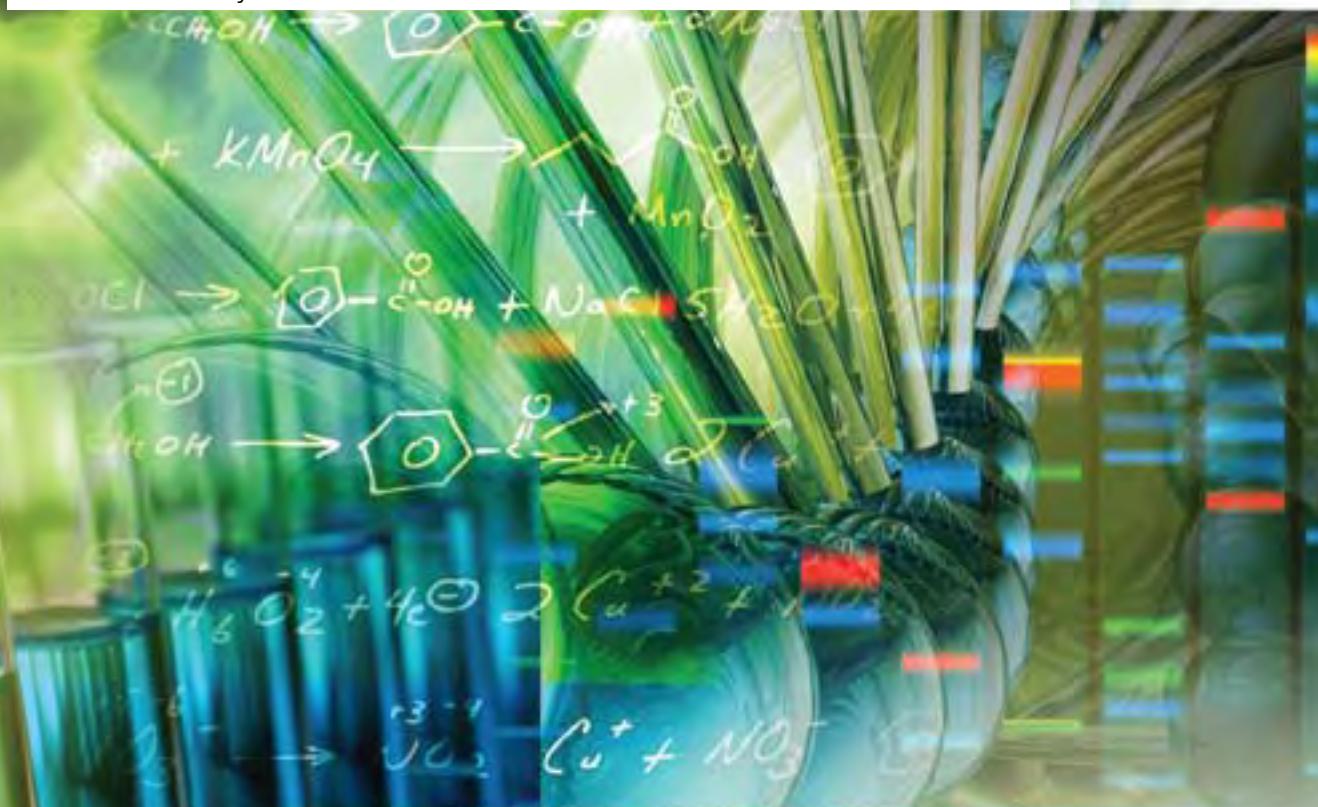


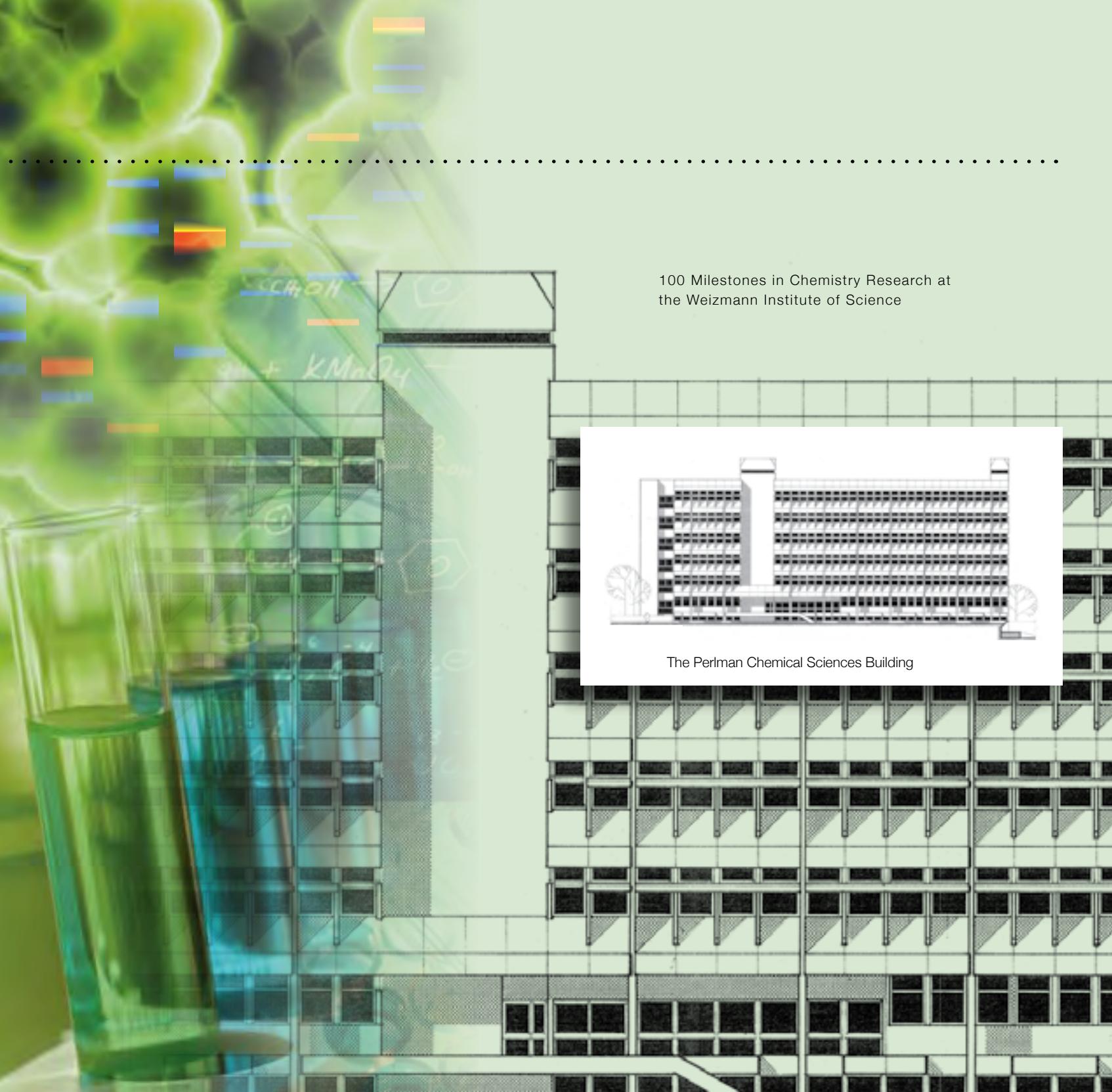
# 100 Milestones

in Chemistry Research at the Weizmann Institute of Science



CELEBRATING 35 YEARS OF  
THE PERLMAN INSTITUTE OF CHEMICAL SCIENCES





100 Milestones in Chemistry Research at  
the Weizmann Institute of Science

The Perlman Chemical Sciences Building

“ THE MOST ALL-PENETRATING  
SPIRIT BEFORE WHICH WILL OPEN THE  
POSSIBILITY OF TILTING NOT TABLES,  
BUT PLANETS, IS THE SPIRIT OF FREE  
HUMAN INQUIRY. ”

DMITRI MENDELEEV, (1834-1907)  
BEST KNOWN FOR HIS PERIODIC  
TABLE OF THE ELEMENTS

22	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	31	Ga	Ge	As	Se	Br	Kr	
23	Titanium	Titanium	Chromium	Manganese	Iron	Cobalt	Nickel	Copper	Zinc	32	Gallium	Silicon	Phosphorus	Sulfur	Chlorine	Argon	
40	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	49	In	50	51	52	53	54	
41	Zirconium	Niobium	Molybdenum	Techneium	Ruthenium	Rhodium	Palladium	Silver	Cadmium	47	Antimony	Selenium	Arsenic	Bromine	Chlorine	Krypton	
72	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	81	Tl	82	83	84	85	86	
73	Hafnium	Tantalum	Tungsten	Rhenium	Osmium	Iridium	Platinum	Gold	Mercury	80	Thallium	Lead	Bismuth	Poison	Atmosphere	Radium	
104	Rf	105	Db	106	Sg	107	Bh	108	Hs	109	Mt	110	Ds	111	Rg	Uub	Rn
	Rutherfordium	Dubnium	Seaborgium	Bohrium	Hassium	Meltanium	Darmstadtium	Roentgenium	Ununbium								

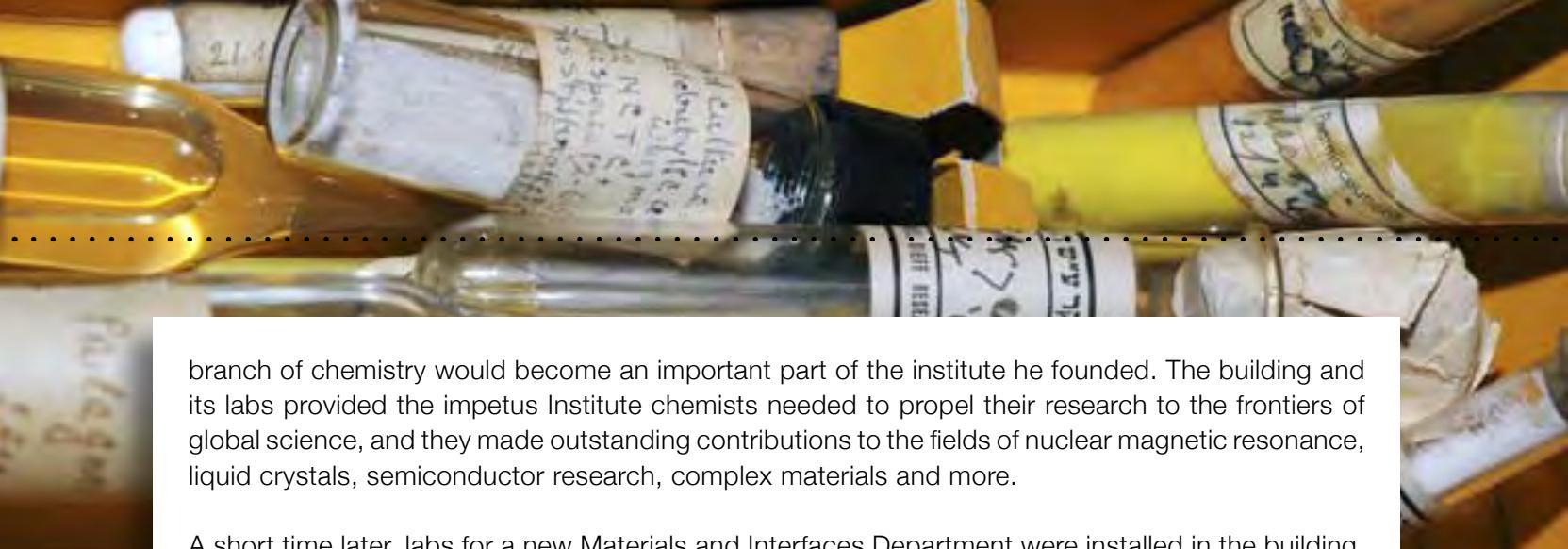
57	La	58	Ce	59	Pr	60	Nd	61	Pm	62	Sm	63	Eu	64	Gd	65	Dy	66	Tb	67	Ho	68	Er	69	Tm	70	Yb	71	Lu
	Lanthanum	Cerium	Praseodymium	Nd	Neodymium	Terbium	Europium	Eu	Promethium	Samarium	Europium	Eu	Gadolinium	Gadolinium	Terbium	Terbium	Dysprosium	Dysprosium	Holmium	Holmium	Thulium	Thulium	Ytterbium	Ytterbium	Yttrium	Yttrium	Yttrium		
89	Ac	90	Th	91	Pa	92	U	93	Np	94	Pu	95	Am	96	Cm	97	Bk	98	Cf	99	Es	100	Fm	101	Md	102	No	103	Lr
	Actinium	Thorium	Protactinium	Uranium	Neptunium	Plutonium	Americium	Curium	Berkelium	Cf	Californium	Curium	Curium	Curium	Berkelium	Berkelium	Cf	Cf	Berkelium	Berkelium	Curium	Curium	Mendelevium	Mendelevium	Amberberium	Amberberium	Lawrencium		



**C**hemistry was the first field of research at the Weizmann Institute of Science, and it will play a significant role in shaping the Institute's future. The Institute's founder and first President, Dr. Chaim Weizmann, was a chemist who strongly believed in the value of basic research; but he also knew how to seize an opportunity and turn scientific findings into useful applications. He said: "I trust and feel sure in my heart that science will bring to this land both peace and a renewal of its youth, creating here the springs of a new spiritual and material life. I speak of both science for its own sake and science as a means to an end." But Weizmann, the visionary who foresaw the need for first-rate science in the land of Israel, could not have imagined the Institute – now one of the world's top multidisciplinary research centers – that has grown up around the original chemistry labs. If he were to visit the Institute today and peek into the various labs where physics, genetics, robotics or brain research is conducted, he might be amazed at the scientific questions we are daring to address. If he were to enter the chemistry labs, he would be doubly amazed – both by the advances that enable scientists to control chemical processes and delve into the secrets of nature with ever greater precision, and by the breadth of a field that currently encompasses everything from global weather phenomena to the atomic structure of biological molecules.

The Faculty of Chemistry was officially created in 1971, when all the Institute's various departments were organized into five faculties. Coinciding with the 100<sup>th</sup> anniversary of Dr. Weizmann's birth, the faculty experienced a "Big Bang": A significant, generous gift, made by Harold Perlman of Chicago in memory of his parents several years before, in 1969, enabled the establishment of the Perlman Institute of Chemical Sciences and the construction of the Perlman Chemical Sciences Building, dedicated in 1974. The six-story edifice's 7,435 sq. meters, home to the Isotope Research and Chemical Physics Departments, housed some of the most advanced chemistry labs of that day.

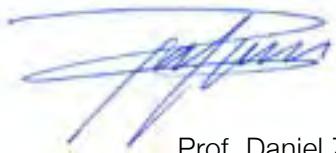
Harold Perlman was a philanthropic visionary and pioneer who understood the central role that materials science would come to play in chemical research; indeed, over the next 40 years this



branch of chemistry would become an important part of the institute he founded. The building and its labs provided the impetus Institute chemists needed to propel their research to the frontiers of global science, and they made outstanding contributions to the fields of nuclear magnetic resonance, liquid crystals, semiconductor research, complex materials and more.

A short time later, labs for a new Materials and Interfaces Department were installed in the building, where they continue to produce top-notch research to this day. Truly, the impact of the scientific activity taking place in the Perlman Chemical Sciences Building has gone far beyond the physical walls, leading to the development of additional research fields at the Weizmann Institute. Among these are the Structural Biology Department – which can boast a number of impressive achievements in recent years – and the Environmental Sciences and Energy Research Department.

Looking back over the record of the achievements of Weizmann Institute scientists in the various areas of chemistry, the creation of the Perlman Institute of Chemical Sciences and the Perlman Chemical Sciences Building stands out as a landmark. After that point in time, one can see chemical research branching out in all sorts of new directions. Like the spot on a tree trunk where the strongest limbs begin spreading out, giving shade to an entire patch of ground, the completion of institute and building in 1974 represents the generation of multiple new directions in the evolution of the Faculty of Chemistry, enabling its varied branches to spread and grow.



Prof. Daniel Zajfman  
President  
Weizmann Institute of Science

# 1934

The Daniel Sieff Research Institute was founded by British philanthropists and friends of Dr. Chaim Weizmann, Israel and Rebecca Sieff, in memory of their son. The building featured up-to-date labs and equipment, including Weizmann's lab and office. Part of the Organic Chemistry Department is still housed in the historic building, as is Dr. Weizmann's memorial laboratory.





# 1938

When the electrodes are bombarded by positive ions of argon or nitrogen or mercury, at pressures of 10<sup>-4</sup> mm., identical negative ion curves are produced, whatever the gas of positive ion. The probable cause of this is that these peaks are about 16, 24, 32, etc. In this set of curves, using positive ions of hydrogen or mercury, the peak at mass number 16 (possibly C<sub>2</sub>H) is about twice as intense as any of the other peaks. The energy and intensity of the positive ion current in a properly degassed apparatus is detectable even under vacuum conditions causing new results about the formation of hydrogen are reported being probably due to oxygen in the surface. Nitrogen positive ion current is low.

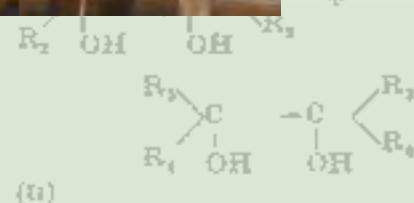
The apparatus was used several runs taken. Analysis curves were now entirely those obtained in argon, nitrogen, and oxygen vapour. The main peaks in oxygen were at mass numbers 16 and 32, representing O<sub>2</sub><sup>-</sup>. The O<sub>2</sub><sup>-</sup> peak was very intense, being about as high as it was in the other gases. It was increased by a factor of about 0.5. The O<sub>2</sub><sup>-</sup>, which was so intense in argon and oxygen vapour, was barely perceptible in the other peaks.

The oxygen was then all pumped off the electrodes bombarded with positive ions, after removing the liquid air traps. The analysis curves of negative ions remaining in the apparatus was still O<sub>2</sub><sup>-</sup>, being 24 times as intense as any other peak. For the ions produced at the cathode E, of our apparatus, the main peaks were those of mass numbers 24 and 32. Re-flushing the apparatus considerably reduced the O<sub>2</sub><sup>-</sup> peak from the cathode, but had no marked effect on the ions from E<sub>2</sub>.

The results in oxygen, which are in agreement with those already published<sup>1</sup>, appear to show that both O<sub>2</sub><sup>-</sup> and O<sub>3</sub><sup>-</sup> are produced by positive ions of oxygen capturing two electrons from the surface, as was previously suggested. However, these ions can also

When a high yield of light negative ions is produced by Hg<sup>+</sup> ions, the number of Hg<sup>-</sup> ions formed will be considerably decreased. This may account for the fact that the O<sub>2</sub><sup>-</sup> peak is not as intense as it would be if there were no Hg<sup>+</sup> ions.

A group of Institute chemists found that amino acids, the building blocks of proteins in all living things, can be broken down when mixed into water and exposed to ultraviolet light. The initial byproduct of this breakdown was ammonia (NH<sub>3</sub>). The scientists noted that some amino acids broke down faster than others, while those with phenyl groups also underwent side reactions "leading to an insoluble coating on the quartz walls and to the formation of an unpleasantly smelling volatile product." They surmised that amino acids in green plants might be broken down in a similar way by simple chemical reactions involving water and light.



In both cases the characteristic reaction is the migration of the hydrogen atom H\* of the alcoholic R<sub>1</sub>OH group.

# 1938

A good deal of research in the Daniel Sieff Research Institute concerned the uses of natural and agricultural products, with the aim of strengthening the country's nascent economy. Its scientists applied the fermentation techniques developed by Dr. Weizmann to such materials as orange and grapefruit peels, creating useful chemical compounds and substances with new properties. In other research, fennel and anise oils were found to contain compounds that were chemically similar to the hormone estrogen, and these were proposed as a source of synthetic estrogen.



# 1940

Petroleum products were an important subject of Institute research; its scientists looked for ways of improving the refining process and of producing new industrial chemicals and materials. Methods for "cracking" the oil to create higher octane fuel were investigated, and an anti-knock compound developed. Institute research also led to a method for producing a type of synthetic rubber.



# 1941

During WWII, Institute scientists adapted their research to the creation of drugs and other substances that had been imported from Germany. When the war began, the scientists' efforts turned to the production of the quinine substitutes Atabrine and plasmoquine for treating the malaria that still plagued the population in Palestine and the Allied troops serving in the region. Another drug to come out of Institute labs at that time was Evipan, a barbiturate-based painkiller. A summary of research from that period reported the development of methods for the production of 22 new compounds, including "anti-malarials, disinfectants, hypnotics, hormones, etc."



# 1947

The Institute envisioned by Dr. Weizmann was to be a regional center for scientific advancement, its scientists working in fruitful collaboration with labs in such respected institutions as the University of Cairo. As late as 1947, Institute scientists were publishing the results of research conducted in collaboration with chemists at the American University of Beirut.



# 1949

The Daniel Sieff Research Institute officially became the Weizmann Institute of Science, in honor of Dr. Weizmann's 75<sup>th</sup> birthday. The new Institute was initially made up of five departments: two chemistry (isotope research and polymer research), together with biophysics, biochemistry and microbiology, and applied mathematics. The latest in scientific equipment – including a mass spectrometer and an X-ray diffraction unit – was installed in the Institute's labs.



TABLE I

MEASURED DIELECTRIC CONSTANTS, REFRACTIVE INDEXES AND DENSITIES OF SOLVENTS AND POLYCYCLIC SPIRANS

Solvent

Benzene at 30°

Toluene at 30°

Toluene at 90°

$\alpha$ -Methylnaphthal-

DIELECTRIC CON-

$\epsilon \times 10^4$        $\Delta\epsilon \times 10^4$   
Compound

at

0      -1  
32     30  
60     56  
86     81  
115    108  
145    136  
176    164  
208    194  
248    228  
310    ...  
658    ...

Compound III

at

0      -3  
77     79  
90     94  
98     102  
108    111  
120    123

Among the thousands of chemical compounds explored in the labs of the Institute were polycyclic spirobypyrans — chemicals that change their color when exposed to light or heat. These substances were interesting because the change was reversible: Turn off the light, and they revert back to the original color. A team of Institute scientists teased out the chemistry of this change, finding how the distribution of electric charges on the spirobypiran molecules affected the color change. These color-changing chemicals became the basis of ground-breaking work on optical data storage by Weizmann Institute scientists.

$\epsilon \times 10^4$        $\Delta\epsilon \times 10^4$

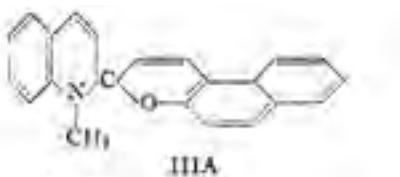
Compound III in benzene

0	-3
0.11	6
.21	8
.36	12
.47	19
.55	23
.67	25
.78	27

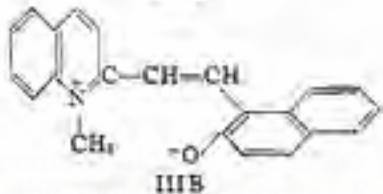
$\epsilon \times 10^4$        $\Delta\epsilon \times 10^4$   
Compound III in  $\alpha$ -methylnaphthalene

0	-5
0.60	17
1.14	35
1.54	50
2.21	71
2.75	97
3.49	100
3.95	121

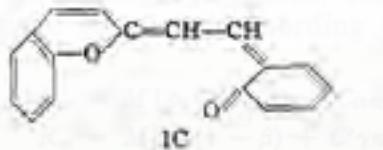
employed. No corrections for solvent polarization<sup>15</sup> had to be introduced. The densities were measured in a bicapillary pycnometer of about 7 ml. capacity. The molecular refractions were both measured experimentally and calculated from bond refraction data,<sup>14</sup> and the average



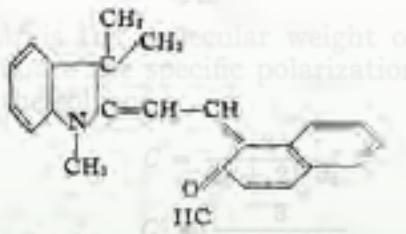
III A



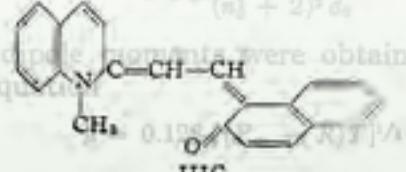
III B



I C



III C



III C

molecular weight of the solute,  $R_D$ , for polarization and refrac-

tion measurements,  $\Delta\epsilon = \epsilon - \epsilon_0$ ,  $\Delta n^2 = n^2 - n_0^2$ ,  $\Delta d = d - d_0$ .

The dipole moments were obtained from the usual equations:

$C = \frac{1}{2} \left( \frac{\epsilon - 1}{\epsilon + 2} \right) d_0$

$C = \frac{1}{2} \left( \frac{n^2 - 1}{n^2 + 2} \right) d_0$

$C = \frac{1}{2} \left( \frac{d - d_0}{n^2 - 1} \right) d_0$

The data for the solvents used are recorded in Table I.

The results are summarized in Tables II and III. Here  $\Delta\epsilon$ ,  $\Delta n^2$  and  $\Delta d$  are defined by  $\Delta\epsilon = \epsilon - \epsilon_0$ ;  $\Delta n^2 = n^2 - n_0^2$ ;  $\Delta d = d - d_0$ . They were measured with an accuracy of  $\pm 0.0002$ ,  $\pm 0.0004$  and  $\pm 0.00003$ , respectively.  $R_D$  denotes the molecular refraction calculated from bond-refraction data.

# Reversible Formation and Eradication of Colors by Irradiation at Low Temperatures. A Photochemical Memory Model

# 1951

ultraviolet light at 213°K. This color change phenomenon (named, "photochromism") in compounds related to dyes and spiropyran esters has been reported in many publications.

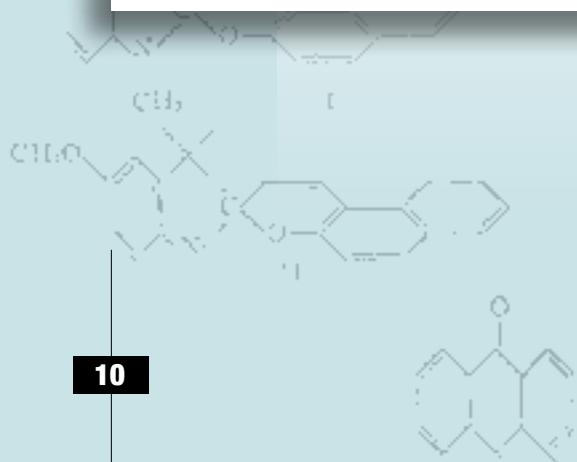
When the coloration are maintained they remain ultraviolet irradiation rates of decay of color are temperature of the solution the original color.

In a preliminary colored form of violet irradiation which it is stable eradicated by cycle can be re-solution.

This phenomenon compounds and aim of this paper

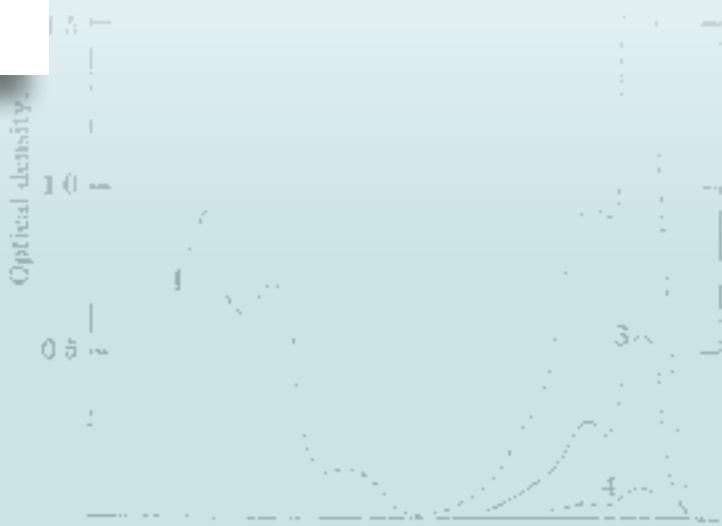
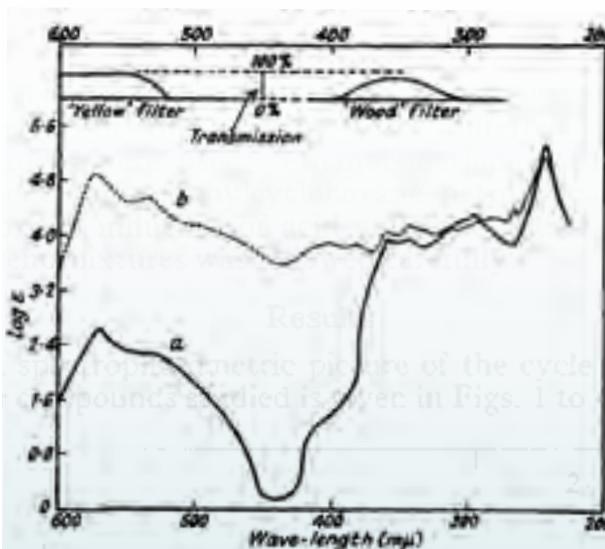
A suggestion from a member of the Electronics Department to an Institute chemist led to one of the seminal papers in the field of optical data storage.

The two scientists realized that chemical compounds that change their color under a beam of light – and remain stable until changed back again with a second action – might perform high-speed memory storage functions similar to the electronic computer, then in its infancy. The chemist proposed a memory storage system based on the properties of these compounds, and he invented the term “photochromism,” still applied to the field today.



10

irradiation with the 365 m $\mu$  group of the above



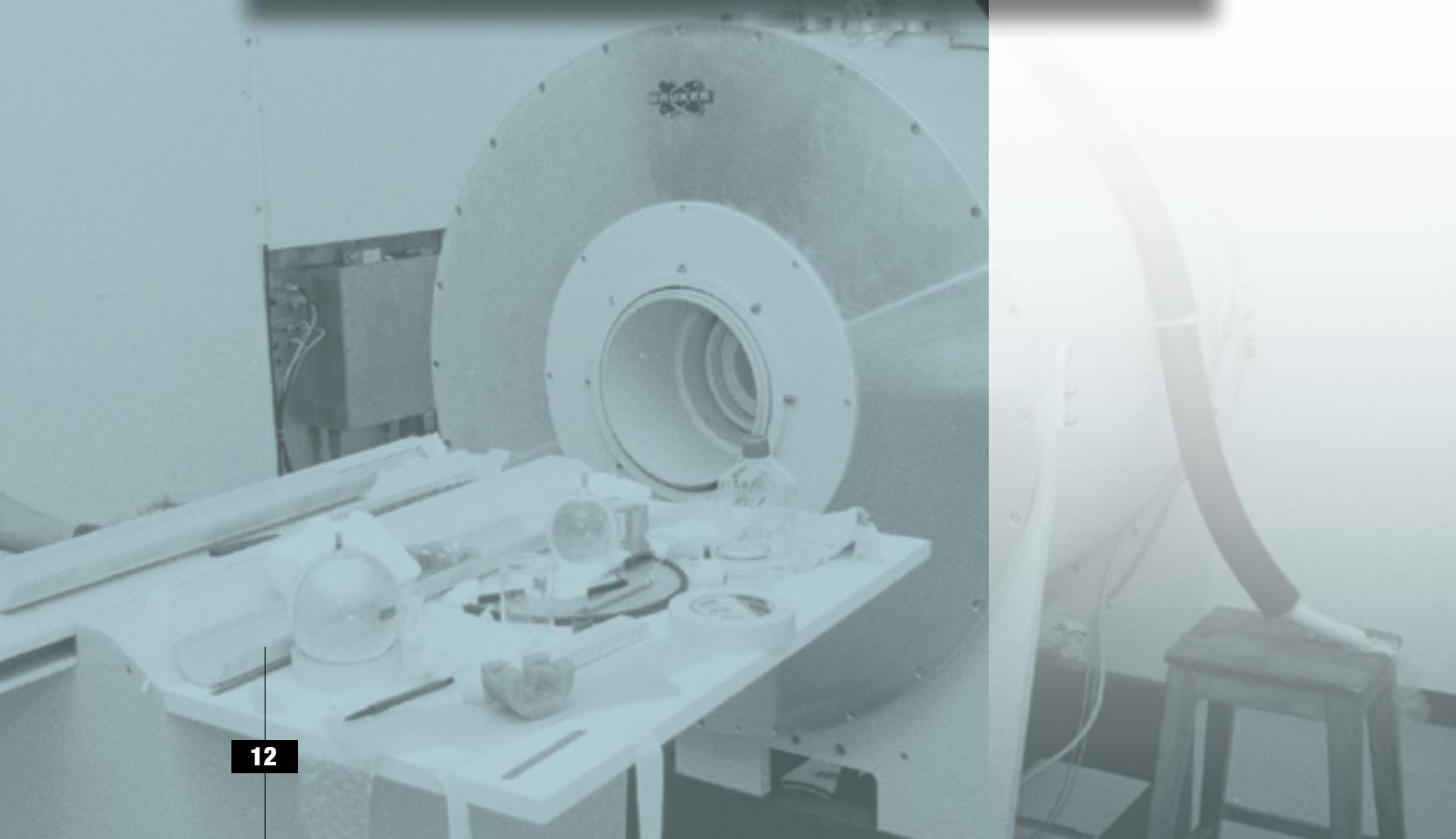
# 1952

The Weizmann Institute was a world leader in isotope research, and it boasted a unique apparatus for separating isotopes – elements that are heavier or lighter than the regular ones, due to a non-standard number of neutrons in the atomic nucleus. The Weizmann facility produced heavy oxygen, and for many years, it supplied most of the world's demand for this isotope. Heavy oxygen is used in a wide variety of research in chemistry, physics, biology and medicine, and in PET scan technology.



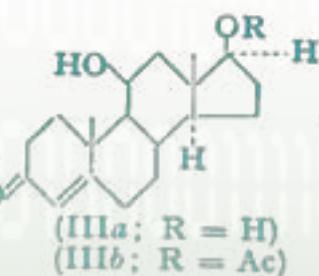
# 1954

Weizmann Institute scientists constructed a high-resolution nuclear magnetic resonance (NMR) spectrometer, one of the first such devices to be built in the world and a forerunner of present-day magnetic resonance imaging (MRI) scanners. The machine was used for pioneering spectroscopic studies, as well as to investigate molecular structure and dynamics.

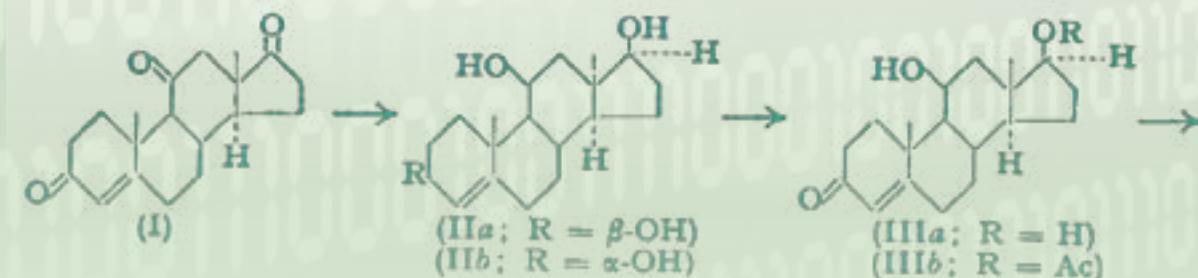


# 1954

W EIZAC, the first electronic computer in the Middle East, and one of the first in the world, was a coup for the mathematics department, but the Institute's chemists were among the first to benefit from it. Crystallographers and polymer scientists, for instance, found they could do several weeks worth of calculations in a mere hour or so.



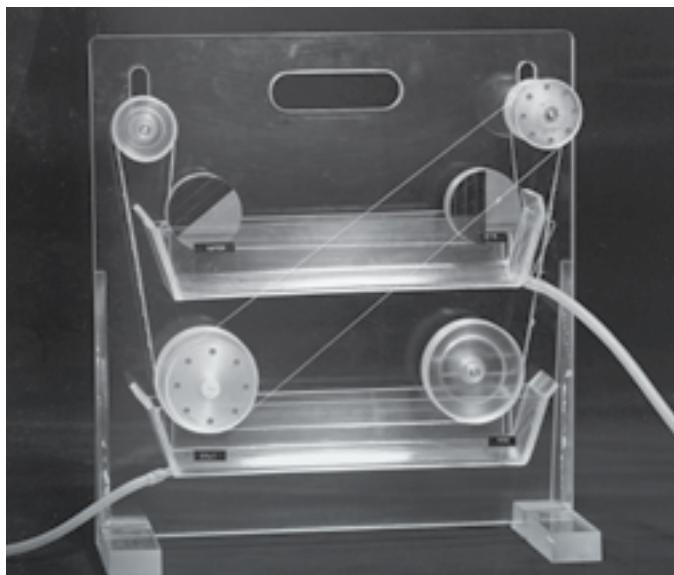
simply and in excellent hydrolysis.



11-Ketotestosterone (**IVa**) was prepared simply and in excellent yield by oxidation and subsequent hydrolysis.

# 1955

One of the dreams of Institute scientists was to build functioning “mechanoochemical machines” that would work in the same way as living tissue. A team of scientists created one such device out of collagen fibers, which are found in animal connective tissue. When subjected to dissolved salt, the fibers expanded or contracted, thereby operating a set of wheels. Though the dream was ahead of its time, the research advanced the study of the properties of living tissues, enabling the scientists to gain crucial insight into the dynamics of biological materials.



# OPENING CEREMONY

*of the*

## INTERNATIONAL SYMPOSIUM ON MACROMOLECULAR CHEMISTRY

# 1956

THE

A landmark international symposium on Macromolecular Chemistry was held at the Institute. This meeting signaled the rising standing of the Institute chemists in the global science arena, especially their “pioneering work on polyelectrolyte chemistry.” Touted uses for the new synthetic polymers highlighted at the symposium included blood clotting, soil conditioning and films for reservoirs to prevent evaporation.

SYNTHÉSE  
DU SYMPOSIUM INTERNATIONAUX  
DE LA CHIMIE MACROMOLÉCULAIRE  
SOUS LES AUSPICES DE  
LA COMMISSION DES MACROMOLECULES  
DE L'UNION INTERNATIONALE DE CHIMIE  
PURE ET APPLIQUÉE  
ET DU WEIZMANN INSTITUTE OF SCIENCE

*et*  
DEDICATION

MICHAEL AND ANNA WIX AUDITORIUM  
THE WEIZMANN INSTITUTE OF SCIENCE, REHOVOT

OPENING CEREMONY  
*of the*

## INTERNATIONAL SYMPOSIUM ON MACROMOLECULAR CHEMISTRY

UNDER THE AUSPICES OF  
THE COMMISSION ON MACROMOLECULES OF  
INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY  
THE WEIZMANN INSTITUTE OF SCIENCE, REHOVOT

*and*

DEDICATION  
*of the*

MICHAEL AND ANNA WIX AUDITORIUM  
THE WEIZMANN INSTITUTE OF SCIENCE, REHOVOT

Tuesday, April 3, 1956, 10.00 a.m.

### OUVERTURE

*du*

## SYNTHÉSE DU SYMPOSIUM INTERNATIONAL DE LA CHIMIE MACROMOLÉCULAIRE

SOUS LES AUSPICES DE  
LA COMMISSION DES MACROMOLECULES  
DE L'UNION INTERNATIONALE DE CHIMIE PURE ET APPLIQUÉE  
ET DU WEIZMANN INSTITUTE OF SCIENCE, REHOVOT

*et*

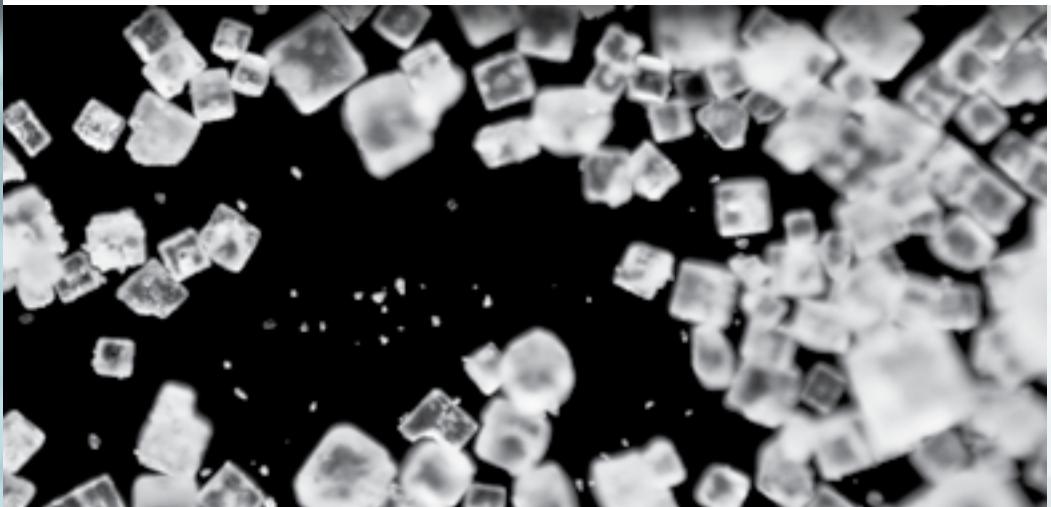
### DEDICATION

MICHAEL AND ANNA WIX AUDITORIUM  
THE WEIZMANN INSTITUTE OF SCIENCE, REHOVOT

Mardi, 3 avril 1956, 10.00 h.

# 1957

**H**ow does one measure the molecular weight of a new polymeric substance when it's dissolved in a solution? This is not a trivial question, as accurate measurement is the basis of nearly all chemical experimentation and theory. An Institute scientist attempting to determine the molecular weight of polyelectrolytes in solution using a light scattering technique found that the method would only work if he added a pinch of cooking salt to the solution. He then provided the chemical explanation as to why this should be so.



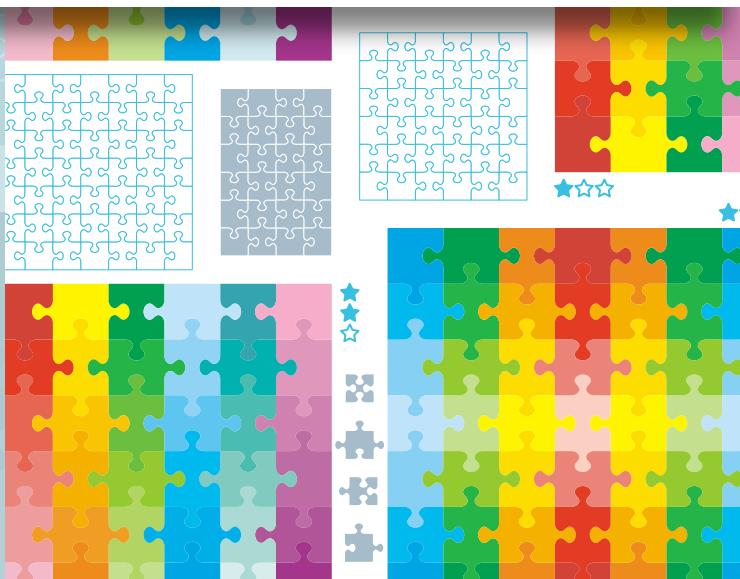
# 1959

Throughout the Institute's early decades, Weizmann chemists investigated the structure, properties, and performance of polymers — long molecules consisting of strings of smaller subunits. (DNA, proteins, polysaccharides and synthetic plastic materials are all polymers.) Among other things, the scientists studied the properties of electrically-charged polymers (polyelectrolytes) and their interactions with ions and other small molecules. Practical inventions to come out of this research included a spray-on polymer solution for preserving fruit, special plastics for covering greenhouses, fire retardants, improved polyesters, pesticides and specialized membranes.



# 1960

The still-growing Weizmann Institute underwent reorganization as new fields of research opened up. The chemistry departments in 1960 included photochemistry, organic chemistry, isotope research, x-ray crystallography and infrared spectroscopy. The NMR Department was absorbed into Nuclear Physics in 1962, and a Chemical Physics Department was established.



## Studies on the Antitumor Effect of Cucurbitacins\*

SIMON GITTER, RUTH GOURLEY, PHIA STEPHAT, AND DAVID LAVIE

• • • • • • • •  
*Hegel's Medieval Re*

# 1961

The car-  
dihydroela-  
ture, and  
cucurbitas

Three c  
inhibition  
Satyoma 1

Morphogenesis with relatively high ing capacity measured

The cucurbitacins are a group of substances which have been found in various species of the Cucurbitaceae family. The species of this plant family include *Cucurbita*, *Elatostema*, *Citrullus colocynthus*, etc. They have been known for their cathartic properties since remote times. In the last few years the cucurbitacins have been the object of more detailed studies, and complete structures have been proposed for elatericin A (I), elatericin B (IIa), and elaterin (IIb) (8) (Chart 1). All are tetracyclic triterpenes,<sup>1</sup> differing in the nature of their genated functions in ring A (e.g., I and IIa), or in the tertiary acetoxy group occurring in the side chain (IIb), as described in

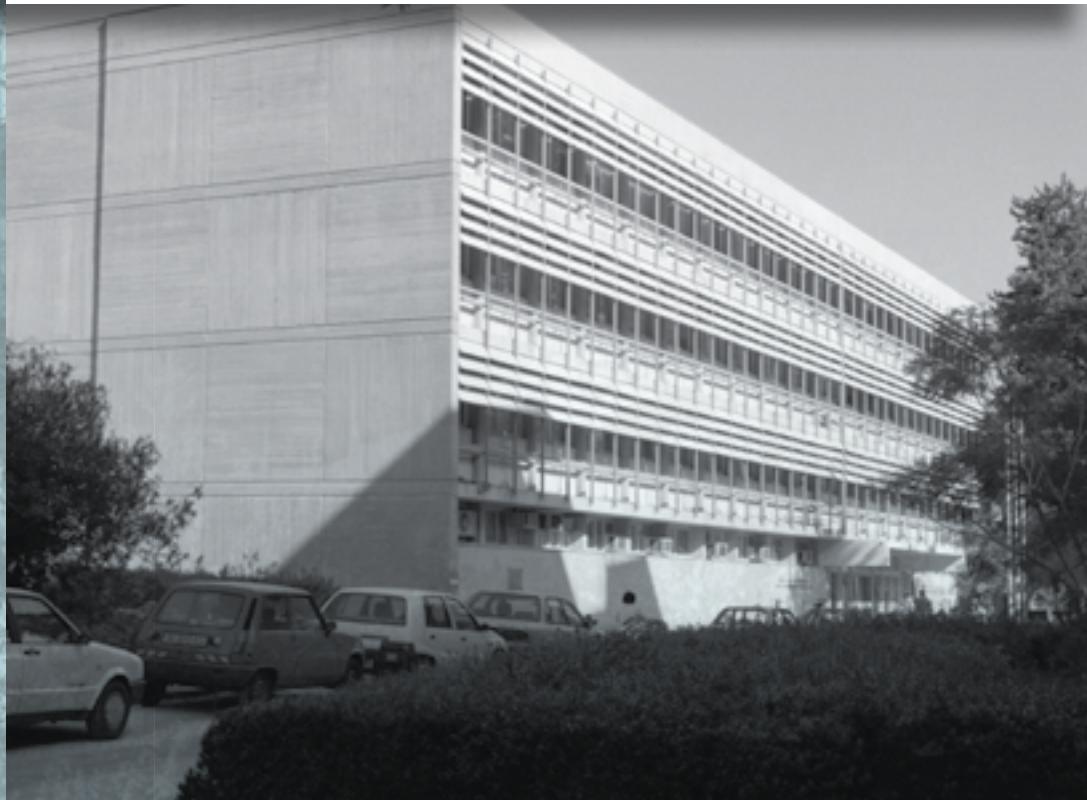


c) was prepared from the hydroxyl of elaterin by acid-catalyzed degradation experiments. The product was identified as 4-hydroxy-4-methylpent-2-enoic acid (4-HMP), the side chain of elaterin A, the side chain of elaterin B, and *trans*-4-hydroxy-4-methylpent-2-enoic acid (4-HMP) was obtained (10).

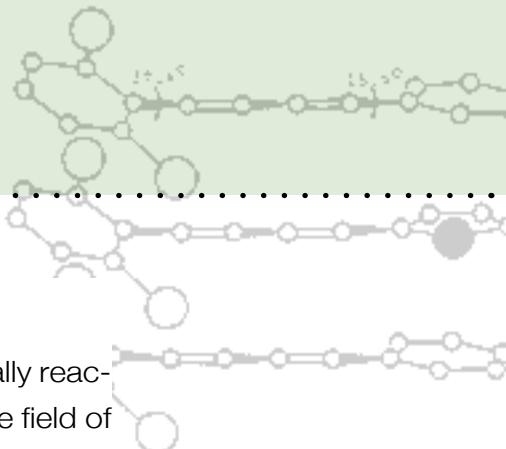
## MATERIALS AND METHODS

# 1964

A new building was erected adjoining the Daniel Sieff Research Institute to accommodate advances in chemistry research. Originally named for Ernst. D. Bergmann, the first scientific director of the Institute, the building housed the Organic Chemistry Department.



(1.3)



# 1964

We wished molecules of **3** to conferences in faces during respectively, terminated in structured by si within the state of 2 to translational symmetry guest molecules of **3** is, of **5a** to **5b**, *i.e.*, the optical yields primarily reflect the nature responsible for cyclodimerization we prepared, by growth glass bulbs,<sup>2</sup> large (1–6 g) containing 15% of **3** in **1**, radiated as above. The consistently found to crystals affording dextrorotatory material,  $[\alpha]_D +$  or — optically active **5** to a lesser many-fold enhancement nickel reductive degradation of (+)-**5** [*or*(-)-**5**] led to (-)-**6** [*or*(-)-**6**],  $[\alpha]_D$  ca.  $10^{\circ}$ ,<sup>11</sup> while acetylation of (+)-**5** afforded (-)-**7**,<sup>12</sup>  $[\alpha]_D$  ca.  $5^{\circ}$ .

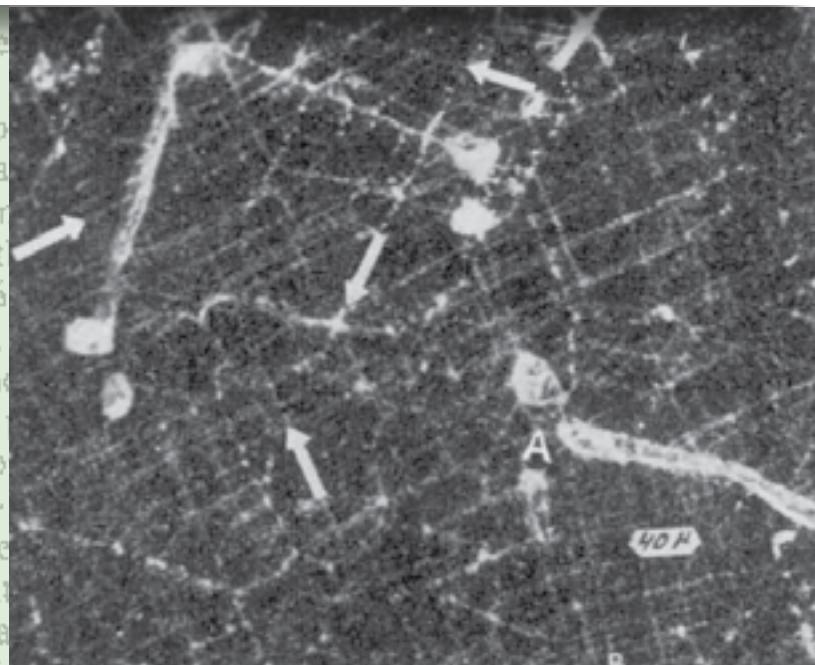
**21**

Diagram of a mixed crystal structure of **1**<sup>3</sup> showing the enantiomeric photodimers **5**.

the optical yield of this and the absolute configuration of the crystal (*i.e.*, whether the is in Figure 1 or as in its parent cyclobutane photodimer crystal, or one having determined. When will indicate which face of **1** or **3** is the more re will provide insight into ground-state molecules.

Finally, the simple production of active samples from optically inactive is highly relevant to current hypo biological origin of optical activity o

**Acknowledgment.** We thank Prof. and F. L. Hirshfeld for valuable di D. P. Robinson and Z. Shabani for

# 1965

Synthesizing antibiotic and other drug compounds for therapeutic use means they should be produced cheaply and efficiently on an industrial scale. Institute scientists took a novel approach, developing a range of chemically active polymers that are used for the preparation of various substances, including antibacterial compounds and biologically active peptides.

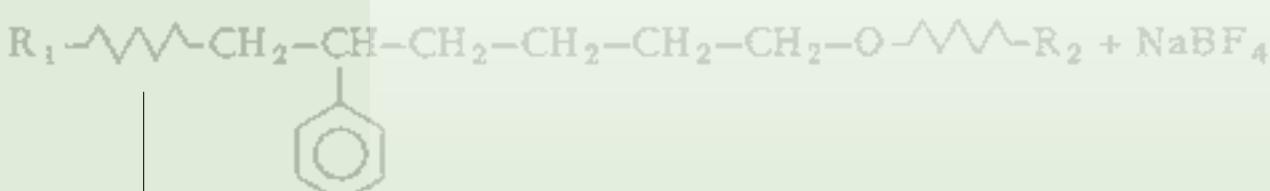
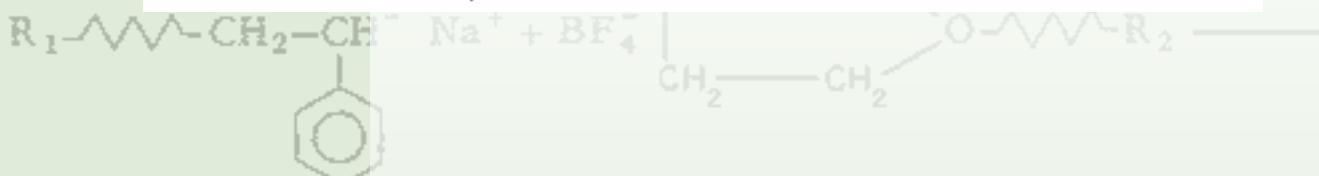
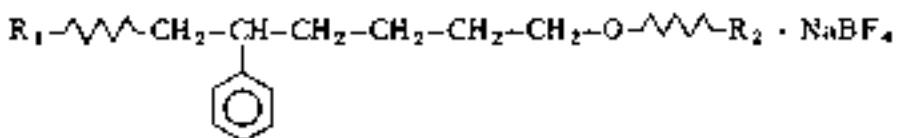
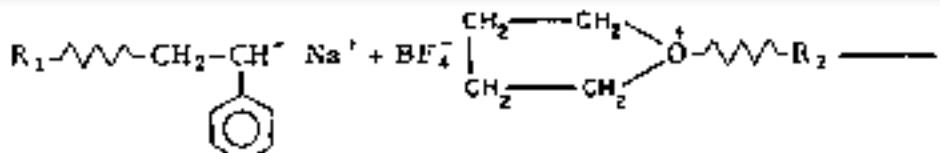


## MUTUAL TERMINATION OF ANIONIC AND CATIONIC "LIVING" POLYMERS\*

# 1966

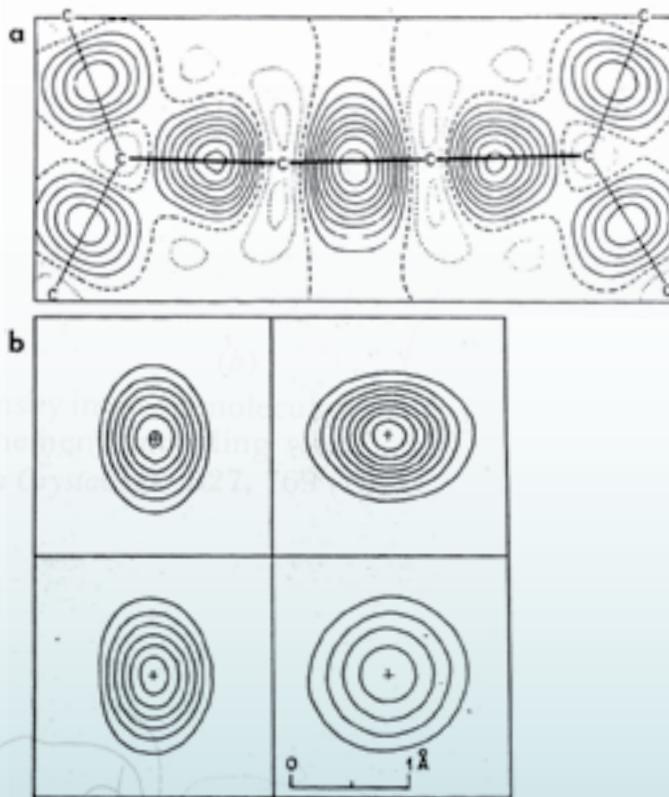
The most important feature of the anionic "living" polymers described by Szwarc, Levy, and co-workers is their ability to grow under living conditions. This mechanism is different from that of cationic polymerization, which is controlled by the addition of a proton acceptor (2).

Until recently, all living polymers were cationic molecules. An anion usually terminates the polymer chain by reacting with the proper counterion. Institute chemists found a new way of terminating the polymer chain growth by mixing two types of living polymers, one with a negative charge at the end of the chain (anionic), and the other with a positive charge (cationic). This resulted in a new type of "block co-polymer" having different properties than either of its constituent polymers.



# 1966

The chemical bonds between the atoms in molecules are functions of the electrons that are shared between them. Understanding the nature of these bonds goes to the very heart of chemistry. An Institute chemist developed a method for “dissecting” molecules to reveal the distribution of their electrons and thus how the various atoms bind to each other. This method, which provided scientists with a deep understanding of chemical processes, has become a standard tool in a number of areas of chemistry.



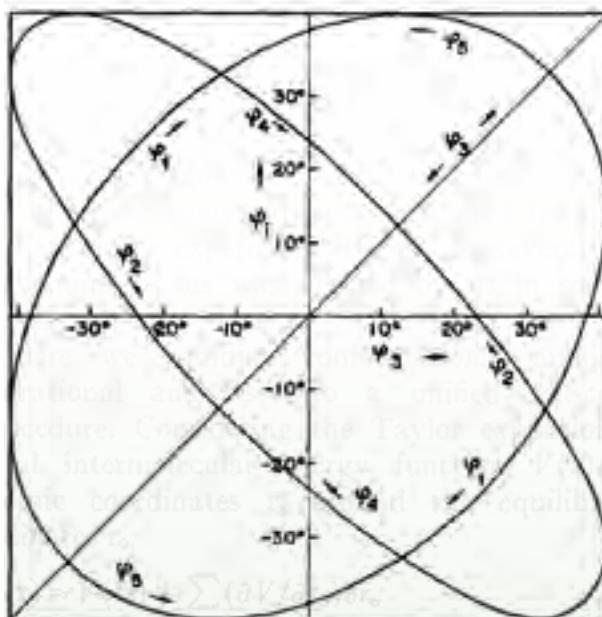
series of medium rings,  $C_5-C_{12}$ , were systematically calculated to obtain better agreement with experimental data on conformations and enthalpies. Recently he revised his calculations for  $C_6-C_{12}$ .

# 1968

## MUTUALLY CONSISTENT CONFORMATIONAL VIBRATIONAL ANALYSIS

**S**cientists often investigate the structure and reactivity of substances at the molecular level and need to quantify the forces that hold molecules together or those involved in various molecular reactions. Institute scientists developed a method, called the "consistent force field," for calculating the forces exerted within the molecule. This method makes it possible to elucidate the structure of molecules, as well as to calculate the binding energy of their components. In biological systems, it allows researchers to determine and quantify the structure of a protein or to compute the binding energy needed to activate molecules such as enzymes.

In the present case of empirical energy calculations in alkane molecules, the calculation of equilibrium spectra, strain energies from the same energy series from  $n$ -butane. The optimization of energy parameters by a least-squares method to obtain best fit with experimental data related to all above-mentioned calculations. With optimized parameters, the degree of success of our calculations depends only on the assumed functional form of the intramolecular energy. By examining a number of suggested energy functions we learn much about their properties, and by selecting the fittest we improve systematically the capability of empirical and semiempirical energy functions.<sup>10</sup>



$$+ \frac{1}{2} \sum_{\alpha, \beta} (\partial^2 V / \partial r_\alpha \partial r_\beta) \delta r_\alpha \delta r_\beta + \dots, \quad (1)$$

attribute simultaneously the appropriate physical meaning to each term in the series.

### A. The First Term Represents the Strain Energy

Our computer program calculates  $V(r)$  for a given conformation  $r$  for any cycloalkane or  $n$ -alkane molecule, from a set of energy functions.

### B. Equilibrium Conformation

The vanishing of the second term, i.e., the solution of the set of equations