Henry Ford Hospital Medical Journal

Volume 15 | Number 2 Article 8

6-1967

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Recommended Citation

Parsons, Jonathan; Holcomb, John B.; and Beher, William T. (1967) "X-Ray Diffraction Powder Data for Steroids: Supplement VIII," *Henry Ford Hospital Medical Journal* : Vol. 15 : No. 2 , 133-138.
Available at: https://scholarlycommons.henryford.com/hfhmedjournal/vol15/iss2/8

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Henry Ford Hosp. Med. Journal
Vol. 15, Summer 1967

X-Ray Diffraction Powder Data for Steroids: Supplement VIII

Jonathan Parsons,* John B. Holcomb,* and William T. Beher**

This supplement continues a series of publications which began as a separate section, with the Dec. 1958 issue, and has been supplemented periodically since then. Other publications have been March 1961 (Supplement I) Sept. 1962 (Supp. II); March 1963 (Supp. III); March 1964 (Supp. IV); Dec. 1964 (Supp. V); Sept. 1965 (Supp. VI) and Dec. 1966 (Supp. VII).

A convenient way to determine the nature of minute quantities of crystalline materials is to use x-ray powder diffraction. By placing a few grains of powder in a small beam of monochromatic x-rays, a characteristic series of concentric cones, all having their apexes at the same point, are generated by the reaction of the x-rays with the systematically spaced atoms comprising the crystal. The intensities and geometric arrangement of the latter cones can be recorded on a film which is appropriately placed, giving rise to so-called x-ray diffraction powder patterns consisting of circles, arcs, or lines. These patterns can give one an insight into the atomic arrangement much below the limit of visual microscopic examination. In order to identify materials by this method, it is necessary to have standard patterns available with which to compare the pattern obtained from an unknown substance.

The steroids are a group of biologically important compounds for which good x-ray diffraction powder patterns are possible. Since 1956, this laboratory has been assembling this type of data as standards to use for identification purposes. The data supplied with this paper comprise a new supplement to the series of steroid data papers first published in the Henry Ford Hospital Medical Bulletin in 1958.[1] Including this set, data for 502 steroids have been assembled in this laboratory.[1-8]

Table I is a classified list of the 26 steroids included in this supplement. Each steroid for which data is reported has been re-crystallized in our laboratory and has had the melting point indicated in Table I checked with the chemical literature.

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The steroid data for this group of compounds is given in Table II with the numerical listings in Table I serving as a key. Interplanar atomic spacings in angstrom units are listed in the columns marked d(A); the relative intensities, in columns marked I/I_1. As with the previous papers in this series, photographs of these patterns are to be found at the end of this paper for use in making quick visual comparisons of patterns.

In order to conserve space, all the sets of pattern data in Table II have been combined into one page. Note that some sets continue from one column to the next.

ACKNOWLEDGMENTS

The authors wish to thank Professor William Klyne, Westfield College, London, England for supplying some of the steroids for which data has been reported.

The continued financial support of the Joint Committee on Powder Diffraction Standards through its agency, the American Society for Testing and Materials, is greatly appreciated.

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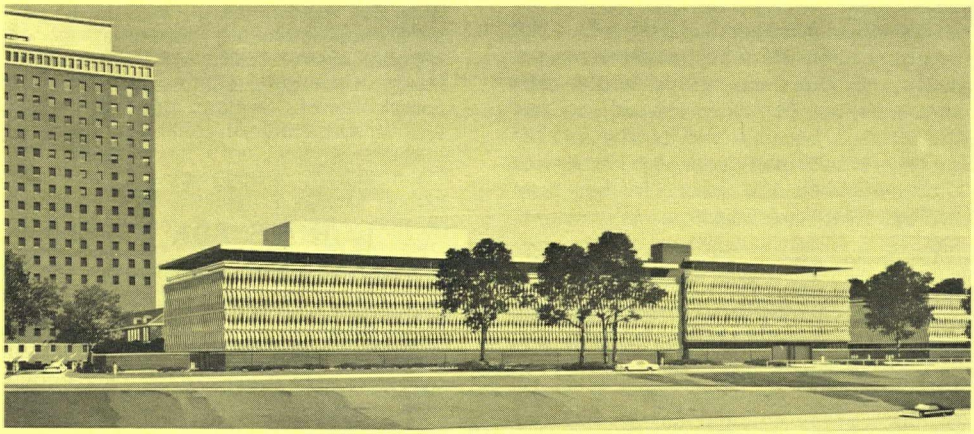
HFH IN THE NEWS

Published for alumni and friends of Henry Ford Hospital, Detroit, Michigan
Editor: C. E. Rupe, M.D. **Summer, 1967**



Photo, Albert Kahn Associated Architects & Engineers, Inc.

NEARING COMPLETION is this new General Services Building and Parking Structure on the northwest corner of the Henry Ford Hospital grounds. Although similar in exterior design to the hospital parking garage across the street, this building will have a below-grade level for housing a central kitchen, radiotherapy department, general stores and mechanical equipment. On the first floor will be the hospital's purchasing department and an emergency power installation. The building will provide 900 additional parking spaces available to patients in six above-grade floors. It was designed by Albert Kahn Associated Architects and Engineers, with Darin and Armstrong the general contractor.

CORONARY CARE UNIT IS EXPANDED

Following a year in operation, the Coronary Care Unit at Henry Ford Hospital has been expanded from eight to 10 monitored bed and may go to 12, according to Gerald M. Breneman, M.D., cardiologist in charge. Probably the largest in Michigan, the unit counted 502 admissions during its first 12 months. It is independent of the hospital's Special Care Unit and is designed for patients suffering from or in danger of myocardial infarction.

The Unit, on F-5, presently consists of five semi-private rooms and an adjoining nurse's station. Here visual and audible signalling systems immediately alert the staff to any changes in every patient's heart beat. Equipment at each bed includes in-the-wall oxygen supply and suctioning devices, cardiac monitors and a "memory module" which keeps 15 seconds of heart activity stored on tape at all times.

Also available in the Unit are resuscitative equipment, an electrical defibrillator, bed boards to provide a firm surface for cardiac massage and emergency drugs. Duty nurses are permanently assigned and specially-trained in recognizing electrocardiographic rhythm changes, administering oxygen and artificial respiration, performing cardiac massage and in anticipating other emergencies. A cardiology resident is present on the floor at all times.

DR. RUPE HEADS NEW EDITORIAL BOARD

With this Summer 1967 issue, the 14-year-old Henry Ford Hospital Medical Bulletin has changed its name, acquired a new editor and editorial board, a redesigned cover and a permanent base of operations. Now titled the HENRY FORD HOSPITAL MEDICAL JOURNAL, the quarterly publication becomes the responsibility of Dr. C. E. Rupe, editor, who succeeds Dr. Philip J. Howard, retired. Dr. Howard became first editor of the Bulletin in 1953 and concluded his service with the March 1967 issue. He has been named Consulting Editor.

Dr. Rupe, who is chief of the Fourth Medical Division of the Hospital, will be assisted by Dr. Melvin A. Block, associate surgeon, Division of General Surgery; and Dr. T. N. James, chairman, Section on Cardiovascular Research, as associate editors; and an editorial board consisting of Dr. P. D. Bartlett, chairman of the Department of Biochemistry and Molecular Biology, Edsel B. Ford Institute for Medical Research; Dr. Howard Duncan, Division of Rheumatology; Dr. R. H. High, chairman, Department of Pediatrics; Dr. R. C. Mellinger, of the Endocrinology Division; Dr. L. B. Stevenson, of the Department of Gynecology and Obstetrics; and Dr. D. Emerick Szilagyi, chairman, Department of Surgery.

Named to the position of assistant editor is Mrs. Enisse Chimes, who also has responsibility for other hospital publications in a newly established Publications Office. Robert H. Mohr continues as Medical Art Director.

The Medical Journal publishes papers from current or former staff members of the Henry Ford Hospital or the Edsel B. Ford Institute for Medical Research. The Journal will continue to cover a broad field of medical interests and will include case presentations, experimental studies in either the basic or clinical sciences as well as philosophically-oriented papers. The new editors and editorial board hope to maintain the high standards which have been set in the first 14 years of the publication.

Long is New Controller

Following the recent retirement of C. G. Puterbaugh, a veteran of more than 25 years' service at Henry Ford Hospital, Herbert E. Long has assumed the position of controller, it is announced by the board of trustees and the advisory board. Mr. Puterbaugh continues on the staff as a consultant. Mr. Long, a fellow of the American Association of Hospital Accountants, was associate controller of the hospital from 1963-66. A B.S. graduate of Miami University (Ohio), he had been comptroller of Cleveland Metropolitan General Hospital before coming to Detroit.

HONORS FOR STAFF

"For distinguished service in opening new horizons of progress", Dr. Harold M. Frost, chairman of the Department of Orthopedic Surgery, was one of five Michigan men who were given "Wolverine Frontiersman" awards by the Economic Club of Detroit during its annual Michigan Week observance. Dr. Frost was honored for his distinguished research in surgery, which won the Ludvic Hektoen Gold Medal Award for basic research from the American Medical Association. Another award recipient was Comedian Danny Thomas, a native of Deerfield, Mich.

The University of Michigan has conferred the Sesquicentennial Award on Dr. Fred A. Henny, chief of the Dentistry and Oral Surgery Division. Award recipients were judged on "knowledge, wisdom and the courage to serve".

Dr. Brock E. Brush, chief of Division One, General Surgery, has been appointed to serve on the committee on medical staff survey of hospitals by the Michigan State Medical Society.

An electron micrograph of an ultra-thin section of a vanadium pentoxide gel is part of the "Once Invisible" traveling exhibit sponsored by the Smithsonian Institution, and shown recently at the Museum of Modern Art in New York City. The micrograph was contributed by Dr. John H. L. Watson, Department of Physics in the Edsel B. Ford Institute for Medical Research.

Death Claims Four Staff Members

JOHN GASTON MATEER, M.D. 1890-1966

Named consultant in 1964 after almost half a century of service to medicine, Dr. Mateer died Sept. 2, 1966. He had been Chairman, Department of Medicine, from 1952 to 1963. Before that he had held the position of Physician-in-Charge of the Division of Gastroenterology for 32 years, starting in 1920.

A graduate of the Johns Hopkins Medical School, he interned and continued in a medical residency there before coming to Henry Ford Hospital in 1920. Dr. Mateer was a member of Phi Beta Kappa, Alpha Omega Alpha, the American Clinical and Climatological Association, the American College of Physicians, and the American Association for the Study of Liver Diseases. He had been treasurer of the American Gastroenterological Association for seven years, its president in 1950, and a member of the governing board for 13 years.

In April 1966 at his alma mater, The College of Wooster, Ohio, Dr. Mateer witnessed the ground breaking for a new science building bearing his name — the gift of his many friends and patients.

F. JANNEY SMITH, M.D., 1888-1966

A senior consultant to the Cardiology Division at the time of his death on November 9, 1966, Dr. Janney Smith had been on the hospital staff since 1915. He became physician in charge of the Cardiorespiratory Division following his graduation, internship and residency training at Johns Hopkins University. He received his A.B. degree in 1909 and his M.D. in 1913 from Johns Hopkins.

He was a member of the American Medical Association, the American Clinical and Climatological Association, the American Heart Association and the Michigan State Medical Association. Dr. Smith was elected a Fellow of the American College of Physicians in 1936 and was a diplomate of the American Board of Internal Medicine.

FRANK ROBERT MENAGH, M.D., 1890-1967

Dr. Menagh, who died Feb. 12, had been chief of the Division of Dermatology from the time it was organized as an integral part of the Department of Medicine until 1953, when he became a consultant. He came directly to Henry Ford Hospital after receiving his M.D. degree from Johns Hopkins University School of Medicine in 1918, and had served here continuously except for an interruption during World War I when he was a first lieutenant in the Medical Corps. He was one of the first two interns to receive training at this institution.

Dr. Menagh was a member of the American Medical Association, the American Academy of Dermatology, the Society for Investigative Dermatology, the Society for the Study of Asthma and Allied Disorders; the Michigan State Medical Society, and a member and past president of the Detroit Dermatological Society. Dr. Menagh was elected a fellow of the American College of Physicians in 1929, and was a diplomate of the American Board of Dermatology. He was an emeritus fellow of the American Academy of Allergy.

THOMAS GAHAGAN, M.D. 1926-1967

Associate surgeon in the Division of Thoracic Surgery, Dr. Gahagan died May 5, 1967. He had been an intern at the Hospital in 1951 and returned in 1953 as a resident in general surgery. His appointment in 1959 as Associate Surgeon followed a two-year military leave serving with the Air Force.

Dr. Gahagan received his B.A. degree from Michigan State College (East Lansing) in 1947 and his M.D. from the Wayne State University College of Medicine in 1951. He was certified by the American Board of Surgery in 1958 and the Board of Thoracic Surgery in 1961. He became a member of the American College of Surgeons in 1961 and of the American Association for Thoracic Surgery in 1963.

12 ASSOCIATES NAMED TO PERMANENT STAFF

Twelve new associates are now serving their first year on the permanent staff of Henry Ford Hospital.

John R. Anderson, M.D. has returned to the Ophthalmology Department after a 28-month absence. He was an ophthalmology resident here from 1960-64.

Eduardo Arciniegas, M.D. who had been a resident in thoracic surgery in 1962 and a resident in cardiology in 1964, is now an associate surgeon in thoracic surgery.

Nihat Bakirci, M.D.; Saul A. Rosenblum, M.D., and Harvey I. Wilner, M.D., became Radiology Department associates last Fall. Dr. Bakirci, who interned at Grace Hospital Detroit, had his residency in radiology at Mt. Carmel Hospital, Detroit, and comes now from the Hacettepe Medical Center, Turkey, while Dr. Rosenblum was formerly radiologist for the Colorado Hill Hospital, Dayton, O., and Dr. Wilner had been on an NIH fellowship in neuroradiology at Columbia Presbyterian Hospital.

Robert W. Brownlee, M.D., associate in the Sixth Medical Division, was formerly on the staff of Riverview Hospital, Windsor, Ontario.

Richard M. Lee, Ph.D., formerly of the University of Maryland, is now associate, Division of Psychology, Department of Neurology and Psychiatry.

Robert B. MacIntosh, D.D.S., now associate in the Department of Dentistry and Oral Surgery, had been a resident in the department from 1963-65.

John D. Moroney, M.D., associate in the Department of Pediatrics, was formerly chief of pediatrics at the U. S. Air Force MacDill Hospital, Florida.

Alvin Schwarz, M.D., joined the hospital's permanent staff on May 15 as associate physician in the department of radiology. He had been in private practice following a residency in radiology at Wayne State University, Detroit General Hospital.

Joseph D. Shore, Ph.D., was post-doctoral fellow, Nobel Medical Institute, Stockholm, before becoming associate in the Department of Biochemistry and Molecular Biology, Edsel B. Ford Institute for Medical Research.

Lester Weiss, M.D., associate in the Department of Pediatrics is also director of the Cytogenetics Laboratory here. Previously he had been in private practice in Philadelphia for five years and also director of the Cytogenetics Laboratory at St. Christopher's Hospital for Children in Philadelphia.

NEWS OF ALUMNI

Dr. Marvin Revzin, formerly associate oral surgeon at Henry Ford Hospital, has taken a three-year leave of absence as associate dean of the University of Detroit's School of Dentistry to head a new dental health project at the University of Saigon in Vietnam. The program is supported by the U. S. Agency for International Development (AID) in association with the American Dental Association and U. of D. To assist in the project, Dr. Revzin hopes to attract 12 dental professors from the U.S. each year. No stranger to the Far East, Dr. Revzin was with Project HOPE in Indonesia in 1961.

Dr. Donald Norris and his wife, Dr. Bonnie Hepburn, who have just completed their internships at Henry Ford Hospital, have become the nation's second husband-and-wife team to enlist in the Army Medical Corps. They will serve a two-year hitch in West Germany both with the rank of captain.

Hospital to Get Betatron

A Brown-Bovari betatron, capable of accelerating electrons to high velocities corresponding to 35 million volts of energy, will be installed this Fall in the new radiation therapy facility at Henry Ford Hospital. To be housed in a specially-designed, below-grade, shielded area of the new Service Building, the Swiss-made betatron will be the largest and most spectacular machine planned for patient treatment and followup. Also included will be two radio-active cobalt units, with future plans for installation of a linear accelerator. Among other features will be a localization room with a transverse tomograph and treatment simulator. The Henry Ford Hospital tomograph, made in Japan, is believed to be one of the first in this country. Worldwide, only about 30 of the betatrons are now in use, the manufacturers say.

Table I

Index to Steroid X-ray Diffraction Powder Data

Pattern Number	Name	Molecular Formula	Melting Point (Uncorr.) °C
	Halogen substituted		
1	5α-Cholestan-2α-bromo-3-one	$C_{27}H_{45}OBr$	173.5-174
	Monohydric alcohols		
2	$\triangle^{5,16}$-Androstadien-3β-ol	$C_{19}H_{28}O$	140-141.5
3	$\triangle^{5}$-Androsten-3β-ol	$C_{19}H_{30}O$	136.5-138
4	$\triangle^{16}$-Androsten-3β-ol	$C_{19}H_{30}O$	127-128
5	5α-Pregnan-20α-ol	$C_{21}H_{36}O$	143-144.5
6	5α-Pregnan-20β-ol	$C_{21}H_{36}O$	141-143
	Dihydric alcohols		
7	$\triangle^{5}$-Androsten-3β,17α-diol	$C_{19}H_{30}O_2$	197-199
8	5α-Pregnan-3β,20α-diol-diacetate	$C_{25}H_{40}O_4$	168-170
9	5β-Pregnan-3α,20β-diol-diacetate	$C_{25}H_{40}O_4$	111-113
	Monoketones		
10	$\triangle^{3,5}$-Androstadien-17-one	$C_{19}H_{26}O$	83-85
11	$\triangle^{4,16}$-Androstadien-3-one	$C_{19}H_{26}O$	134-136
12	$\triangle^{4}$-Androsten-3-one	$C_{19}H_{28}O$	105.5-106.5
	Monohydroxy-monoketones		
13	$\triangle^{4,6}$-Androstadien-3-one-17β-ol	$C_{19}H_{26}O_2$	203-205
14	$\triangle^{4,9(11)}$-Androstadien-3-one-17β-ol-17α-methyl	$C_{20}H_{28}O_2$	170-172
15	5β-Androstan-3-one-17α-ol	$C_{19}H_{30}O_2$	142-144
16	5β-Pregnan-20-one-3α-acetoxy	$C_{23}H_{36}O_3$	100-102
	Monohydroxy-diketones		
17	$\triangle^{4}$-Androsten-3,17-dione-16α-ol	$C_{19}H_{26}O_3$	184-186
18	$\triangle^{5}$-Androsten-16,17-dione-3-ol-16-oxime	$C_{19}H_{27}O_3N$	248-250
19	5β-Pregnan-11,20-dione-3α-acetoxy	$C_{23}H_{34}O_4$	131-134
20	5α-Pregnan-16-en-12,20-dione-3β-acetoxy	$C_{23}H_{32}O_4$	177-179
	Dihydroxy-monoketones		
21	$\triangle^{4}$-Androsten-3-one-11α,17β-diol	$C_{19}H_{28}O_3$	180-182
22	$\triangle^{4}$-Androsten-3-one-11α,17β-diol-17α-methyl	$C_{20}H_{32}O_2$	156-159
23	5β-Pregnan-20-one-3α,21-diol-21-acetate	$C_{23}H_{36}O_4$	182-184
	Trihydroxy-monoketones		
24	$\triangle^{4}$-Pregnan-3-one-17α,20β,21-triol	$C_{21}H_{32}O_4$	188-190
	Tetrahydroxy-monoketone		
25	$\triangle^{4}$-Pregnan-3-one-11β,17α,20α,21-tetrol	$C_{21}H_{32}O_5$	258-260
	Amino steroid		
26	$\triangle^{5}$-Androsten-17β-amino-3β-ol	$C_{19}H_{31}ON$	165-167

TABLE II

d,A	I/I_1
1	
12.9	.09
10.8	.40
9.45	.16
8.88	.09
7.67	.06
6.64	.20
6.20	.30
6.02	.18
5.68	.30
5.34	1.00
5.05	.40
4.73	.40
4.46	.18
4.29	.18
3.83	.18
3.64	.08
3.50	.09
3.28	.18
3.21	.18
3.14	.19
3.05	.20
2	
12.1	.07
9.94	.18
7.86	.09
6.66	.65
6.19	.10
5.96	.30
5.72	.14
5.56	.19
5.28	1.00
4.90	.50
4.58	.20
4.43	.20
4.22	.09
3.86	.18
3.67	.08
3.53	.06
3.39	.08
3.33	.12
3.11	.05
2.92	.05
2.86	.05
2.75	.05
2.64	.05
2.47	.07
2.30	.05
3	
12.9	.10
11.6	.18
10.9	.25
9.98	.10
8.85	.10
7.77	.10
7.22	.13
6.95	.13
6.46	.07
6.20	.09
5.83	.60
5.50	1.00
5.13	.20
4.92	.35
4.64	.16
4.47	.13
4.23	.12
4.10	.12
4.03	.12
3.89	.11
3.55	.09
3.43	.07
3.01	.06
4	
15.3	.20
11.0	.20
9.87	.19
7.79	.08
6.97	1.00
6.24	.35
5.79	.11
5.44	.80
4	
5.13	.55
4.94	.40
4.65	.65
4.41	.14
4.31	.06
4.14	.11
3.99	.20
3.85	.17
3.75	.08
3.66	.06
3.45	.11
3.23	.08
3.15	.07
3.04	.11
2.89	.06
2.84	.05
2.74	.06
2.67	.04
2.58	.08
2.32	.06
2.22	.05
2.18	.07
2.00	.08
5	
11.7	.35
10.3	.19
8.56	.11
7.07	.11
6.64	.16
6.34	.55
5.99	.45
5.80	1.00
5.53	.30
5.35	.45
5.24	.20
4.81	.45
4.74	.45
4.58	.35
4.40	.25
4.18	.25
3.95	.09
3.78	.11
3.71	.13
3.49	.04
3.33	.13
3.09	.10
3.03	.08
2.83	.09
2.65	.08
2.56	.06
2.40	.05
2.25	.08
2.17	.07
2.04	.04
1.98	.06
6	
13.5	.04
12.5	.06
10.9	.08
10.2	.07
8.28	.11
7.54	.08
6.77	.08
6.15	.65
6.05	.55
5.81	.55
5.38	1.00
5.14	.30
4.99	.50
4.83	.08
4.60	.06
4.33	.06
4.24	.08
4.12	.09
3.97	.10
3.81	.19
3.45	.12
3.36	.04
3.30	.04
6	
3.09	.07
2.97	.06
7	
14.5	.20
11.1	.09
8.95	.07
7.79	.20
7.35	.45
7.07	.40
6.64	.55
6.47	.50
6.16	.35
5.87	.17
5.35	1.00
5.11	.80
4.91	.70
4.70	.30
4.45	.13
4.26	.50
3.98	.14
3.91	.16
3.44	.19
3.35	.15
3.19	.09
3.13	.07
3.05	.10
2.71	.10
2.66	.08
2.57	.07
2.45	.12
8	
14.8	.25
9.91	.16
8.31	.14
7.52	.13
7.15	.14
6.06	1.00
5.81	.80
5.63	.75
5.45	.25
5.23	.18
4.80	.70
4.76	.80
4.61	.30
4.33	.20
4.17	.30
4.10	.17
3.91	.11
3.79	.13
3.66	.11
3.56	.11
3.24	.12
3.11	.14
3.00	.11
2.49	.05
2.46	.04
2.36	.07
2.26	.09
2.21	.10
2.13	.07
2.09	.07
1.88	.07
9	
9.61	.16
6.76	1.00
6.17	.35
5.94	.50
5.64	.55
5.32	.13
5.04	.16
4.83	.95
4.69	.25
4.35	.35
4.12	.35
4.00	.25
3.83	.20
3.74	.20
3.59	.25
3.37	.20
10	
9.31	.25
6.35	.95
5.69	1.00
5.44	.95
5.13	.60
4.78	1.00
4.63	.15
4.09	.17
3.78	.09
3.58	.13
3.48	.14
3.29	.13
3.22	.13
3.09	.20
2.90	.25
2.85	.15
2.78	.04
2.71	.09
2.67	.11
2.56	.09
2.39	.13
2.32	.13
2.21	.06
2.15	.06
2.06	.06
11	
10.3	.10
8.86	.07
7.18	.09
6.05	.30
5.77	1.00
5.16	.06
4.88	.55
4.55	.11
4.43	.13
4.31	.08
4.04	.12
3.82	.17
3.53	.09
3.38	.04
3.22	.14
3.11	.04
2.97	.09
2.78	.04
2.51	.04
2.38	.06
2.31	.04
2.18	.04
2.08	.08
12	
11.7	.20
9.14	.25
7.46	.10
6.15	1.00
5.64	.12
5.03	.65
4.93	1.00
4.59	.35
4.33	.08
4.20	.11
4.06	.25
3.85	.07
3.73	.11
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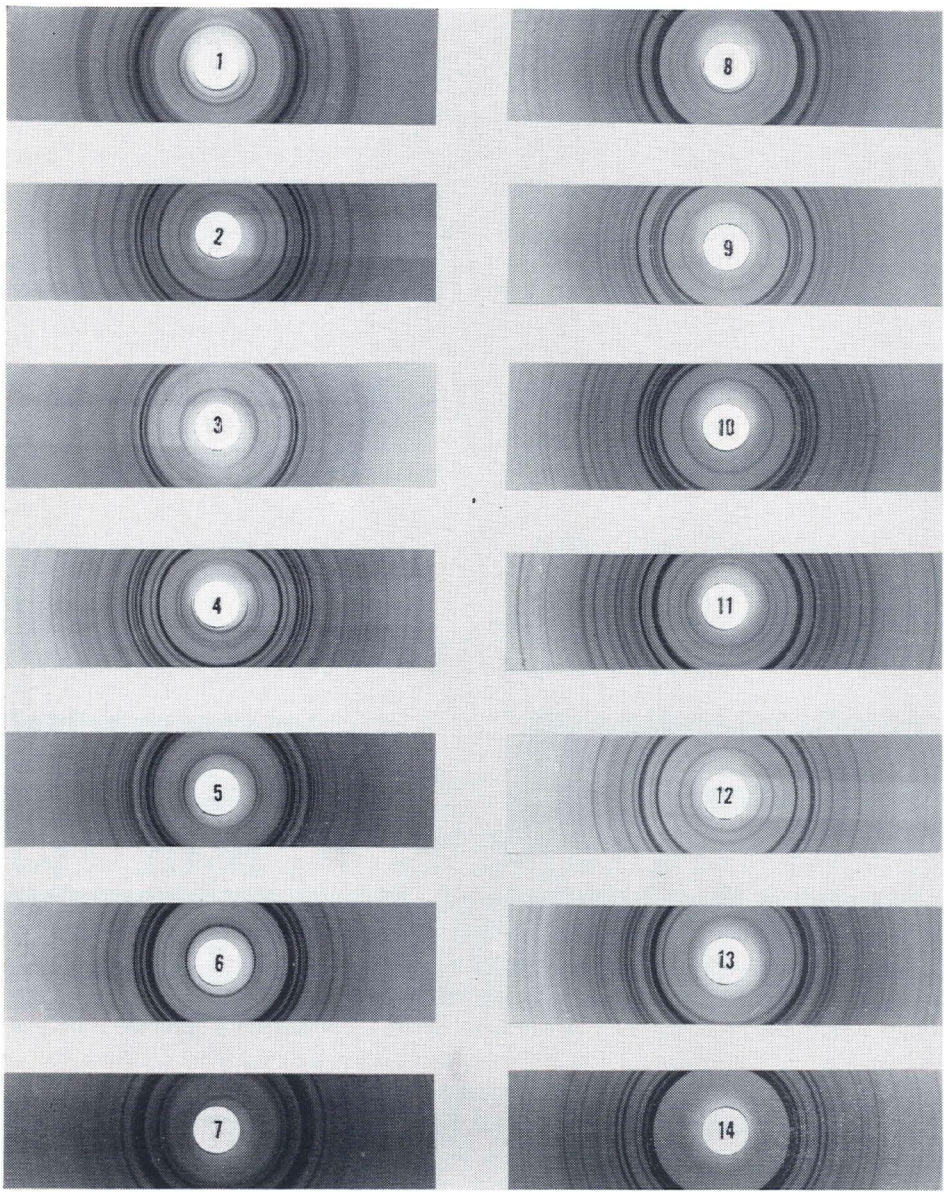
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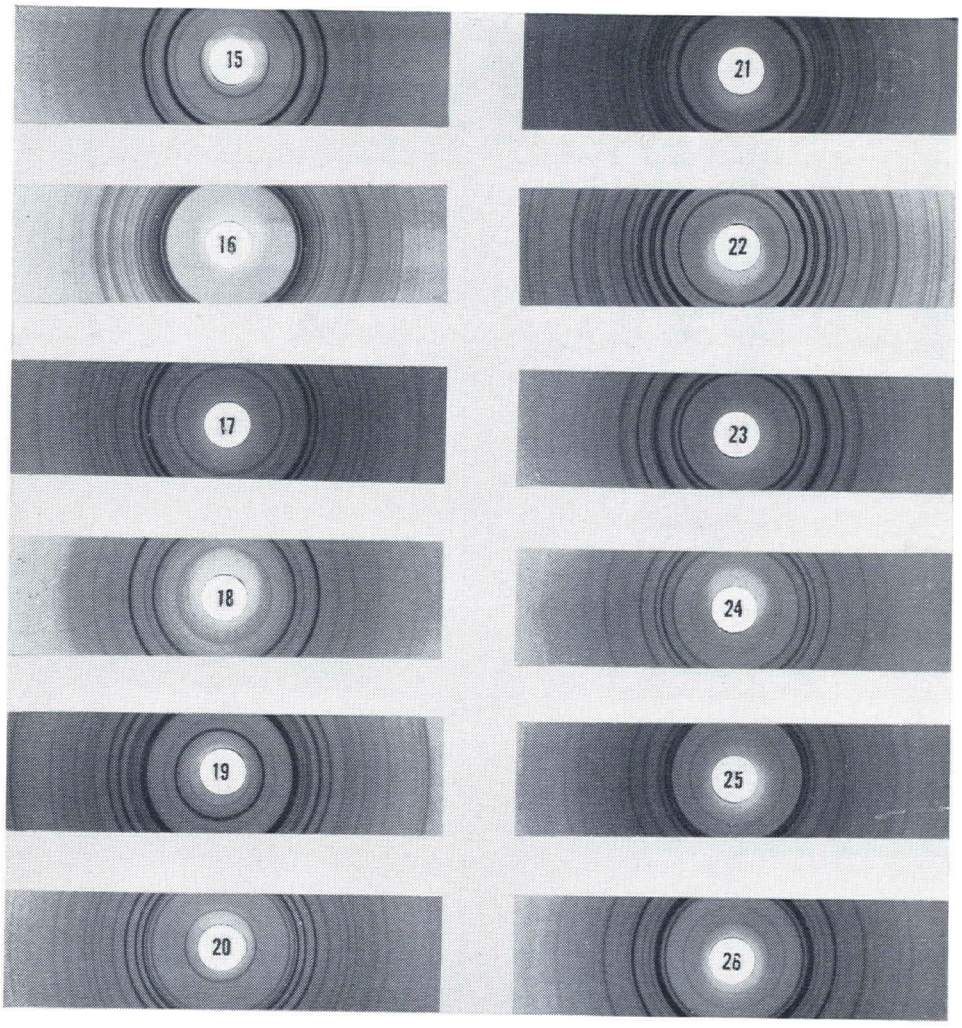
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