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PROGRESS IN CONCEPTS OF CONFORMATIONAL SWITCHING AND MOLECULAR --ETC(U)
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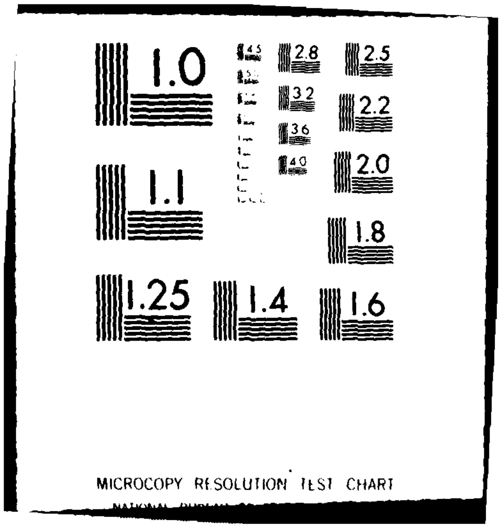
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The importance of molecular conformational changes as switching mechanisms in proposed molecular electronic devices is stressed. Primarily two types of phenomena are considered; a molecular tunnelling analogue to a NOR gate and a variety of soliton phenomenon. These include soliton switching, soliton valving, proton tunnelling and soliton generation, soliton reversal, and soliton transport as a memory device. Also briefly considered is the proposed uses of the valence-bonded surface contact and the very small electrochemical cell in the controlled synthesis of molecular devices.

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CONTENTS

PROGRESS IN CONCEPTS OF CONFORMATIONAL SWITCHING AND MOLECULAR ELECTRONIC DEVICES

Forrest L. Carter
Chemistry Division

Introduction

The concept of electronic switching at the 'molecular' size level has been developed in the two previous Electroactive Polymer Program (EAP) Annual Reports (1). Possible 'molecular' phenomena which might function as gates or switches were tabulated in the First Annual EAP Report (1a) and a general scheme for building computers using a chemical synthetic method was outlined. The Second Annual EAP Report (1b) extended these concepts while emphasizing: 1) the enormous versatility of chemical moieties to function as Control Groups in electron multibarrier tunnel switches; 2) the promise of soliton propagation in conjugated systems to facilitate various device functions; and 3) the importance of self-organization as a synthetic construction principle. While the above considerations were arrived at independently, for historical completeness it should be noted that earlier in 1974, Aviram and Ratner (2) had developed the important concept of 'molecular' rectifiers although they had not discussed linking the particular molecule to external effects.

This report stresses the importance of molecular conformational changes as switching mechanisms in electron tunnel switches and particularly in phenomena involving soliton propagation. Accordingly, a molecular tunnelling analogue to a NOR gate is discussed and a variety of soliton phenomenon will be proposed. These include soliton switching, soliton valving, proton tunnelling and soliton generation, soliton reversal, and a soliton memory element. Thereafter a soliton input to a bistable chemical memory is described as well as a new valence-bonded surface contact. In the last section the use of very small electrochemical cells is suggested as a promising technique for the controlled synthesis of molecular devices.

NOR Gate Molecular Analogue

Among the most promising of switching mechanisms tabulated earlier [1a] is that of electron tunnelling in short periodic structures. This mechanism was based on the quasi-classical approach of Pschenichnov [3]; in NRL Memorandum Report 4680.

Manuscript submitted October 7, 1981.

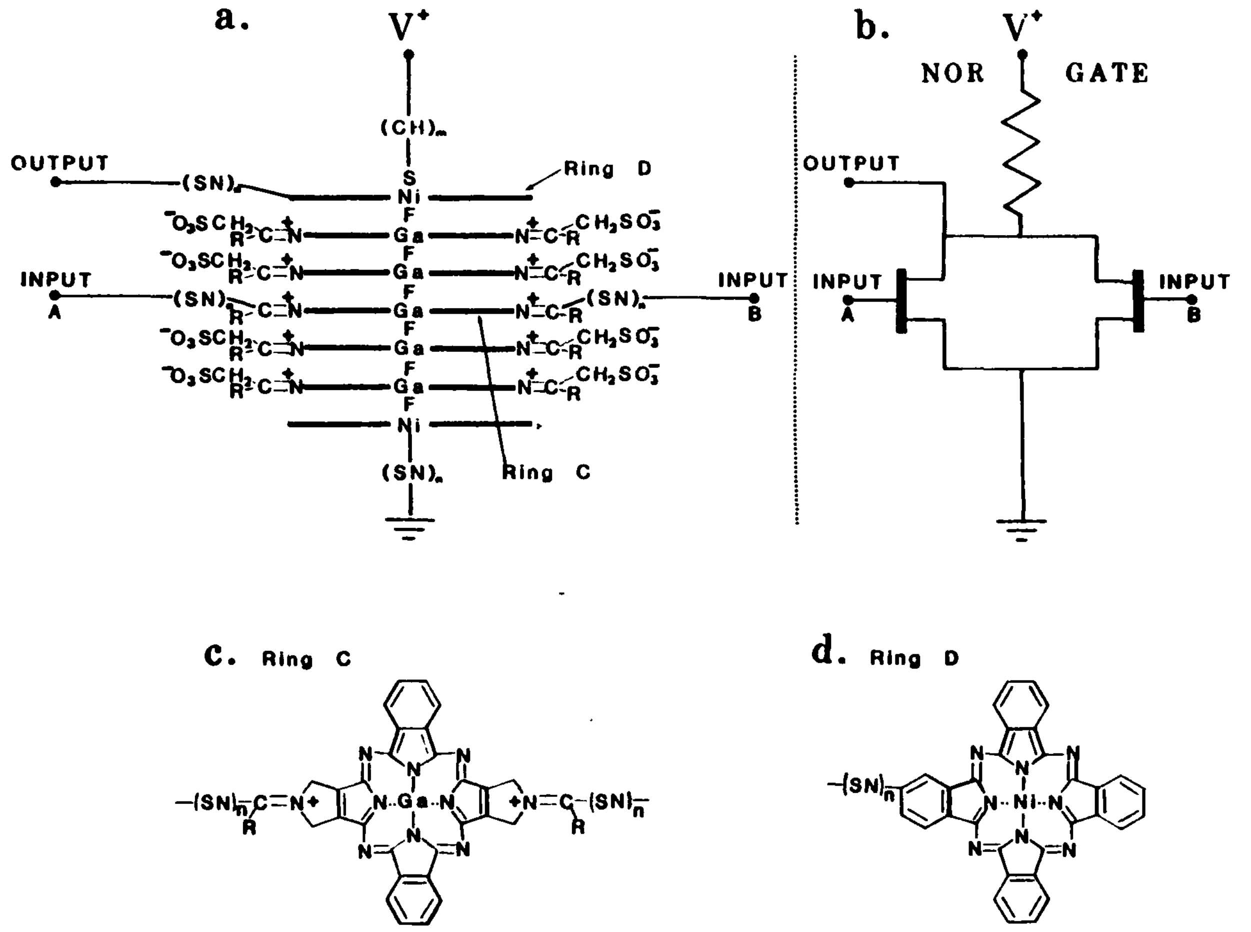


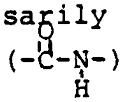
Fig. 1: A molecular analogue to a NOR gate based on a stacked fluorine bridged gallium pthalocyanine-type ring. The bridging fluorines result in an insulating barrier between the rings while the terminal sulfurs provide a strong multivalent bond to the $(SN)_n$ and more resistive $(CH)_n$ conductors.

the mathematics of tunnelling through an arbitrary set of square well potentials is formulated [4]. The analytic soliton obtained will be soon specialized and applied to the current problem of tunnelling through periodic barriers. In the first EAP Review [1a] molecular analogues of semiconducting NAND and NOR gates were offered; however the NOR gate was based on the special properties of the CuS crystal structure with its alternating insulating and conducting layers. The structure now offered is more properly a 'molecular' analogue.

In Fig. 1a the structure of an analogue to the electronic switch in Fig. 1b is based on a fluorine bridged stack of gallium phthalocyanine rings similar to the compounds recently reported by Kuznesof, Wynne, Nohr, and Kenny [5]. The stack is composed primarily of rings of type C (Fig. 1c) where the $-(SN)_x-$ linkage is replaced by the $-CH_2-SO_3$ group. Clearly the rings C are carriers for the Control Group or the Dummy Control Groups having the quaternary imino nitrogen groups $>C=N^{+}<$. The two kinds of Control Groups define the periodic potential necessary for tunnelling; Control Groups permit modification of the potential and, hence, the tunnelling to be switched on or off (Ref. 1b).

The D rings (Fig. 1d), nickel phthalocyanine moieties, provide links to both the ground and the negative potential through Ni-S bonds (Fig. 1a); as well as to the $(SN)_n$ - Output lead. These terminating rings also serve to provide a suitable environment for the stacked bridged phthalocyanine rings. Control through the Input $-(SN)_n-$ leads A or B occurs via an electron flow down the $-(SN)_n-$ chain to neutralize the quaternary imino nitrogen. The neutralization of either nitrogen would change the potential of that ring sufficiently to sharply cut off the electron tunnelling through the rings. Although Control Groups switch the electron tunnelling on or off primarily by the relocation of charge, there is always associated with that charge relocation a configurational or conformational change. In switching phenomena involving solitons, conformational change is of first importance.

Soliton Switching in Conjugated Systems

On a microscopic scale a soliton is a non-linear structural disturbance that moves in one or two dimensions like a "particle." Associated with this pseudo-particle is a definite energy, momentum and velocity. Davydov [6] postulated in 1976 that a soliton traveling thousands of Angstroms down a α-helix might be the signal transport mechanism associated with bond breaking in A.T.P. The bond energy associated with that phenomenon is only four times thermal background and normally would have been lost in the thermal background before traveling far. Accordingly, soliton transport is associated with the motion of a disturbance moving without energy loss. In the α-helix the motion of this 'solitary' wave is necessarily linked to the stretching of the polypeptide amide bond  $(-\overset{O}{\overset{\|}{C}}-\underset{H}{\underset{|}{N}}-)$ through its dipole moment.

SOLITON TRANSPORT

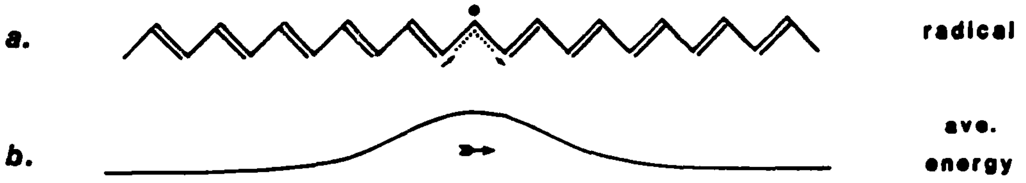
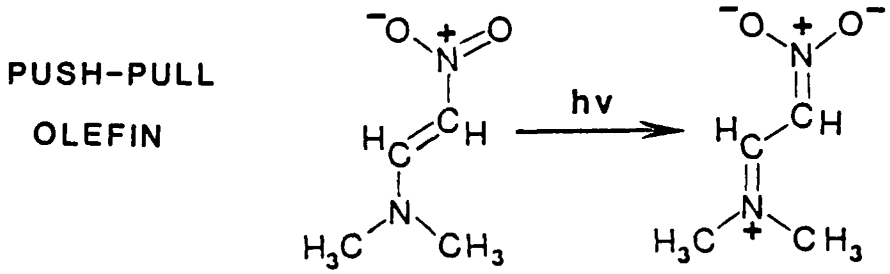


Fig. 2: The motion of a radical soliton in a conjugated system is associated with the motion of a "phase boundary" or "kink" between ordered single-double bond domains (adapted from Ref. 1b, Fig. 4).

In conjugated systems the corresponding dipole moment may be absent, however, single-double bond rearrangement is possible and that presumably provides the necessary mechanism for soliton propagation. A schematic picture of a soliton moving from left to right is indicated in Fig. 2. At the soliton center there exists a moving 'phase' or 'domain' boundary with respect to the conjugation. It should also be made clear that plus and minus charged solitons exist as well as radical solitons and that the disturbance at the soliton center is much larger than suggested in Fig. 2. The passage of a soliton through a conjugated system generally results in the exchange of single and double bonds. This effect will play a major role in soliton switching, as discussed below.

The 'push-pull' disubstituted olefin, 1,1-N,N-dimethyl-2-nitroethenamine is of special interest because it can be photoactivated to undergo an electron transfer from the amine nitrogen to the nitro-oxygen [7]. At the same time there is a conformational change involving the olefinic double bond:



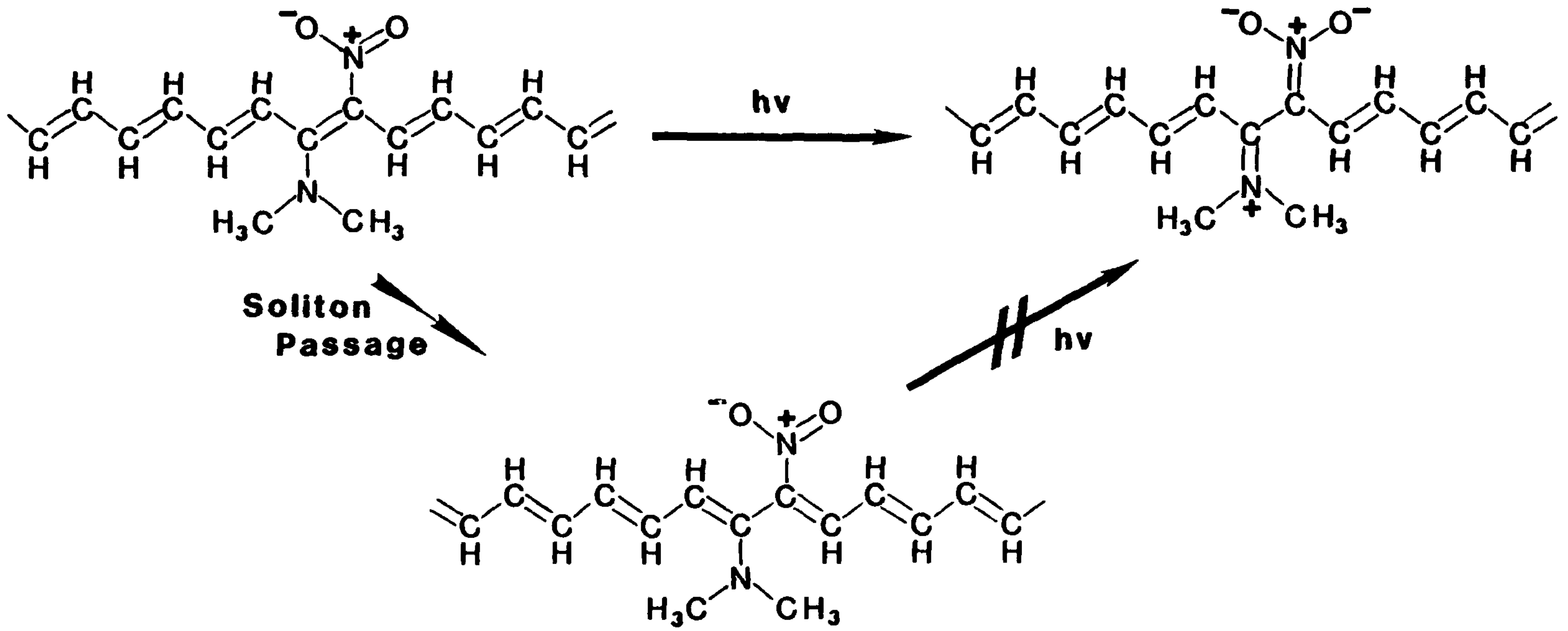


Fig. 3: A push-pull disubstituted olefin imbedded in transpolyacetylene can a) be switched off by the propagation of a soliton, or b) be used as a soliton detector.

Now imagine that the double bond is part of a larger polyacetylene chain as indicated in Fig. 3. Under polarized photoactivation it should still undergo electron transfer. However if a soliton has been propagated down the polyene chain then that photoactivation process can no longer take place (see Fig. 3). Thus the soliton has switched off the internal charge transfer reaction. (Note also that the absorption spectra of the push-pull olefin can serve as a detector for the passage of the soliton.)

This soliton switching concept can be extended to two chains and two different push-pull structures or extended chromophores. This is indicated in Fig. 4 where the conformation of chain 1 has switched off the nitro-amine chromophore but does not prevent the photoactivation of the sulfur containing chromophore. The passage of a soliton down chain 1 will turn the first chromophore on and the second off; a soliton moving down chain 2 will turn both of them off. In Fig. 5 the concept of soliton gang switching is generalized where A, C, and D, are generalized electron acceptors, conjugated connectors, and electron donors, respectively. Notice that each chromophore, separated from each other by dotted lines, has a different relationship to the conformations of chains 1, 2 and 3. This relationship is summarized in Table 1 where eight different chromophore-chain relationships are indicated as possible. Only the first 4 relationships indicated in Table 1 are illustrated in Fig. 5. For reasons to be offered shortly, the chromophores are identified as channels in Table 1. In Fig. 5 note that the relationship of the leftmost chromophore to each chain is such that the chromophore is subject to photoactivation; in Table 1 this set of relationships is indicated by a vertical row of 1s. However the second chromophore or channel is turned off by the 1st chain, while the third channel is turned off by the 2nd chain. In short the chromophores or channels are so arranged that the passage of a soliton down any of the three

Table 1. Three Chain Gang Switching

Channel [a]	1	2	3	4	5	6	7	8
Chain [b] 1.	1	0	1	1	1	0	0	0
Chain 2.	1	1	0	1	0	1	0	0
Chain 3.	1	1	1	0	0	0	1	0

[a] A channel is only open if a vertical column is all ones.

[b] Soliton passage through a chain changes all ones to zeros and vice versa.

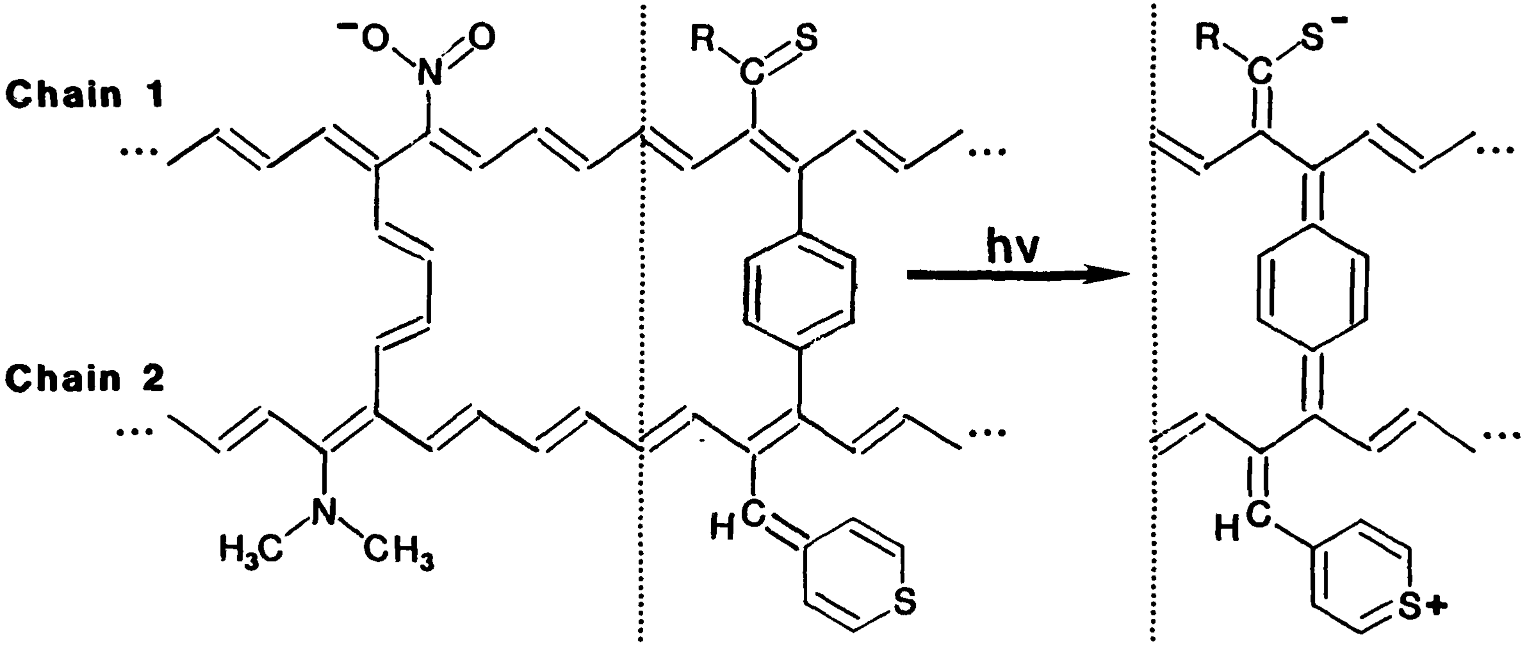


Fig. 4: Soliton switching involving two transpolyacetylene chains and two chromophores. The second sulfur chromophore can be photoactivated but not the first.

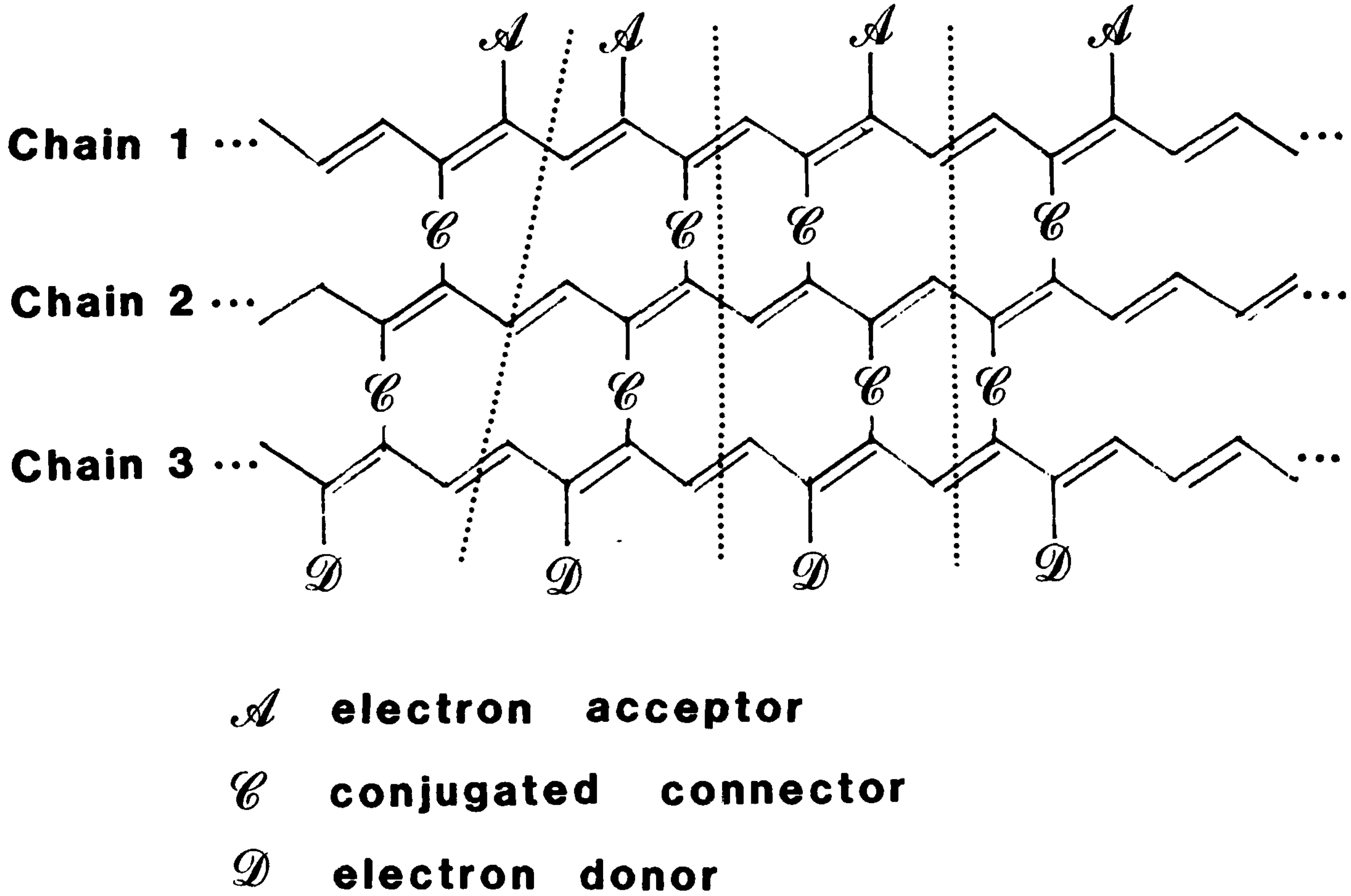


Fig. 5: Soliton gang switch showing four of eight possible different arrangements chromophores can have relative to three conjugated chains.

chains turns off any soliton that is on and turns on one of the others.

Table 1 then expresses the concept that soliton propagation can be used to perform gang switching where three input states can control 8 different output channels. By separating the chromophores by about 100Å the density of such switches can be estimated to be as high as 10^{18}/cc! It should be remembered however that soliton propagation is less than the speed of sound.

The next generalization as shown in Fig. 6 goes beyond our meager knowledge of soliton propagation. Here we have replaced the electron acceptor and donor groups with molecular 'wires' or filaments of $-(SN)_n-$. Here the question is, "Can the conformation of the chains 1, 2, and 3 control the conduction of electrical charges in the different 8 channels as suggested in Table 1? One question to be asked is, "Does band conduction in $(SN)_x$ convert to soliton propagation across the chains and back again to band conduction?" Note that in such a case, pairs of signals must be sent to restore conformation back to the original state in each channel.

Soliton Valving

Soliton propagation in a conjugated system can lead to a valving behavior as well as to a switching action. This is suggested in Fig. 7 and Table II. Fig. 7 illustrates three conjugated half-chains joining at a single carbon or branch carbon. The passage of a soliton from A to B (or from B to A) moves the double bond at the branch carbon from the A chain to the B chain. In the upper right portion of Fig. 7 we note that a soliton moving from B to C moves the double bond to the C chain. Thus in Fig. 7 we note those soliton propagations that correspond to a clockwise rotation of 120°. In short, those propagations behave like a group operation. The first two entries in the SEND column of Table II in each section correspond to a rotation clockwise, while the last two of each section correspond to a counter-clockwise rotation of the bridgehead double bond.

Note that this behavior is not like the operation of a three-way valve where one branch is cut off from the other two. In this case of soliton valving, Table II shows that communication is cut off from just one direction, not two (see NOT SEND column).

It would be surprising to the author if this effect is not used somewhere in nature in the directed synthesis of natural products.

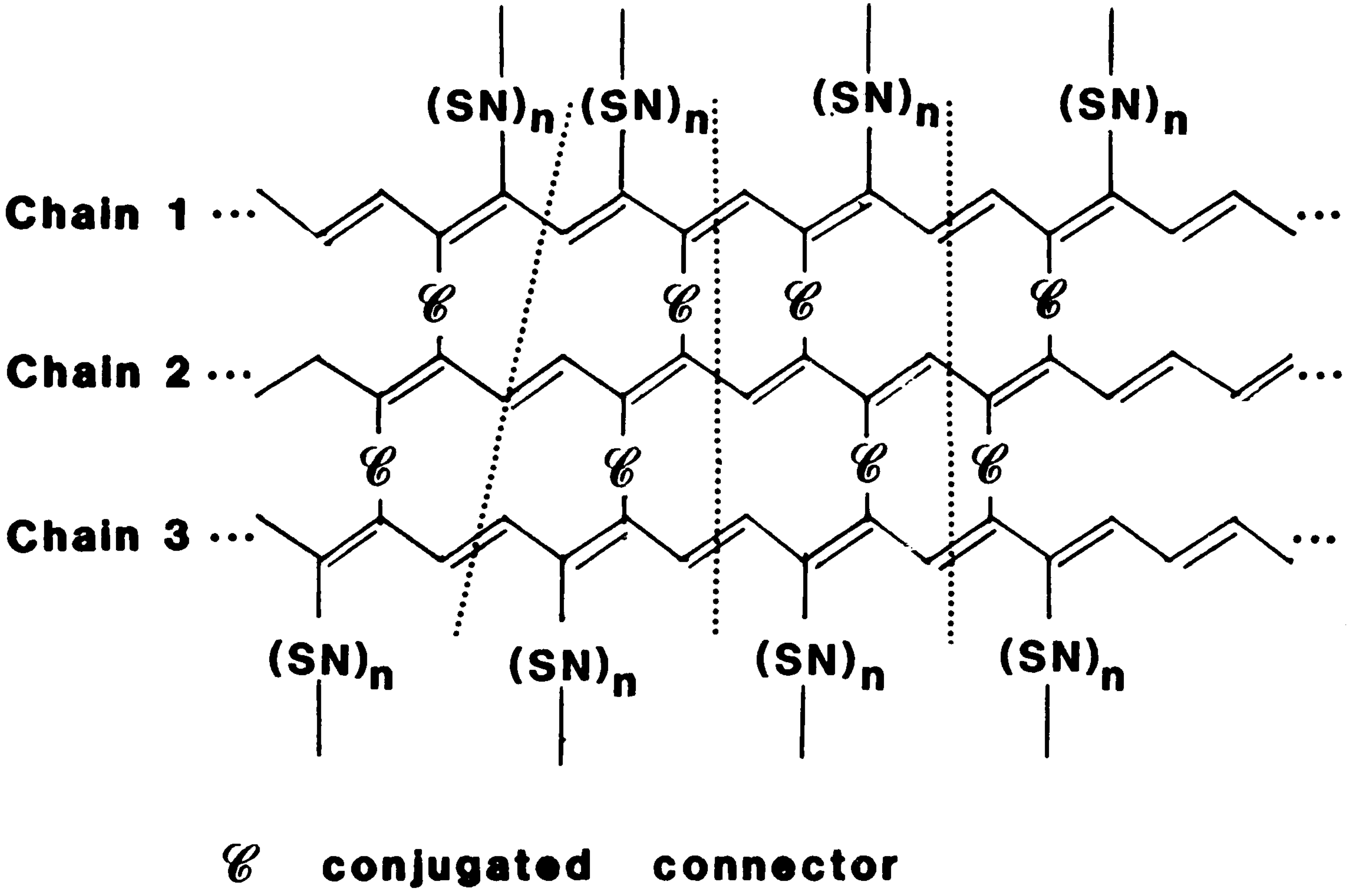


Fig. 6: Gang switching is conceptually extended by replacing the electron acceptor and donor of each chromophore or channel with an electron conductor.

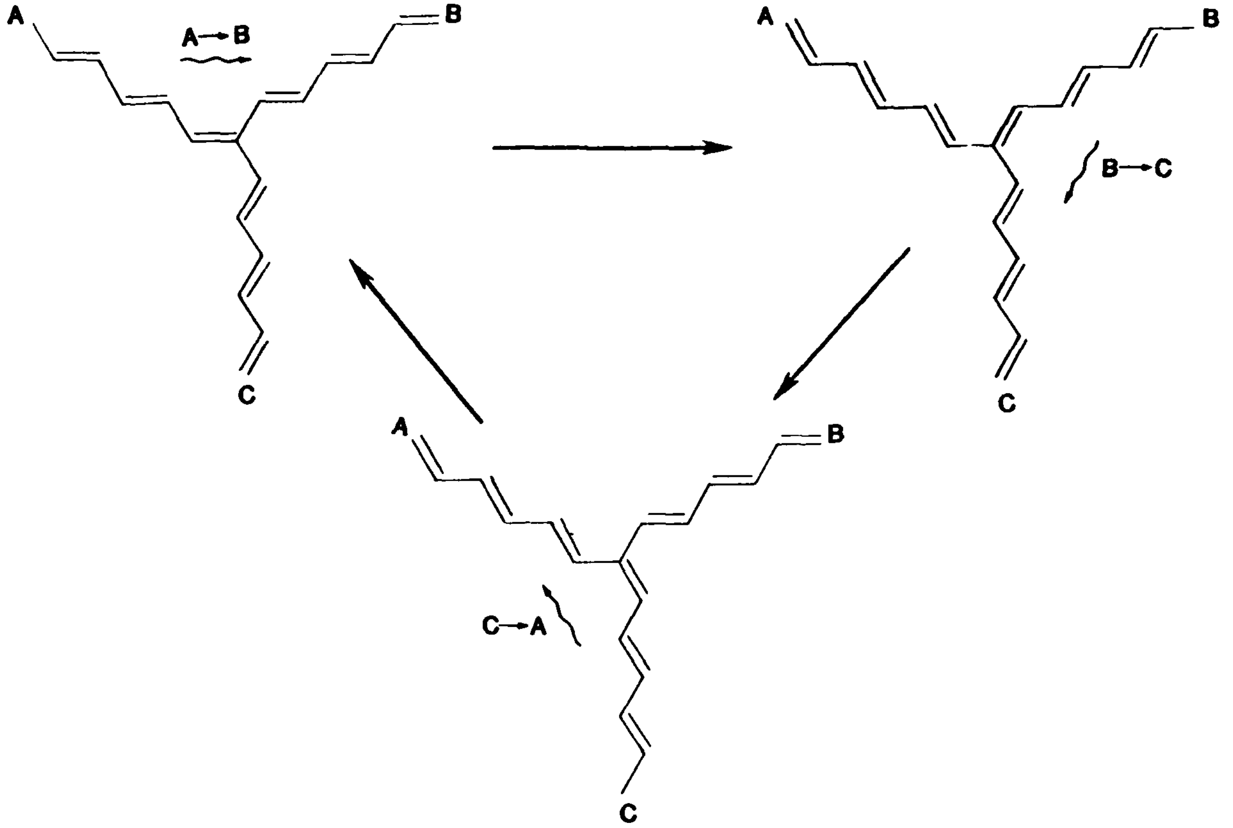


Fig. 7: The propagation of a soliton from A to B corresponds to a clockwise rotation by 120° of the upper left hand configuration. This valve like action is related to but not isomorphous to a threeway valve.

Table II. Soliton Valving

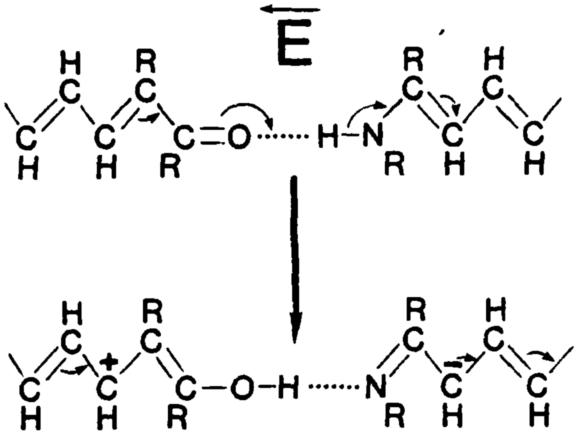
Double Bond* on Chain	Send	New Double Bond Position	Not Send
A	A → B	B	B → C
	B → A	B	C → B
	A → C	C	
	C → A	C	
B	B → C	C	A → C
	C → B	C	C → A
	A → B	A	
	B → A	A	
C	A → C	A	A → B
	C → A	A	B → A
	B → C	B	
	C → B	B	

*i.e., the double bond on branch carbon

Proton Tunnelling and Soliton Generation

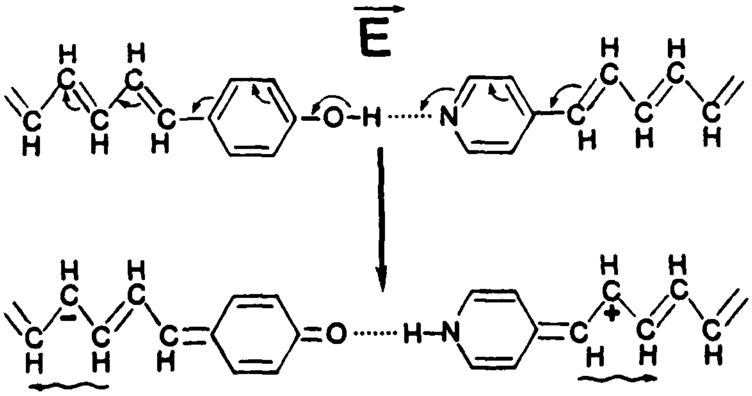
The asymmetric nature of most hydrogen bond led to the suggestion of their possible use as 'molecular' rectifiers [2] and to their tabulation as a possible switching mechanism in 1979 [1a]. In the same EAP report [1a] we included hydride ion (H^-) as well as proton (H^+) transfer mechanisms in our discussions but like Aviram and Ratner [2] earlier, omitted suggesting a method for coupling the tunnelling current to an external current or other phenomenon (ignoring any displacement current effects). Below we offer a mechanism that not only relates proton and hydride ion tunnelling to an external current but also provides a mechanism for the generation of solitons.

In a chemically naive form the proton tunnelling is indicated below as taking place between a secondary amine and a ketone group in the presence of an electric field of strength E. The proton donor and acceptor groups are both adjacent to extended conjugated systems, in this case trans-polyacetylene.



As the proton, H^+ moves to the left to form a new bond with oxygen, valence electrons (usually π electrons) move to the right as is indicated by the curved arrows. After the conformational changes occur, as indicated in the lower equation, we can imagine a trivalent carbon anion being formed on the right and a carbonium ion being formed on the left. Further motions of these charged states to the right and left respectively are suggested by the curved arrows in the lower equation above. Moreover, since the proton tunnelling is necessarily associated with conformational changes induced by an electric field it seems that the necessary elements for charged soliton formation are present. Accordingly we anticipate that a negative soliton will move to the right while a positive soliton will propagate to the left.

Consider another example:



Several changes are made in the proton tunnelling scheme for soliton generation just above. The electric field direction is reversed and the chemical system is apt to be more stable. In addition, the presence of aromatic terminal groups will mean that the potential at which proton tunnelling is first induced will be higher. That is, a bias can be chemically built in. Furthermore, by the proper choice of terminal groups, the chemist will have considerable control over that bias. In this case, proton tunnelling will occur to the right leaving behind a quinonylidene terminal group.

At this point (lower equation), the system has generated two solitons of opposite charge moving in opposite directions; but then soliton generation stops. If the potential is increased sufficiently, then a hydride ion (H^-) can leave the right hand nitrogen, hopping back to the oxygen and generating two more solitons of the same charges and moving in the same direction as before. Moreover, when the solitons depart and their potential has dropped sufficiently for the hydrogen to see primarily the electric field E, then proton tunnelling will occur again and generate two more solitons. In short we will have an oscillatory generation of solitons.

Soliton Reversal

As a pseudo-particle, a hydrodynamic soliton has a definite energy, shape, and momentum; and like a particle one might consider reflecting it from a suitably stiff surface. At the molecular level the same consideration occurs, but here it is clear that the correct reflector is of molecular origin. Soliton reversal is indicated in two different modes in Fig. 8. The first mode involves two trans-polyacetylene chains connected in a conjugated manner to a tricyclic pentaene. In Fig. 8a we see that the chains are connected in such a way that the number of double bonds in the reversing tricyclic moiety remains constant.

In the single chain soliton reverser of Fig. 8b the reverser moiety is a partially hydrogenated coronine. In this case the soliton advances to the left and proceeds clockwise around the molecule. The valence π electron motion is indicated sequentially by the numbered curved arrows. Note that the electron motion indicated by the tenth arrow can occur only after electron motion indicated by the first arrow is completed. This suggests the theoretical possibility that the soliton never traverses around the hydrocoronene moiety first clockwise and then counter clockwise but is only reflected at the first ring atom while the molecule undergoes a concerted conformation change. In this single chain case, the chain remains in the same conformational state before and after the soliton has been reversed since the soliton passes over the same chain twice.

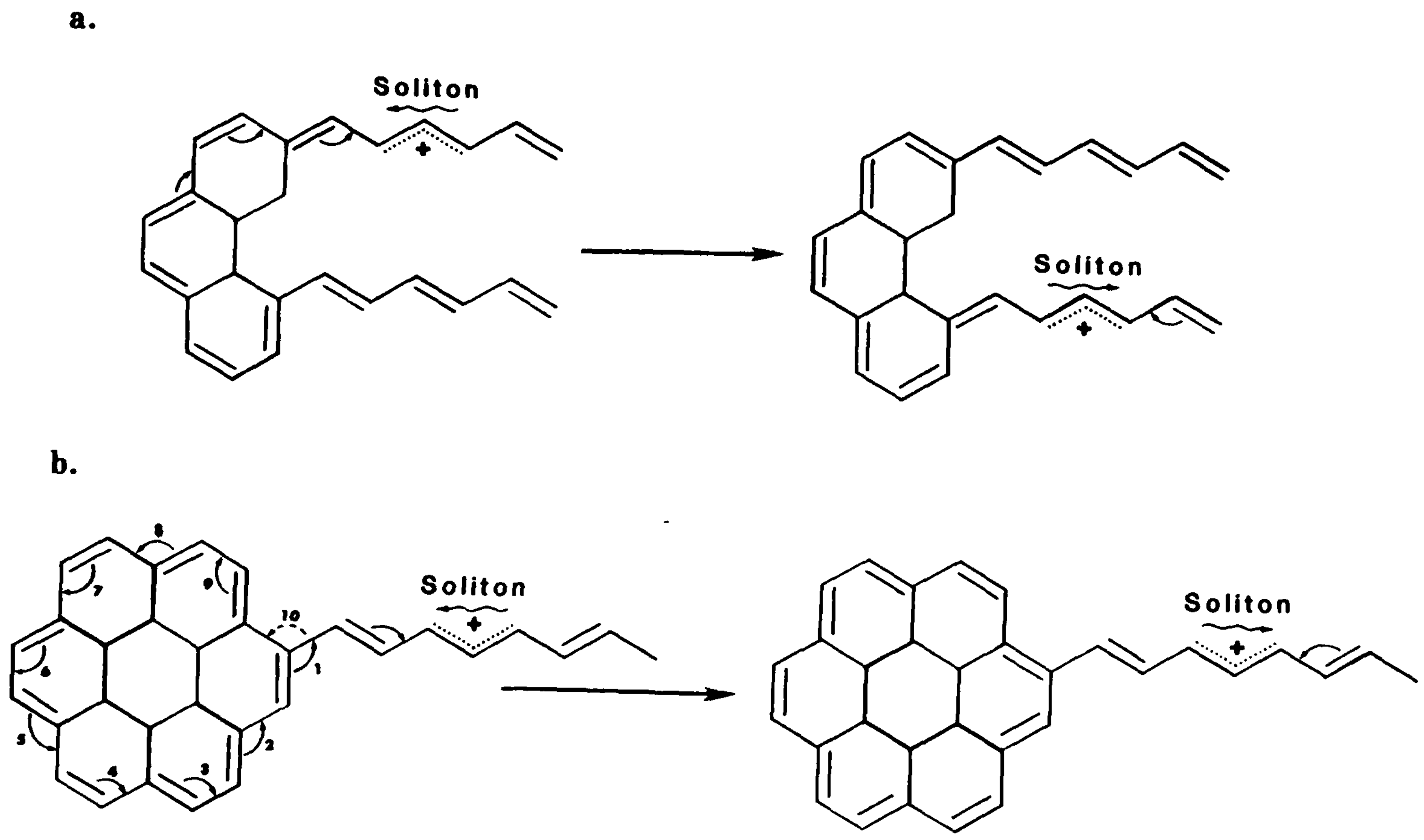


Fig. 8: Molecular double chain (a) and single chain (b) soliton reversers are illustrated.

Soliton Memory Element

In the discussion above we have presented all the components necessary to postulate a Soliton Memory Element. A simple example of such an element is indicated in Fig. 9. In such an element the access time of an information bit (soliton or no soliton) and the number of bits clearly depend on the soliton velocity and the lengths of the conjugated polymer linking the soliton generator and the electron tunnel switch. The velocity of a soliton is energy dependent but only approaches phonon velocity as an upper limit. A soliton is estimated to propagate 100Å in somewhat less than 10^{-10} sec.

In Figure 9 we show the possibility of storing four bits (in duplicate) at any one time; two on the upper chain and two on the lower chain. The illustration implicitly suggests using the simultaneous arrival of both the positive and negative solitons to trigger the electron tunnel switch. This technique then provides a built-in defense against some soft errors.

While soliton devices may not be very fast, one can store information at great densities. Assume that soliton separations along a trans-polyacetylene chain are approximately 200Å. If the chains are packed on 50Å centers then the density of soliton information bits can be an astounding 2×10^{18} bits/cc.

Bistable Chemical Memory

The configuration of the soliton generator and the soliton reverser can be used as input to another memory element, namely the bistable chemical memory element, first discussed in Ref. 1b. This element can be independently written and read. It is a static conformational storage device that depends on the existance of two valence states, $M^{\delta+}_{(low)}$ and $M^{\delta-}_{(high)}$, of a transition metal. At the bottom of Fig. 10a we see that one metal atom is acting as a Control Group for an electron tunnel switch (the read device) while the Driver controls the valence states in the metal ring by the development of Driver + and - charges. If these Driver charges are reversed to - and + then with the resulting movement of the bridging ligands, B, the valence states of the metal atoms are exchanged, with the ligands B moving toward the new high valence $M^{\delta-}$ atoms.

While the nature of the Driver moiety has not been specified as yet, it is clear that the Driver charges could be reversed by accepting two pairs of solitons from a soliton generator as suggested in Fig. 10b. Thus the Driver charges can be reversed by three different mechanisms: 1) charge flow under a potential difference; 2) photoactivation (dipole transition); and 3) charged pairs of solitons. Of the three the last would seem to be the most versatile mechanism.

SOLITON MEMORY ELEMENT

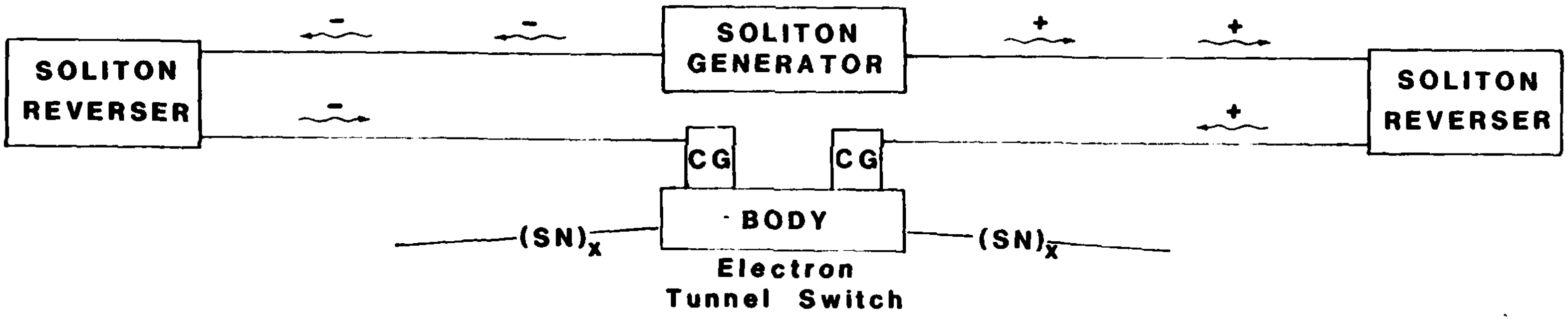


Fig. 9: Solitons may be temporarily stored on transpolyacetylene chains connecting the soliton generator first to the soliton reversers and then to the Control Groups (CGs) of the multi-barrier electron tunnel detector (switch).

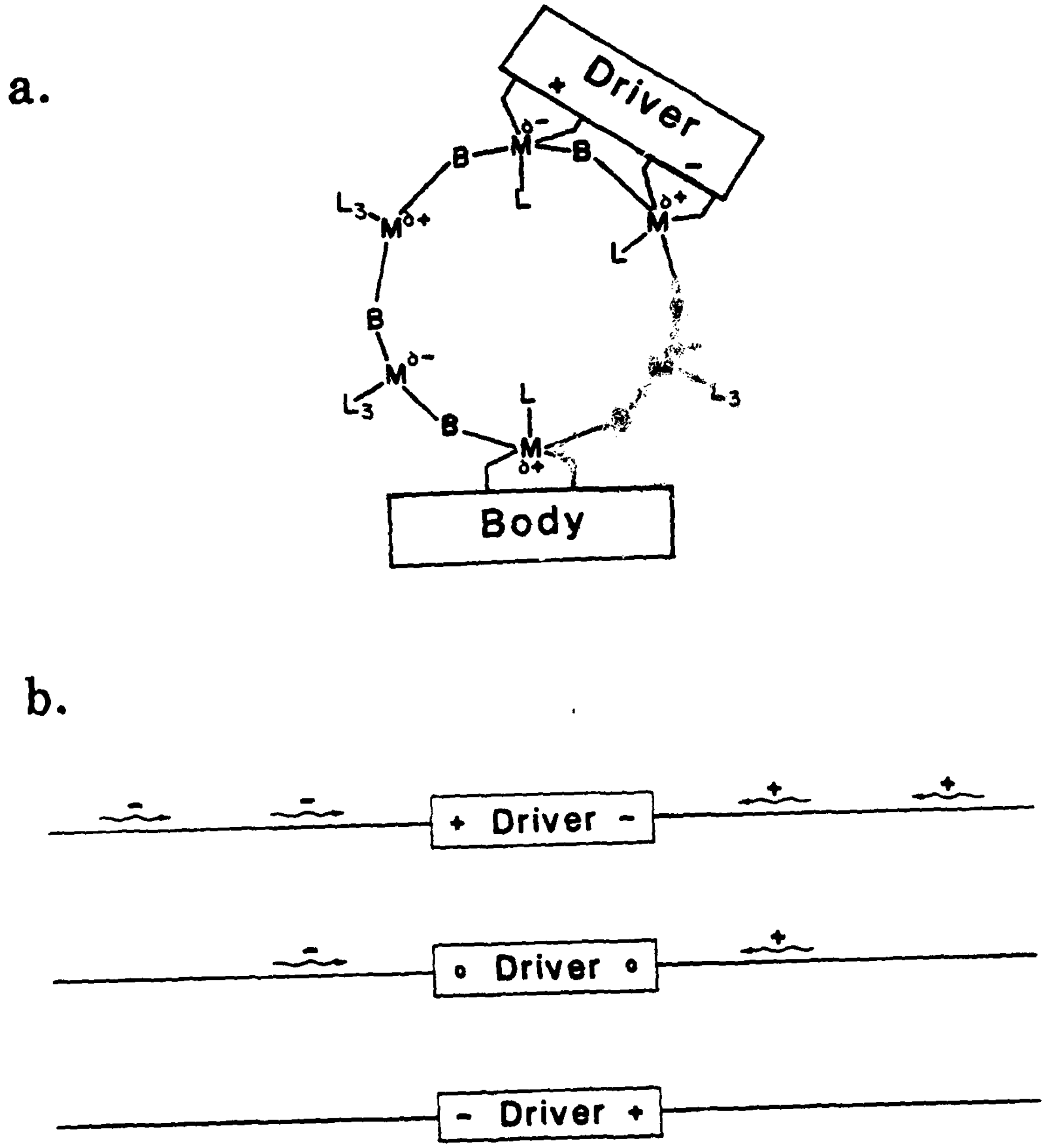


Fig. 10: The bistable chemical memory unit of Ref. (1b) is shown in a) while b) illustrates the reversal of the Driver charges by two pairs of solitons. The read device of the chemical memory is a multibarrier tunnel switch whose BODY and one Control Group is shown at the bottom of Fig. 10a.

A New Valence-Bonded Surface Contact

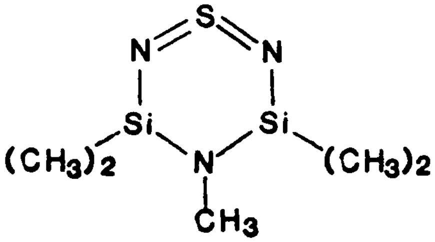
In the first EAP Annual Report it was suggested that the preferred method of communicating electrically with a molecular switch was via a direct Valence-Bonded Surface (VBS) contact (Ref. 1a, p. 129). Here a conducting polymer is covalently bonded to a metal surface (like Pt) by first exposing the metal surface to a reactive trimethoxysilane and then chemically modifying the attached silane to form:

$$\text{metal-Pt-O-Si(OCH}_3)_2\text{CH=CH-CH=N-(SN)}_x$$

This approach however results in a short insulating section between metallically conducting $(SN)_x$ and the Pt metal. This potential problem would appear to be avoidable by noting the recent preparation of the sulfur diimides by Scherer and Wies (8):

$$(CH_3)_3Si{-}N{=}S{=}N{-}Si(CH_3)_3$$

I



II

and of $(SN)_x$ from species I by Milliken (9).

Since in both sulfur diimides nitrogen is bonded to tetravalent silicon we can reasonably anticipate that the diimide could bond directly to the clean surface of semiconducting silicon thus:

$$\text{semiconducting-Si-N=S=N-Si(CH}_3)_3$$

although a sulfur link to the surface might be stronger. Then for successive treatments of the modified Si surface by first SCl_2

$$\text{(semi)-Si-S-N=S=N-Si(CH}_3)_3 + \text{SCl}_2$$

$$\downarrow \; - \text{ClSi(CH}_3)_3$$

$$\text{(semi)-Si-S-N=S=N-S-Cl} + (\text{CH}_3)_3\ \text{SiN=S=NSi(CH}_3)_3$$

$$\downarrow \; - \text{ClSi(CH}_3)_3$$

$$\text{(semi)-Si-S-N=S=N-S-N=S=N-Si(CH}_3)_3\text{SCl}_2$$

and then sulfur diimide, one can increase the size of the chain each time by $-(SN)_2-$ increments. Whereas Milliken produced $(SN)_x$ by the sublimation of the black powder reaction product of SCl_2 and $((CH_3)_3SiN)_2S$ (I) the above approach permits the control of the length of the $(SN)_x$ by units of $-(SN)_2-$ provided the SCl_2 treatment does not cleave the Si-N or SiS-N bonds at the surface. These bonds however are reasonably sterically protected by the bulk silicon. Finally we note 1) that if the bulk silicon is heavily doped one has a VBS contact of low resistance; and 2) that the nature of the silicon doping could result in a diode behavior.

Future Developments in Synthesis

The synthesis of future molecular devices constitutes a problem of extreme importance where ultimately one must make the maximum use of the principles of self-assembly and self-organization. However, before those principles are fully known other techniques also invite exploration. Such a technique might well involve very small electro-chemical cells. The advantages of such a cell are numerous and include:

1) Rapid turnover of solutions - that is the amount of solution used as reagents and rinse would be very small.

2) An electron potential can be used to drive many electric cell reactions to completion and hence avoid some of the problems suggested by the well-known mass action principle.

3) By reversal of current and the pole position it may be possible to grow conducting copolymer chains of definite length depending on the number of potential reversals. Thus:

$$(+\text{metal})\text{ABABABAB}^{+} + \text{A}^{-} \rightarrow (+\text{metal})\text{ABABABABA}$$

$$(-\text{metal})\text{ABABABABA}^{-} + \text{B}^{+} \rightarrow (-\text{metal})\text{ABABABABAB}$$

where A^- and B^+ are mixed in solution but react only with the end of the chain under the right potential.

4) Directed spatial structuring of small components should be possible using an electric field. For example, the growth of the charged polymer chain in 3) above could be achieved in an electric field so that it always stretched from left to right. In this case the field must be reversed each time the chain end reacted and changed the sign of its charge.

Summary

Modern chemistry begins with structural information; from the interatomic distances and angles not only can you predict properties and lifetimes of processes but also synthetic approaches. We have shown that structural or conformational information can provide the key to switching at the molecular level ranging from electron tunnelling and soliton switching to soliton valving, reversal and generation. Since many bulk properties of electroactive polymers are dependent on molecular conformation, these materials may prove to be the key to chemical synthesizing molecular devices. While most of the examples given are drawn from organic chemistry, the bistable chemical memory suggests that inorganic examples will become plentiful; the enormously rich field of transition metal chemistry has hardly been mentioned as an area to be searched for molecular switches.

In the last sections new opportunities in the development of valence surface contacts and the advantages of using small electrochemical cells for synthetic microfabrication of future molecular electronic systems were described.

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