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X-RAY DIFFRACTION POWDER DATA FOR STEROIDS: SUPPLEMENT II

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THE ASSEMBLY of x-ray diffraction powder data for steroids began at this Institute in 1955 with the realization of the potentialities that lay in the use of x-ray diffraction for the identification of intermediates involved in the organic synthesis of steroids and for identification of micro-crystals occurring in medical and biological materials.[1] To make the latter types of analyses feasible by x-ray diffraction, it is necessary to have available sets of standard data[2] which are characteristic of particular chemical compounds much in the manner in which individual finger prints are characteristic of particular persons.

The original publication[3] of steroid data by the authors appeared as Part II of the Henry Ford Hospital Medical Bulletin for December 1958. The first set of supplementary data[4] was published in 1961 but did not carry the designation Supplement I. It is intended that future data in this series will be serially numbered as supplements following the designation of this paper as Supplement II. The present sets of data for 44 steroids bring the total number published to date by the authors to 208.

The conditions of x-ray exposure, film development and melting point determination were the same as previously reported.[4] Table I is a classified index for the present group of steroids, giving the molecular formulas and uncorrected melting points. All steroids reported in this paper were recrystallized from ethanol unless otherwise indicated. Table II lists the interplanar spacings in angstrom units (d,A) and relative intensities were determined by visual comparison with a calibrated set of intensity strips. Table I serves as a key to the consecutively numbered data groups of Table II and also to the numbered pattern photographs of Figure 1.

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Table I

Index To Steroid X-ray Diffraction Powder Data

Pattern Number	Name	Molecular Formula	Melting Point (Uncorr.) °C
	C_{18} Steroids		
1	$\Delta^{1,3,5}$-Estratrien-3, 17β-diol-3, 17-diacetate	$C_{22}H_{28}O_4$	127-129
2	$\Delta^{1,3,5}$-Estratrien-3, 17β-diol-3, 17-dipropionate	$C_{24}H_{32}O_4$	105-106.5
	Steroid hydrocarbons		
3	5α-Androstane	$C_{19}H_{32}$	49-50
4	Cholestane	$C_{27}H_{48}$	80.5-81.5
	Monohydric alcohols		
5	$\Delta^{5,7}$-Cholestadien-3β-ol-3-benzoate	$C_{34}H_{48}O_2$	141-143
6	Δ^{5}-Cholesten-3β-ol-3-decanoate	$C_{37}H_{64}O_2$	82-84
7	Δ^{5}-Cholesten-3β-ol-3-heptanoate	$C_{34}H_{50}O_2$	111-112
8	Δ^{5}-Cholesten-3β-ol-3-hexadecanoate	$C_{43}H_{76}O_2$	76-77
9	Δ^{5}-Cholesten-3β-ol-3-hexanoate	$C_{33}H_{56}O_2$	96-97
10	Δ^{5}-Cholesten-3β-ol-3-isobutyrate	$C_{31}H_{52}O_2$	129-130
11	Δ^{5}-Cholesten-3β-ol-3-nonanoate	$C_{36}H_{62}O_2$	74-75
12	Δ^{5}-Cholesten-3β-ol-3-octadecanoate	$C_{45}H_{80}O_2$	78.5-80
13	Δ^{5}-Cholesten-3β-ol-3-octanoate	$C_{35}H_{60}O_2$	107-107.5
14	Δ^{5}-Cholesten-3β-ol-3-pentanoate	$C_{32}H_{54}O_2$	95-96
15	Δ^{5}-Cholesten-3β-ol-3-phenylacrylate	$C_{36}H_{52}O_2$	159-161
16	Δ^{5}-Cholesten-3β-ol-3-hydrogen succinate	$C_{31}H_{50}O_4$	175-180
17	Δ^{5}-Cholesten-3β-ol-3-tetranoate	$C_{31}H_{52}O_2$	150.5-151
	Dihydric alcohols		
18	5α-Androstane-3α, 17β-diol	$C_{19}H_{32}O_2$	227.5-229
19	5α-Androstane-3β, 17β-diol	$C_{19}H_{32}O_2$	168-170
20	5β-Pregnan-3α, 20α-diol diacetate	$C_{25}H_{40}O_4$	180-181.5
	Monoketones		
21	$\Delta^{3,5}$-Cholestadien-7-one	$C_{27}H_{42}O$	109-110
	Triketones		
22	4-Androsten-3, 11, 17-trione	$C_{19}H_{24}O_3$	224.5-226.5
	Monohydroxy-monoketones		
23	5α-Androstane-3β-ol-17-one 3-acetate	$C_{21}H_{32}O_3$	95-96.5
24	Δ^{4}-Androsten-17α-ol-3-one	$C_{19}H_{28}O_2$	220.5-223
25	4-Androsten-17β-ol-3-one 17-acetate	$C_{21}H_{30}O_3$	140.5-141.5
26	$\Delta^{5,16}$-Pregnadien-6α-methyl-3β-ol-20-one	$C_{22}H_{32}O_2$	164-165.5
27	5β-Pregnan-3α-ol-20-one[a]	$C_{21}H_{34}O_2$	149-150.5
28	16-Dehydro-5β-pregnan-3β-ol-20-one 3-acetate	$C_{23}H_{34}O_3$	144.5-146
29	Δ^{5}-Pregnen-16α-methyl-3β-ol-20-one 3-acetate	$C_{24}H_{36}O_3$	184-185
	Dihydroxy-diketones		
30	Δ^{4}-Pregnen-11β, 21-diol-3, 20-dione	$C_{21}H_{30}O_4$	181-183
31	4-Pregnen-11β, 21-diol-3, 20-dione 21-acetate	$C_{23}H_{32}O_5$	146-147.5
	Trihydroxy-diketones		
32	4-Pregnen-11β, 17α, 21-triol-3, 20-dione	$C_{21}H_{30}O_5$	219.5-220.5
33	4-Pregnen-11β, 17α, 21-triol-3, 20-dione 21-acetate	$C_{23}H_{32}O_6$	225-226
	Trihydroxy-triketones		
34	$\Delta^{1,4}$-Pregnadien-11β, 17α, 21-triol-3, 20-dione	$C_{21}H_{28}O_5$	241-243D
	Carboalkoxy acids		
35	Cholanic acid	$C_{24}H_{40}O_2$	165.5-167
36	Ag-3α, 12α-diacetoxycholanate	$C_{28}H_{43}O_6Ag$	
37	Ketocholanic acid		238-240D
	Carboalkoxy esters		
38	Methyl 3, 7, 12-trihydroxy cholanic acid	$C_{25}H_{42}O_5$	158-159
39	Methyl 3, 7-diacetoxy-12-hydroxy cholanate	$C_{29}H_{46}O_7$	184-187
40	Methyl 3α, 7α-diacetoxy-12-ketocholanate	$C_{29}H_{44}O_7$	176-178
	Sopogenins and sopogenin derivatives		
41	6-Methyl diosgenin acetate	$C_{30}H_{46}O_4$	219.5-220.5D
42	Hecogenin acetate	$C_{29}H_{44}O_5$	245-248
43	Tigogenin[a]	$C_{27}H_{44}O_3$	204.5-205.5
44	Tigogenin acetate	$C_{29}H_{46}O_4$	207-208.5

[a]Recrystallized in acetone

Table II

1		2		3	
d,A	I/I_1	d,A	I/I_1	d,A	I/I_1
13.25	0.27	11.63	0.15	10.85	0.41
8.92	0.01	9.88	0.05	7.47	0.11
8.41	0.01	8.55	0.05	6.68	0.08
7.85	0.01	8.15	0.05	5.99	0.73
6.99	0.73	7.73	0.03	5.79	0.10
6.50	0.64	7.17	0.20	5.57	0.05
5.73	0.41	6.92	0.05	5.40	0.11
4.99	0.15	6.51	0.05	4.94	1.00
4.73	1.00	5.89	0.20	4.77	0.04
4.38	0.55	5.19	0.10	4.35	0.05
4.23	0.55	4.91	0.10	4.17	0.27
3.97	0.41	4.51	1.00	4.03	0.01
3.85	0.34	4.34	0.13	3.79	0.02
3.73	0.08	4.18	0.08	3.67	0.02
3.57	0.11	3.97	0.02	3.51	0.08
3.43	0.08	3.75	0.11	3.34	0.08
3.25	0.15	3.57	0.08	3.07	0.08
3.17	0.08	3.41	0.10	2.80	0.01
3.06	0.05	3.23	0.08	2.68	0.01
3.00	0.05	3.19	0.08	2.52	0.05
2.93	0.08	3.09	0.05	2.40	0.07
2.85	0.05	3.03	0.03	2.30	0.02
2.78	0.02	2.93	0.03	2.24	0.02
2.67	0.08	2.75	0.02	2.16	0.07
2.59	0.02	2.70	0.03	2.08	0.01
2.49	0.03	2.59	0.01		
2.42	0.05	2.53	0.02		
2.33	0.03	2.48	0.01		
2.24	0.03	2.45	0.03		
2.15	0.03	2.33	0.01		
2.11	0.05	2.29	0.02		
2.08	0.05	2.23	0.01		
2.04	0.05	2.15	0.02		
1.92	0.03	2.09	0.01		
		1.92	0.02		
		1.79	0.02		

4

d,A	I/I_1
11.02	0.04
9.59	0.30
7.77	0.18
7.30	0.06
6.91	0.04
6.27	0.01
5.58	0.25
5.40	0.02
4.99	1.00
4.68	0.03
4.42	0.04
4.18	0.01
3.95	0.11
3.64	0.08
3.52	0.11
3.42	0.01
3.34	0.01
3.24	0.01
3.11	0.04
2.94	0.02
2.64	0.06
2.49	0.02
2.45	0.01
2.40	0.02
2.24	0.02
2.19	0.01
2.11	0.02
2.07	0.02
2.02	0.01
1.92	0.02
1.87	0.02

5

d,A	I/I_1
14.85	0.07
12.54	0.15
10.72	0.13
8.27	0.03
7.80	0.02
7.08	0.13
6.44	0.02
6.08	0.03
5.83	0.02
5.44	1.00
5.07	0.03
4.85	0.37
4.43	1.00
4.24	0.02
4.13	0.03
3.98	0.05
3.85	0.05
3.69	0.07
3.54	0.03
3.45	0.03
3.34	0.05
3.19	0.01
3.07	0.01
2.95	0.01
2.82	0.02
2.65	0.01
2.50	0.02
2.28	0.05
2.16	0.02
2.13	0.02

6

d,A	I/I_1
12.96	0.02
11.99	0.04
10.03	0.13
8.78	0.09
7.36	0.11
6.36	0.04
5.94	0.07
5.53	0.02
5.21	0.49
5.01	1.00
4.71	0.13
4.49	0.58
4.35	0.09
4.12	0.04
4.00	0.07
3.89	0.01
3.79	0.01
3.67	0.02
3.50	0.04
3.35	0.02
3.11	0.01
2.88	0.03
2.74	0.02
2.65	0.02
2.44	0.01
2.33	0.01
2.22	0.02
2.09	0.02

7

d,A	I/I_1
13.77	0.28
12.68	0.03
10.26	0.20
7.71	0.11
6.50	0.38
5.60	0.08
5.03	0.94
4.58	1.00
4.35	0.15
4.11	0.13
3.91	0.15
3.70	0.05
3.51	0.02
3.39	0.03
3.29	0.03
3.11	0.03
3.00	0.01
2.91	0.04
2.74	0.05
2.55	0.01
2.49	0.01
2.38	0.05
2.31	0.04
2.24	0.04
2.17	0.03
2.11	0.01
2.07	0.03
2.02	0.03
1.95	0.01
1.89	0.01

8

d,A	I/I_1
21.24	0.13
13.37	0.07
10.27	0.10
9.30	0.13
7.59	0.20
7.13	0.03
6.08	1.00
5.81	0.13
5.57	0.20
5.32	0.07
5.08	0.10
4.88	0.10
4.64	0.40
4.45	0.03
4.20	0.40
4.16	0.73
3.80	0.87
3.55	0.07
3.39	0.02
3.24	0.02
3.10	0.03
2.97	0.03
2.77	0.03
2.54	0.01
2.32	0.01
2.26	0.13
2.17	0.03
2.08	0.03
1.94	0.02
1.90	0.03

9

d,A	I/I_1
13.64	0.17
9.07	0.20
7.80	0.13
6.51	0.20
6.13	0.04
5.56	0.09
5.01	1.00
4.70	0.67
4.42	0.13
4.16	0.09
4.05	0.09
3.88	0.20
3.72	0.04
3.63	0.04
3.46	0.02
3.35	0.01
3.16	0.01
3.08	0.01
2.95	0.01
2.86	0.04
2.77	0.01
2.60	0.02
2.51	0.02
2.41	0.02
2.34	0.01
2.26	0.04
2.18	0.01
2.12	0.01
2.08	0.02
2.04	0.01
1.98	0.01

10

d,A	I/I_1
14.63	0.24
10.23	0.05
8.72	0.11
8.20	0.15
7.70	0.04
7.20	0.05
6.47	0.28
5.91	0.04
5.53	0.04
5.23	1.00
4.85	0.75
4.64	0.08
4.50	0.05
4.38	0.05
4.19	0.15
3.94	0.10
3.83	0.11
3.50	0.05
3.38	0.05
3.27	0.04
3.17	0.05
3.07	0.01
2.96	0.01
2.88	0.08
2.76	0.03
2.64	0.02
2.55	0.02
2.44	0.07
2.33	0.01
2.25	0.05
2.20	0.04
2.15	0.04
2.09	0.03
2.01	0.04

11

d,A	I/I_1
9.66	0.15
8.76	0.10
7.73	0.13
7.41	0.05
7.03	0.02
6.71	0.03
6.33	0.05
5.83	0.05
5.42	0.37
5.08	1.00
4.68	0.13
4.54	0.27
4.36	0.15
4.09	0.08
3.93	0.05
3.74	0.07
3.51	0.08
3.04	0.05
2.97	0.03
2.90	0.05
2.71	0.02
2.48	0.01
2.25	0.02
2.18	0.01
2.13	0.01
2.06	0.02

12

d,A	I/I_1
13.92	0.04
10.34	0.07
9.41	0.09
7.60	0.09
7.22	0.06
6.09	1.00
5.81	0.09
5.61	0.20
5.39	0.07
5.11	0.09
4.93	0.04
4.70	0.36
4.51	0.02
4.21	0.36
4.13	0.67
3.80	0.84
3.55	0.04
3.35	0.01
3.25	0.01
3.11	0.02
3.03	0.02
2.26	0.09

13

d,A	I/I_1
13.92	0.20
12.81	0.03
9.21	0.28
7.76	0.11
6.53	0.33
5.63	0.08
5.25	0.04
5.01	1.00
4.61	0.75
4.36	0.28
4.10	0.11
3.90	0.15
3.68	0.05
3.39	0.03
3.24	0.03
3.12	0.01
3.01	0.01
2.91	0.07
2.87	0.01
2.74	0.04
2.63	0.01
2.55	0.01
2.45	0.01
2.35	0.01
2.28	0.03
2.24	0.03
2.15	0.04
2.08	0.05

14

d,A	I/I_1
11.48	0.49
7.31	0.36
6.37	0.02
5.79	0.02
5.26	1.00
5.05	0.02
4.71	0.58
4.53	0.20
4.33	0.07
4.07	0.02
3.79	0.09
3.69	0.11
3.46	0.01
3.16	0.01
3.04	0.09
2.91	0.01
2.81	0.02
2.71	0.01

15

d,A	I/I_1
14.26	0.20
10.05	0.17
8.63	0.09
7.69	0.04
7.28	0.04
6.92	0.20
6.22	0.67
5.50	0.27
5.22	0.24
4.90	0.27
4.73	1.00
4.63	0.17
4.37	0.09
4.26	0.13
4.09	0.11
3.79	0.17
3.63	0.11
3.47	0.11
3.22	0.04
3.08	0.13
2.97	0.09
2.89	0.03
2.79	0.01
2.55	0.01
2.45	0.02
2.31	0.01
2.23	0.04
2.17	0.02
2.14	0.02

16

d,A	I/I_1
12.40	0.03
11.01	0.30
8.82	0.04
7.30	0.11
6.85	0.02
6.14	0.04
5.80	0.02
5.56	0.04
5.09	1.00
4.65	0.73
4.39	0.06
4.25	0.06
3.73	0.20
3.45	0.04
3.28	0.04
3.06	0.05
2.91	0.04
2.80	0.04
2.71	0.03
2.59	0.01
2.53	0.01
2.35	0.04
2.27	0.04
2.20	0.04
2.12	0.02
2.04	0.01

17

d,A	I/I_1
10.06	0.30
9.32	0.30
8.47	0.13
7.57	0.13
7.26	0.07
6.98	0.07
6.24	0.40
5.83	0.13
5.30	1.00
5.08	1.00
4.73	1.00
4.44	0.20
4.20	0.20
4.05	0.03
3.91	0.30
3.74	0.13
3.69	0.20
3.44	0.20
3.33	0.07
3.29	0.07
3.21	0.07
3.15	0.07
3.00	0.07
2.93	0.10
2.78	0.10
2.70	0.07
2.55	0.05
2.47	0.05
2.40	0.05
2.34	0.05
2.28	0.10
2.23	0.10
2.15	0.10
2.10	0.09
2.05	0.05
2.00	0.03
1.96	0.02
1.87	0.02

18

d,A	I/I_1
11.33	0.11
9.51	0.15
6.13	0.04
5.77	1.00
5.20	0.35
4.73	0.40
4.45	0.04
4.17	0.11
3.97	0.08
3.79	0.04
3.60	0.08
3.45	0.06
3.34	0.05
3.20	0.13
2.88	0.01
2.73	0.06
2.61	0.06
2.43	0.08
2.28	0.06
2.25	0.05
2.16	0.04
2.07	0.04
2.02	0.08
1.94	0.02
1.89	0.02

19

d,A	I/I_1
10.92	0.20
8.42	0.28
6.19	0.20
5.93	1.00
5.72	0.88
5.49	1.00
5.11	0.56
4.78	0.11
4.58	0.11
4.36	0.47
4.14	0.24
3.83	0.08
3.76	0.05
3.66	0.11
3.51	0.05
3.40	0.18
3.31	0.18
3.12	0.15
3.03	0.01
2.94	0.08
2.90	0.11
2.83	0.08
2.76	0.11
2.67	0.11
2.59	0.01
2.56	0.05
2.51	0.01
2.47	0.04
2.43	0.03
2.36	0.03
2.31	0.08
2.27	0.08
2.17	0.05
2.12	0.08

20

d,A	I/I_1
7.16	0.63
6.36	0.58
5.82	0.27
5.55	1.00
5.26	0.10
5.02	0.05
4.83	0.10
4.62	0.03
4.47	0.02
4.38	0.37
4.24	0.15
4.06	0.02
3.91	0.27
3.67	0.07
3.59	0.03
3.49	0.03
3.41	0.07
3.29	0.03
3.22	0.10
3.07	0.07
2.98	0.02
2.92	0.02
2.75	0.03
2.59	0.01
2.43	0.01
2.37	0.07
2.31	0.02
2.24	0.05
2.18	0.05
2.09	0.07

21

d,A	I/I_1
15.78	0.50
9.77	0.03
8.67	0.15
7.63	0.10
6.78	0.07
6.11	0.75
5.72	0.20
5.45	0.15
5.19	0.75
4.90	0.37
4.52	0.03
4.32	1.00
4.13	0.03
4.02	0.03
3.87	0.15
3.75	0.09
3.62	0.01
3.50	0.01
3.26	0.15
3.14	0.02
3.04	0.01
2.87	0.03
2.72	0.01
2.58	0.07
2.43	0.03
2.26	0.03
2.15	0.03
2.09	0.03
2.00	0.02

22

d,A	I/I_1
13.29	0.10
8.89	0.05
7.69	0.05
6.35	1.00
5.83	0.09
5.31	0.63
4.94	0.37
4.65	0.50
4.40	0.10
4.10	0.09
3.75	0.15
3.63	0.07
3.50	0.03
3.23	0.02
3.15	0.03
3.09	0.10
3.04	0.10
2.98	0.15
2.89	0.09
2.78	0.05
2.65	0.10
2.57	0.07
2.46	0.10
2.38	0.03
2.32	0.01
2.25	0.03
2.18	0.02
2.13	0.03
2.00	0.03
1.96	0.02
1.92	0.02
1.89	0.01
1.83	0.01
1.79	0.02

23

d,A	I/I_1
11.44	0.20
6.27	0.17
5.84	0.49
5.65	1.00
5.38	0.58
5.15	0.49
4.80	0.67
4.55	0.09
4.22	0.13
3.99	0.04
3.70	0.04
3.59	0.11
3.50	0.09
3.35	0.11
3.22	0.13
3.07	0.27
2.96	0.09
2.90	0.04
2.82	0.07
2.69	0.09
2.63	0.01
2.55	0.02
2.49	0.02
2.36	0.09
2.28	0.09
2.12	0.02
2.07	0.04
2.00	0.07
1.90	0.07
1.78	0.02
1.75	0.04

24

d,A	I/I_1
10.11	0.05
7.60	0.02
6.68	0.15
6.01	0.20
5.74	1.00
5.16	0.48
4.86	0.04
4.60	0.05
4.46	0.28
4.31	0.05
4.07	0.20
3.85	0.09
3.69	0.15
3.48	0.05
3.31	0.18
3.18	0.05
3.01	0.08
2.91	0.03
2.87	0.03
2.76	0.02
2.57	0.05
2.50	0.08
2.41	0.01
2.36	0.01
2.32	0.03
2.28	0.03
2.16	0.05
2.08	0.08
1.91	0.03
1.88	0.04

25

d,A	I/I_1
10.65	0.38
8.01	0.20
7.00	0.28
6.51	0.04
6.33	0.04
6.03	1.00
5.74	0.08
5.45	0.47
5.25	0.11
5.05	0.11
4.83	0.47
4.71	0.11
4.61	0.03
4.31	0.08
3.99	0.38
3.65	0.08
3.51	0.28
3.40	0.07
3.27	0.05
3.15	0.08
3.07	0.05
2.99	0.07
2.88	0.05
2.81	0.08
2.72	0.03
2.66	0.03
2.61	0.03
2.53	0.05
2.47	0.07
2.36	0.01
2.30	0.05
2.23	0.05
2.17	0.04
2.13	0.05
2.04	0.04
1.95	0.03

26

d,A	I/I_1
12.50	0.27
10.56	0.07
7.99	0.09
6.50	0.67
6.29	0.09
6.06	0.49
5.77	0.01
5.50	1.00
5.24	0.58
5.08	0.13
4.84	0.09
4.63	0.17
4.39	0.49
4.28	0.49
4.19	0.02
4.08	0.02
3.90	0.07
3.52	0.09
3.44	0.09
3.27	0.07
3.17	0.01
3.04	0.20
2.95	0.20
2.87	0.03
2.80	0.03
2.75	0.01
2.60	0.07
2.48	0.02
2.41	0.01
2.24	0.07
2.09	0.04

27

d,A	I/I_1
10.85	0.07
9.51	0.04
7 03	0.07
6.61	1.00
6.24	0.13
5.61	0.11
5.39	0.07
5.19	0.67
4.97	0.49
4.68	0.20
4.27	0.11
4.17	0.09
3.89	0.02
3.66	0.07
3.53	0.09
3.34	0.02
3.18	0.07
3.06	0.01
2.92	0.01
2.82	0.01
2.73	0.01
2.66	0.02
2.50	0.09
2.34	0.04

28

d,A	I/I_1
9.56	0.41
8.39	0.01
7.41	0.01
6.56	1.00
6.11	0.01
5.72	0.41
5.32	0.73
4.98	0.03
4.76	0.02
4.48	0.55
4.29	0.04
4.11	0.05
3.90	0.05
3.80	0.08
3.71	0.08
3.55	0.11
3.43	0.15
3.31	0.11
3.16	0.10
3.07	0.02
2.95	0.01
2.89	0.01
2.84	0.08
2.75	0.04
2.66	0.05
2.60	0.08
2.54	0.03
2.45	0.02
2.39	0.03
2.31	0.08
2.25	0.04
2.20	0.01
2.14	0.04
2.11	0.04
2.01	0.04
1.99	0.04

29

d,A	I/I_1
14.49	0.11
11.05	0.02
9.21	0.04
7.56	0.07
6.15	0.09
5.79	0.84
5.49	0.67
5.19	1.00
4.81	0.09
4.44	0.09
4.23	0.13
4.11	0.09
3.92	0.02
3.80	0.01
3.72	0.02
3.50	0.04
3.32	0.13
3.15	0.02
3.07	0.01
2.98	0.11
2.89	0.07
2.82	0.01
2.75	0.02
2.70	0.01
2.64	0.04
2.42	0.04
2.26	0.04
2.12	0.02
2.06	0.04
2.01	0.07
1.96	0.04
1.89	0.04
1.78	0.02

30

d,A	I/I_1
8.29	0.03
7.27	0.11
6.88	0.33
6.50	0.28
6.16	0.33
5.75	0.20
5.09	0.28
4.94	1.00
4.48	0.15
4.19	0.38
3.95	0.11
3.74	0.66
3.59	0.13
3.44	0.11
3.34	0.08
3.15	0.01
3.07	0.13
2.91	0.18
2.78	0.03
2.68	0.05
2.63	0.03
2.58	0.05
2.52	0.03
2.48	0.03
2.37	0.06
2.29	0.02
2.26	0.01
2.23	0.01
2.19	0.02
2.15	0.03
2.09	0.03
2.07	0.03
2.04	0.03
1.98	0.02
1.96	0.03

31

d,A	I/I_1
9.48	0.02
8.32	0.10
7.78	0.01
7.18	0.15
6.43	1.00
6.12	0.03
5.84	1.00
5.36	0.07
4.99	0.05
4.68	0.10
4.37	0.37
4.20	0.10
4.03	0.03
3.78	0.07
3.53	0.13
3.45	0.13
3.32	0.03
3.23	0.02
3.14	0.03
3.07	0.10
2.99	0.10
2.91	0.01
2.80	0.05
2.73	0.07
2.68	0.05
2.62	0.03
2.55	0.01
2.45	0.03
2.40	0.01
2.34	0.02
2.26	0.03
2.20	0.05
2.00	0.02
1.94	0.02
1.88	0.02
1.82	0.02

32

d,A	I/I_1
9.86	0.04
8.83	0.02
7.75	0.05
7.07	0.02
6.75	0.02
6.10	1.00
5.82	0.02
5.50	0.15
5.24	0.03
5.08	0.41
4.91	0.01
4.73	0.11
4.56	0.05
4.38	0.08
3.82	0.08
3.67	0.01
3.45	0.01
3.26	0.03
3.06	0.11
2.96	0.11
2.87	0.03
2.78	0.03
2.54	0.05
2.46	0.02
2.42	0.04
2.31	0.05
2.24	0.02
2.12	0.02
2.08	0.02
2.04	0.02
2.01	0.01
1.97	0.02

33

d,A	I/I_1
8.80	0.20
7.37	1.00
6.84	0.27
6.19	0.27
5.63	0.78
5.39	0.84
5.20	0.67
4.85	0.27
4.33	0.27
4.17	0.36
4.05	0.27
3.79	0.04
3.61	0.11
3.52	0.20
3.16	0.49
2.83	0.20
2.74	0.09
2.68	0.20
2.62	0.11
2.46	0.20
2.38	0.02
2.30	0.09
2.26	0.09
2.22	0.11
2.18	0.04
2.10	0.13
2.00	0.13
1.92	0.09
1.86	0.09
1.80	0.02
1.72	0.04

34

d,A	I/I_1
10.78	0.11
8.80	0.05
6.94	0.05
6.42	0.87
5.89	0.41
5.45	1.00
4.94	0.73
4.55	0.08
4.34	0.20
4.14	0.13
3.80	0.08
3.71	0.20
3.60	0.04
3.49	0.04
3.36	0.10
3.27	0.05
3.20	0.05
3.08	0.04
2.99	0.13
2.94	0.08
2.84	0.01
2.76	0.10
2.66	0.01
2.54	0.05
2.48	0.04
2.36	0.05
2.31	0.08
2.24	0.02
2.19	0.05
2.16	0.05
2.04	0.05
2.01	0.02
1.96	0.04
1.91	0.04

35

d,A	I/I_1
10.65	0.02
8.63	0.09
6.76	0.13
6.26	0.13
5.95	0.36
5.56	0.24
5.11	1.00
4.87	0.09
4.62	0.04
4.42	0.04
4.20	0.07
4.00	0.13
3.78	0.02
3.58	0.07
3.38	0.07
3.25	0.07
2.98	0.04
2.89	0.01
2.81	0.04
2.71	0.04
2.64	0.01
2.43	0.03
2.37	0.04
2.25	0.04
2.20	0.02
2.10	0.03
2.06	0.02
2.01	0.03

36

d,A	I/I_1
14.37	0.13
10.40	0.73
8.01	0.07
5.47	0.13
4.55	0.02
3.95	0.40
3.40	0.01
3.07	1.00
2.79	0.02
2.57	0.30
2.34	0.07
2.16	0.30
1.97	0.10
1.89	0.35
1.65	0.07
1.56	0.10
1.53	0.02
1.48	0.01
1.39	0.01
1.32	0.03

37

d,A	I/I_1
15.11	0.07
10.53	0.15
9.72	0.10
7.80	0.01
6.94	0.01
6.44	0.13
6.17	0.10
5.70	1.00
5.29	0.20
5.01	0.20
4.76	0.03
4.47	0.07
4.27	0.10
4.14	0.24
4.00	0.05
3.87	0.05
3.72	0.05
3.56	0.05
3.45	0.07
3.30	0.05
3.15	0.10
3.03	0.03
2.94	0.03
2.77	0.03
2.64	0.07
2.47	0.05
2.40	0.02
2.36	0.02
2.29	0.03
2.23	0.03
2.12	0.07
2.06	0.05

38

d,A	I/I_1
15.24	0.07
9.36	0.20
7.41	0.40
6.94	0.20
6.49	0.30
6.24	0.53
5.97	0.30
5.45	1.00
5.16	0.30
4.86	0.13
4.54	0.73
4.39	0.20
4.28	0.20
4.05	0.10
3.86	0.13
3.67	0.17
3.55	0.05
3.40	0.20
3.28	0.03
3.16	0.03
3.10	0.03
3.01	0.13
2.91	0.03
2.85	0.03
2.77	0.03
2.71	0.10
2.64	0.10
2.53	0.05
2.48	0.05
2.43	0.07
2.30	0.05
2.24	0.02
2.20	0.13
2.15	0.02
2.04	0.07
1.94	0.03

39

d,A	I/I_1
14.58	0.13
11.85	0.25
9.50	0.38
7.96	0.09
7.52	0.38
7.04	0.75
6.65	0.47
6.13	0.06
5.77	0.66
5.37	0.06
5.09	0.75
4.67	0.32
4.45	1.00
4.19	0.03
3.97	0.56
3.82	0.03
3.65	0.25
3.48	0.19
3.28	0.25
3.16	0.03
3.05	0.13
2.95	0.13
2.83	0.03
2.69	0.06
2.57	0.03
2.44	0.09
2.38	0.13
2.25	0.09
2.20	0.13
2.14	0.03
2.08	0.03
2.02	0.06

40

13.92	0.09
10.72	0.38
8.12	0.38
7.76	0.25
7.05	0.47
6.43	0.02
6.13	0.32
5.81	1.00
5.37	0.38
5.07	0.88
4.86	0.19
4.68	0.06
4.47	0.19
4.29	0.25
4.05	0.25
3.94	0.09
3.68	0.09
3.49	0.09
3.39	0.19
3.22	0.19
2.94	0.06
2.81	0.09
2.72	0.03
2.64	0.09
2.58	0.06
2.53	0.03
2.38	0.03
2.30	0.09
2.19	0.06
2.08	0.06
2.04	0.03

41

d,A	I/I_1
15.50	0.08
11.71	0.11
10.05	0.08
8.35	0.11
6.97	0.05
6.24	1.00
5.87	0.04
5.66	0.27
5.45	0.55
5.10	0.55
4.76	0.05
4.48	0.48
4.37	0.34
4.17	0.05
3.96	0.11
3.75	0.08
3.52	0.08
3.45	0.04
3.35	0.08
3.24	0.20
3.12	0.04
3.04	0.04
2.94	0.02
2.83	0.08
2.73	0.05
2.67	0.01
2.55	0.05
2.50	0.08
2.46	0.01
2.42	0.02
2.37	0.01
2.33	0.04
2.28	0.02
2.21	0.04
2.17	0.02

42

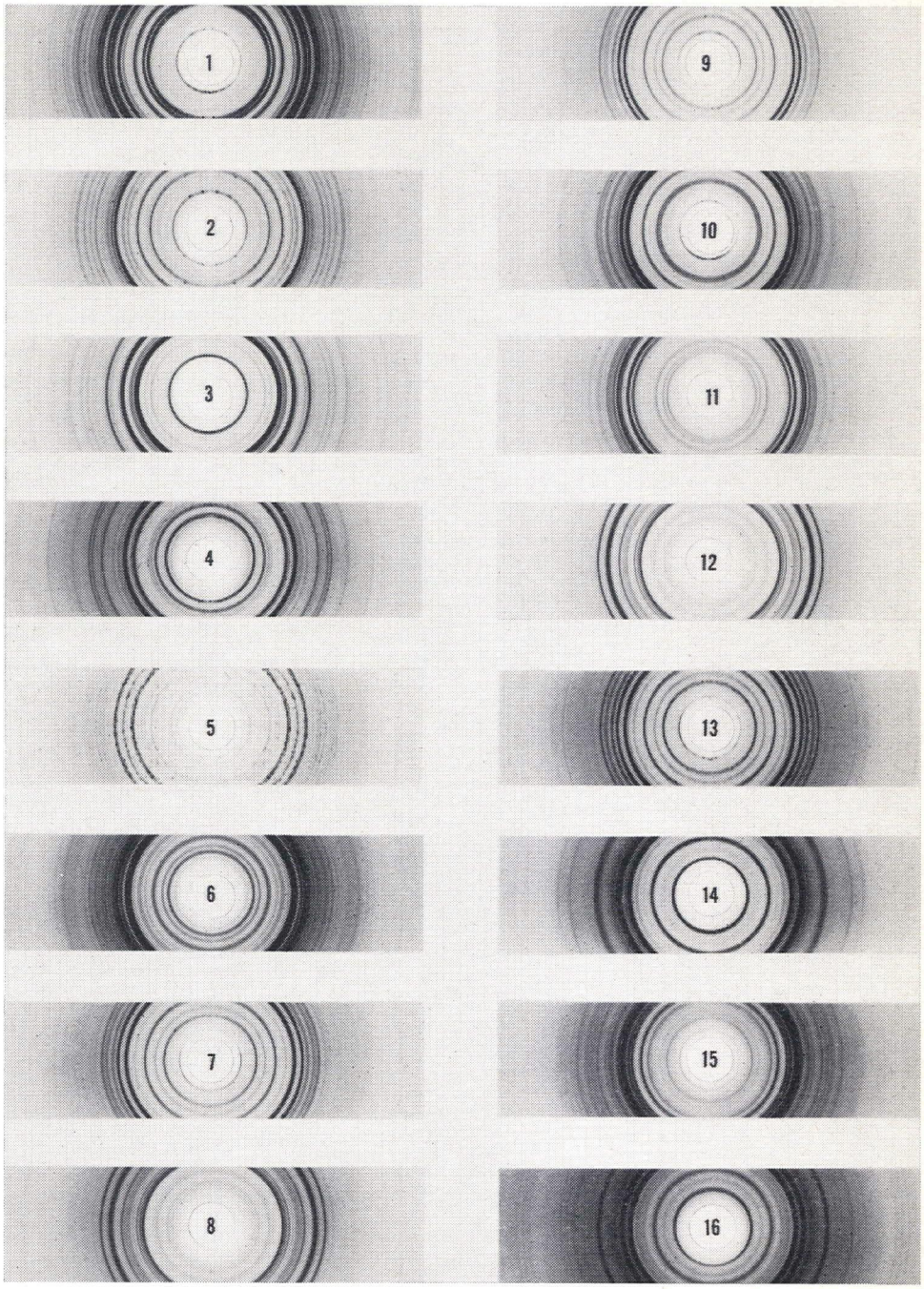
d,A	I/I_1
16.84	0.05
10.53	0.15
8.63	0.02
7.37	0.02
6.66	0.24
6.37	0.05
5.91	0.93
5.56	0.11
5.19	1.00
4.82	0.15
4.58	0.05
4.39	0.04
4.22	0.27
4.00	0.05
3.79	0.02
3.71	0.04
3.57	0.05
3.50	0.05
3.36	0.04
3.14	0.11
3.06	0.02
3.00	0.02
2.91	0.04
2.84	0.04
2.75	0.08
2.63	0.04
2.56	0.04
2.46	0.02
2.37	0.04
2.30	0.01
2.23	0.05
2.14	0.08
2.08	0.05
2.03	0.02
2.00	0.02
1.82	0.08

43

d,A	I/I_1
15.92	0.05
10.34	0.04
9.12	0.08
8.42	0.08
6.76	0.11
6.07	1.00
5.54	0.27
5.17	0.20
4.78	0.55
4.43	0.02
4.17	0.15
4.04	0.13
3.86	0.04
3.63	0.04
3.49	0.02
3.39	0.07
3.30	0.04
3.09	0.04
3.01	0.05
2.86	0.05
2.77	0.02
2.70	0.08
2.44	0.02
2.37	0.05
2.26	0.02
2.22	0.02
2.17	0.02
2.12	0.04
2.08	0.04
1.99	0.02
1.96	0.01
1.90	0.02
1.84	0.01

44

d,A	I/I_1
17.67	0.04
10.53	0.08
9.17	0.04
8.59	0.03
6.71	0.20
6.39	0.04
5.97	0.87
5.63	0.06
5.20	1.00
4.81	0.08
4.62	0.04
4.36	0.04
4.22	0.30
3.99	0.04
3.83	0.01
3.72	0.03
3.60	0.03
3.53	0.02
3.35	0.03
3.25	0.01
3.13	0.15
3.02	0.01
2.90	0.03
2.83	0.02
2.77	0.03
2.64	0.02
2.57	0.02
2.46	0.02
2.38	0.02
2.33	0.01
2.28	0.01
2.23	0.02
2.16	0.02
2.10	0.03
2.04	0.02
2.01	0.03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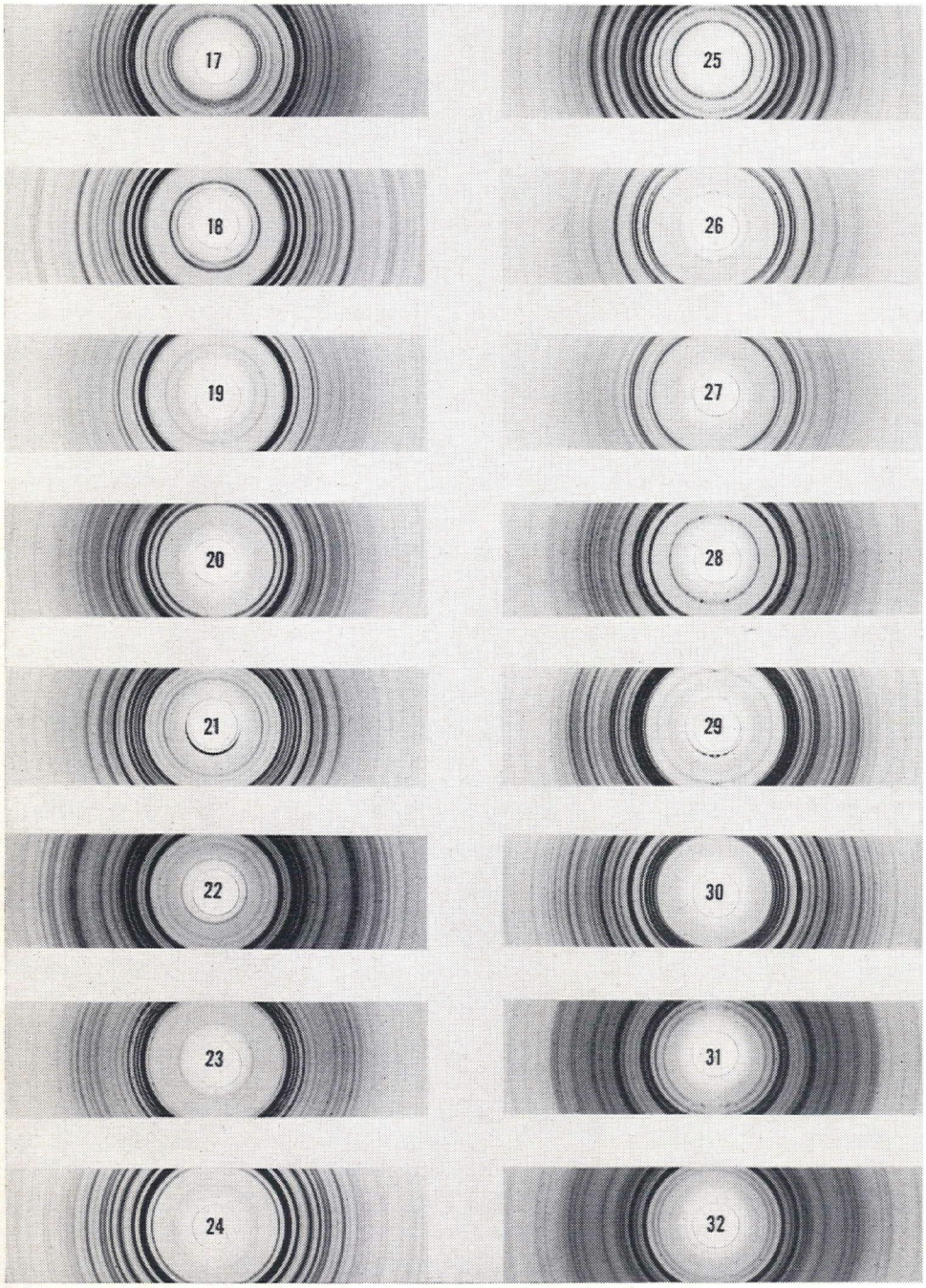
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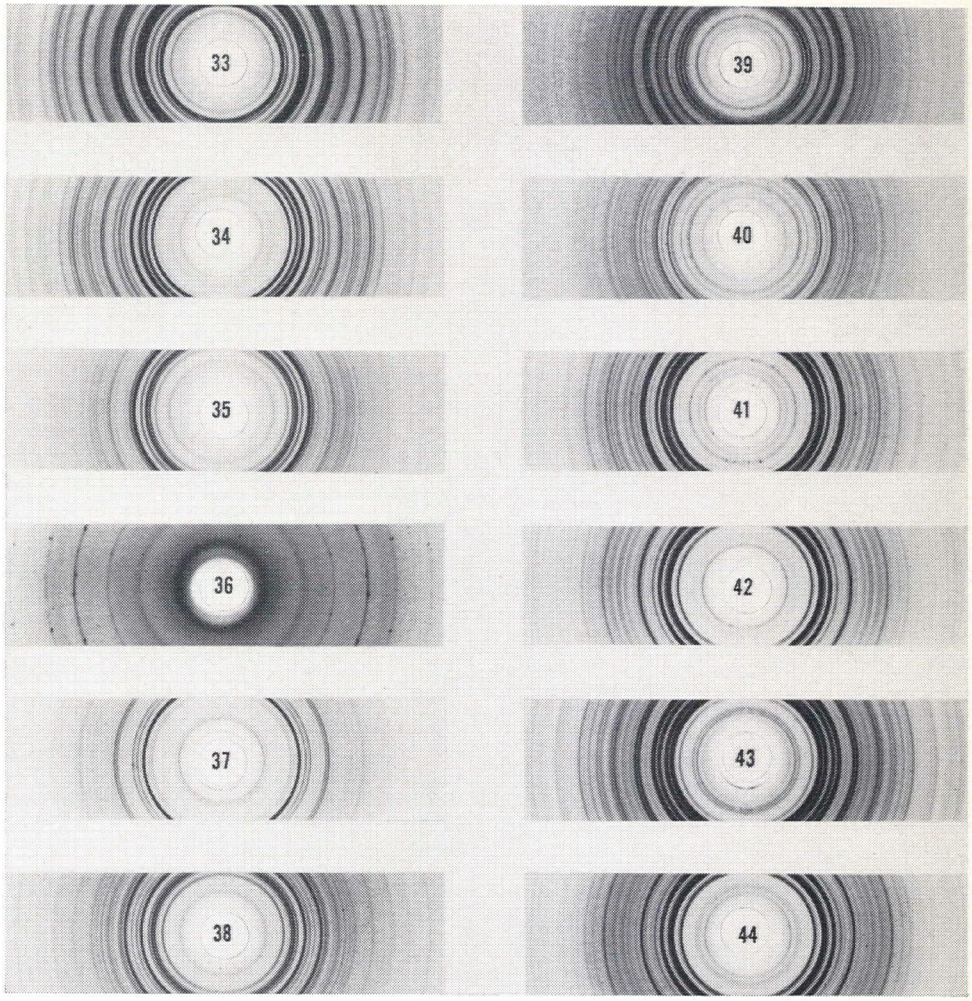
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