc} 1 & 14 & 17 & 16 \end{array} \\ \begin{bmatrix} & -1 & & \\ -1 & & +1 & \\ & +1 & & -1 \\ & & -1 & \end{bmatrix} \end{array} \quad \begin{array}{c} \begin{array}{cc} 1 & 16 \end{array} \\ \begin{bmatrix} & +1 \\ +1 & \end{bmatrix} \end{array}$$

S_{11} S_{12}

1st string

$$\begin{array}{c} \begin{array}{cccc} 1 & 15 & 18 & 16 \end{array} \\ \begin{bmatrix} & -1 & & \\ -1 & & +1 & \\ & +1 & & -1 \\ & & -1 & \end{bmatrix} \end{array} \quad \begin{array}{c} \begin{array}{cc} 1 & 16 \end{array} \\ \begin{bmatrix} & -1 \\ -1 & \end{bmatrix} \end{array}$$

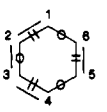
T_{11} T_{12}

2nd string

canonical representation corresponds to the connection table of Table III. The present treatment gives a sound basis to canonization of two-or-more-string reactions, which is not pointed out in the literature.[34]

In general, each matrix representation of a reaction graph can be divided into such pairs of canonical matrices after appropriate similarity transformation. Each pair of canonical matrices corresponds to a reaction string, but not always in 1:1 fashion. The number of pairs is equal to the stringity (the number of reaction strings).

The Diels–Alder addition is characterized by reaction graph $\mathbf{30}_{rg}$ of one string, which can be represented by matrix M_2.



$$M_2 = \begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\ \begin{bmatrix} & 2\text{-}1 & & & & 0\text{+}1 \\ 2\text{-}1 & & 1\text{+}1 & & & \\ & 1\text{+}1 & & 2\text{-}1 & & \\ & & 2\text{-}1 & & 0\text{+}1 & \\ & & & 0\text{+}1 & & 2\text{-}1 \\ 0\text{+}1 & & & & 2\text{-}1 & \end{bmatrix} \end{array}$$

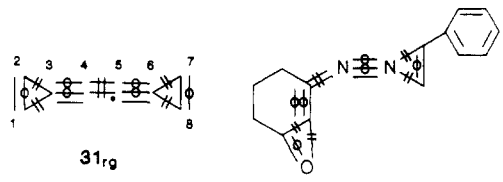
$$\begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\ \begin{bmatrix} & -1 & & & & \\ -1 & & +1 & & & \\ & +1 & & -1 & & \\ & & -1 & & +1 & \\ & & & +1 & & -1 \\ & & & & -1 & \end{bmatrix} \end{array} \quad \begin{array}{c} \begin{array}{cc} 1 & 6 \end{array} \\ \begin{bmatrix} & +1 \\ +1 & \end{bmatrix} \end{array}$$

S_{21} S_{22}

All elements of (0+0) are abbreviated

The matrix M_2 can be regarded as the sum of a pair of canonical matrices (S_{21} and S_{22}), which have nodes 1 and 6 as common terminal nodes. This implies the reaction string has a ring structure.

The reaction graph $\mathbf{31}_{rg}$ of Eschenmoser's epoxyhydrazone fragmentation can be represented by matrix M_3, which is transformed into a pair of canonical matrices (S_{31} and S_{32}).



$\mathbf{31}_{rg}$ $\mathbf{31}$

	1	2	3	4	5	6	7	8
1		+1	−1					
2	+1		−1					
3	−1	−1		+2				
4			+2		−2			
5				−2		+2		
6					+2		−1	−1
7						−1		+1
8						−1	+1	

M_3

	1	2	3	4	5	6	7	8
1		+1						
2	+1		−1					
3		−1		+1				
4			+1		−1			
5				−1		+1		
6					+1		−1	
7						−1		+1
8							+1	

S_{31}

	1	3	4	5	6	8
1		−1				
3	−1		+1			
4		+1		−1		
5			+1		−1	
6				−1		+1
8					−1	

S_{32}

This pair corresponds to the reaction string 1+2−3+4−5+6−7+8−6+5−4+3−1. Thus, the graphical representation of the present method is a versatile aid to understand such treatment.

CONCLUSION

Various two-string reactions are classified in terms of their reaction graphs. Enumeration of representative reaction graphs of two strings is accomplished by the use of Polya's theorem. Matrix representations of reaction graphs are related to Ugi's R matrices in the cases of one-string reactions. Canonization of matrix representations is shown to be achieved on the basis of reaction strings.

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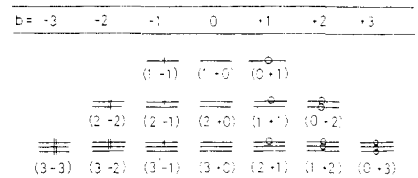
(2) An *out-bond* has bond color of *out* and means a bond disappearing during a reaction. An *in-bond* is of *in* color and represents a bond formed. A *par-bond* is an invariant bond and has bond color of *par*. Bonds appearing in ITS's are referred to as ITS bonds or imaginary bonds. Each ITS bond is represented by a complex bond number (*a b*), wherein integer *a* is the multiplicity of a bond in the starting stage and *b* is the difference in bond multiplicity between the product and the starting stage.



(3) A one-string reaction gives an ITS, or a reaction graph, which contains a reaction string. A two-string reaction provides an ITS, or a reaction graph, having two reaction strings, and so on. The numbering of nodes appearing in an ITS is arbitrary and not canonized in the present paper. The numbering of nodes appearing in a reaction graph may be equal to that of the corresponding ITS. Sometimes, it can be canonized for the purpose of classification reactions. Deletion of in-bonds of an ITS provides the starting stage of the reaction represented by said ITS. This operation is defined as *projection to starting stage* and is abbreviated PS. *Projection to product stage* is abbreviated PP, which is defined as deletion of out-bonds of an ITS.
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