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X-ray Diffraction Powder Data For Steroids: Supplement III

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X-RAY DIFFRACTION POWDER DATA FOR STEROIDS: SUPPLEMENT III

including a

DISCUSSION OF STEROID NOMENCLATURE

JONATHAN PARSONS*, S. T. WONG*, WILLIAM T. BEHER**, AND GIZELLA D. BAKER**

THE X-RAY DIFFRACTION powder data for steroids given in this paper comprise an extension to the sets of data previously published in past issues of the Henry Ford Hospital Medical Bulletin.^{1,2,3} Because there exists a lack of agreement with respect to steroid nomenclature, a section is included with this report explaining some of the ways in which the different steroids are classified and showing methods used for naming the majority of these compounds.

DESCRIPTION OF TABLES

The procedures used for obtaining the present data were the same as previously reported.^{1,2,3} Table II is a classified list of steroids studied in this group. Their molecular formulas and corrected melting point ranges are given. Table III gives for each steroid the consecutively numbered data groups consisting of the interplanar spacings (d) in angstrom units and the relative intensities (I/I_1) with I_1 being the intensity of the strongest line of the group.

PURITY OF STEROIDS

In work with each steroid the following steps are taken in order to ascertain the purity of the compound. (1) An x-ray diffraction powder pattern is obtained for each steroid as received from its commercial source. (2) The steroid is then recrystallized from ethanol, if possible, or from an alternative solvent as indicated in Table II. (3) A new powder pattern and melting point determination are then made for the recrystallized steroid. The melting point range thus determined is checked with that reported in the chemical literature. Any steroid whose melting point differs significantly from the literature reported values is held up for further investigation as to its purity.

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POLYMORPHIC FORMS

When the x-ray diffraction powder patterns before and after recrystallization are identical, and their melting point ranges agree with the literature, only one crystalline form is present and the data is included as representing the ethanol (or other solvent) recrystallized form. Where different patterns are obtained before and after recrystallization two polymorphic forms are present and the data is included for the unrecrystallized form as well as for the ethanol (or other solvent) recrystallized states. In cases where the melting point ranges differ slightly before and after recrystallization, this information is listed in Table II. It should be emphasized that more than two forms for the same steroid often exist and the inclusion of data for only one or two of these polymorphic forms does not mean that other crystalline forms with different x-ray diffraction powder patterns are not possible.

STEROID NOMENCLATURE

Steroid nomenclature is at present in a confused state. An international commission has agreed and formulated a standard nomenclature; however its universal acceptance has not been achieved. Nomenclature in this field has been further confused inasmuch as many steroids have useful pharmacological properties and each drug house manufacturing or marketing a given steroid has conferred its own trivial name to these products. As an example of the multiplicity of names given a single compound, the Merck Index lists 14 names for Δ^4 -Androsten-17(β)-ol-3-one (testosterone). While no attempt will be made to cover all methods of naming a given steroid it is hoped that sufficient background will be provided so that the reader can decipher the structure of a steroid regardless of the system of nomenclature used. This, of course, does not apply to the use of trivial names, a practice which should be abandoned. The only recourse in these cases is to find the alternate chemical nomenclature in drug bulletins, Merck Index, etc.

All of the true steroids are characterized by the presence of the cyclopentano-perhydrophenanthrene nucleus, Figure 1. In the shorthand of the chemist the hydrogens are omitted from the ring structure as in Figure 1a which is fully equivalent to Figure 1 and the hydrogen atoms are understood to be present at each of the carbons which in turn are represented by the junctures of two lines. In certain special cases, e.g. stereo considerations it is necessary to include certain hydrogens in writing the structure. This fully saturated alicyclic nucleus is altered by substitution and dehydrogenation in various steroids.

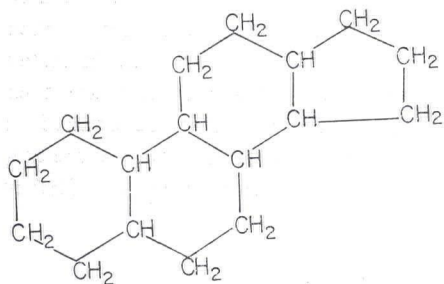


Figure 1

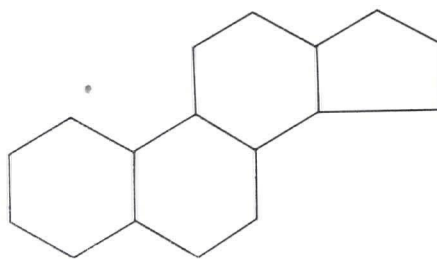


Figure 1a

In order to designate the position of substitution or dehydrogenation the carbon atoms of the nucleus have been assigned numbers which are universally accepted. The numbering and lettering of the cyclopentanoperhydrophenanthrene nucleus is shown in Figure 2.

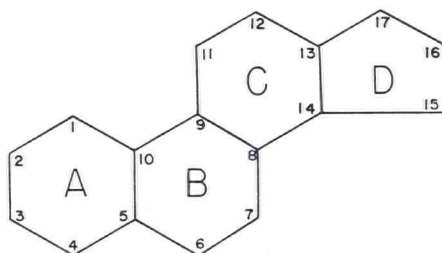


Figure 2

With the exception of the estrogens and a few other compounds all of the steroids have methyl groups substituted for hydrogens at position 10 and 13. Since most steroids contain these methyl groups they are assumed to be present and their presence is not designated as a nuclear substitution. The methyl group at position 10 is missing in the estrane series of compounds. Since the methyl groups are not designated by substitution they have been assigned numbers 18 and 19, Figure 3a. These methyl groups are commonly represented in formulae by heavy strokes, Figure 3b.

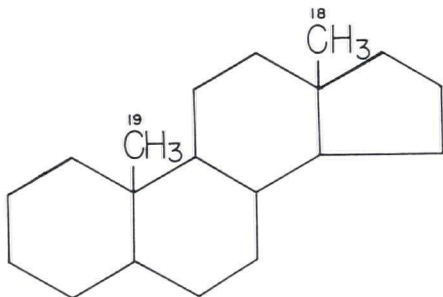


Figure 3a

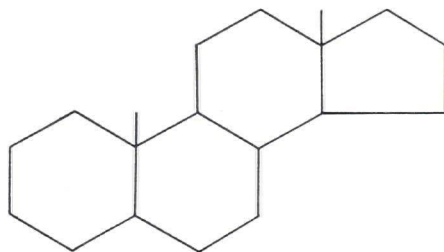


Figure 3b

One of the hydrogen atoms at position 17 may be substituted by a chain of carbons of varying length. Since the order and arrangement but not the number of the carbon atoms in the 17 side chain are the same in all of the steroids substituted at this position, standard numbering of the side chain carbons has been devised. This numbering system is illustrated using the side chain of the cholestane series as an example, Figure 4.

The steroid nucleus has been shown by x-ray diffraction to be planar. The bond angles of carbon atoms in the nucleus are such, that the hydrogen atoms on each of the carbon atoms lie either above or below the plane of the nucleus, (one

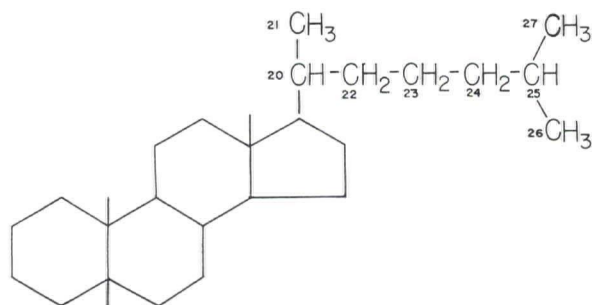


Figure 4

above and one below). The methyl groups (angular methyls) 18 and 19 have been shown to be oriented on the same side of the nuclear plane in all known steroids. The configuration (above or below the nuclear plane) of all other substituting groups are cis or trans (same or opposite side respectively) with respect to the angular methyl groups. Those atoms or radicals cis with respect to the angular methyls are designated to have the β configuration and are always joined to the nucleus by a solid line. Those trans with respect to the angular methyls are designated α and are joined to the nucleus with a dotted line, Figures 5 and 6. If the configuration is unknown the substituent is designated ξ and joined to the nucleus by a wavy line, Figure 7.

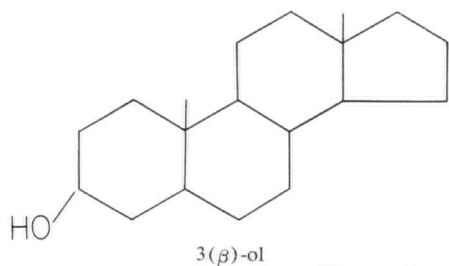


Figure 5

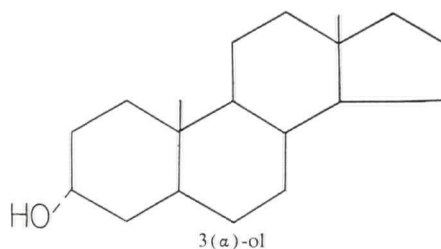


Figure 6

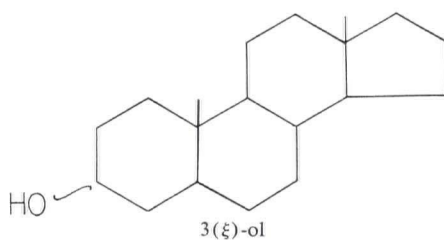


Figure 7

Since some of the carbon atoms in the nucleus contain only one hydrogen atom (position 5, 8, 9, 14), it is necessary to designate the configuration of these hydrogen atoms (α or β) inasmuch as the properties, identity, and nuclear configuration of the steroids depend upon these parameters. Fortunately the configuration of all of these hydrogens with the exception of the one at position five seldom change and

for purposes of nomenclature we can disregard them. The importance of the configuration at position five will become apparent later, it may be either α or β , Figure 8 and 9.

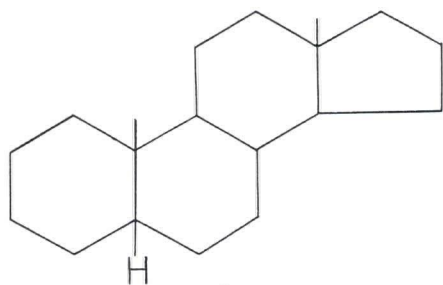
5 α

Figure 8

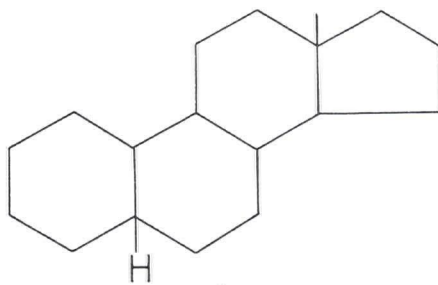
5 β

Figure 9

Most of the steroids commonly encountered may be classified as substitution products of 9 major hydrocarbons which differ only in the configuration of the hydrogen atom at position five and the side chain substitution at carbon 17. The hydrocarbons, their structure and alternate names are shown in structural formulas 10 to 18.

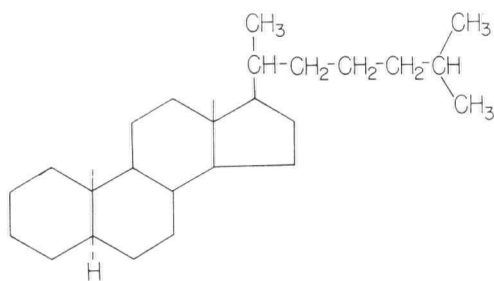
Cholestane
5 α -Cholestane

Figure 10

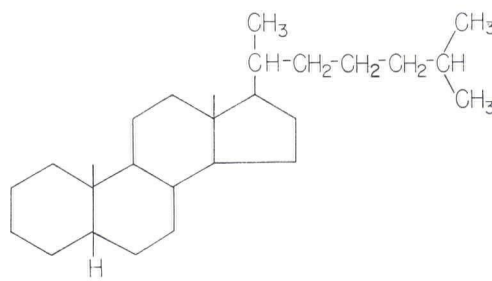
Coprostane
5 β -Cholestane

Figure 11

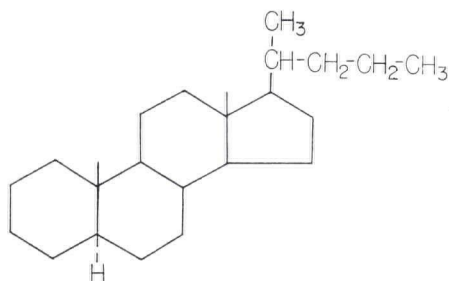
Allocholane
5 α -Cholane

Figure 12

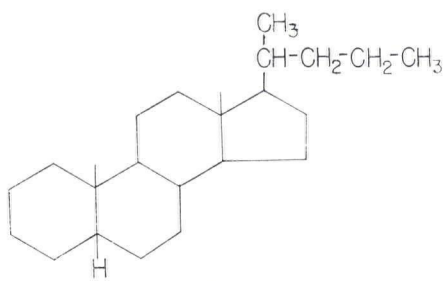
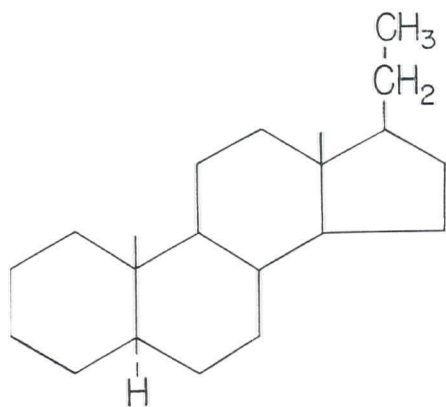
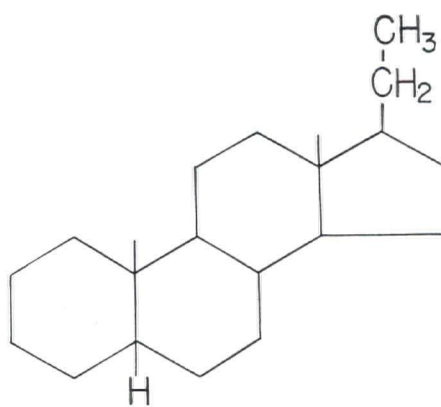
Cholane
5 β -Cholane

Figure 13



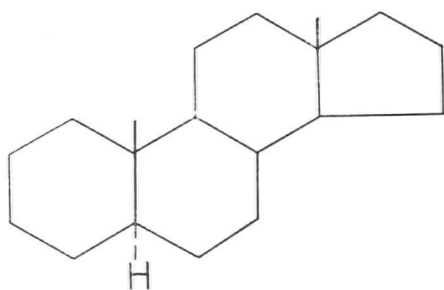
Allopregnane
5 α -Pregnane

Figure 14



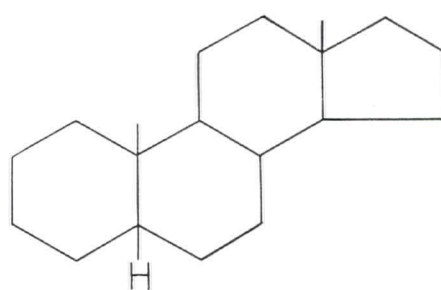
Pregnane
5 β -Pregnane

Figure 15



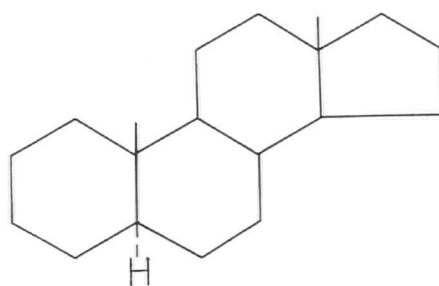
Androstane
5 α -Androstane
Etioallocholane

Figure 16



Etiocholane
5 β -Androstane

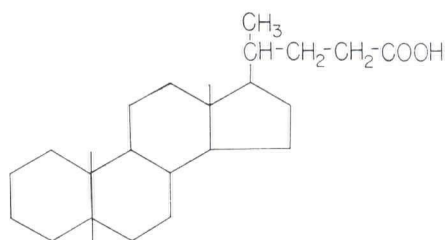
Figure 17



Estrane

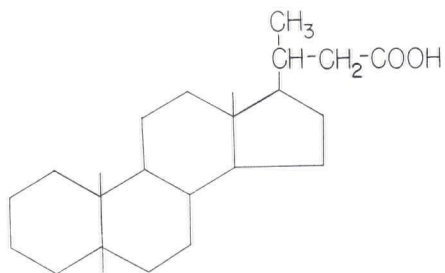
Figure 18

These hydrocarbons may be referred to as stem compounds. One other series of compounds are generally treated as stem compounds, they are cholanic acid, norcholanic acid, bisnorcholanic acid, and etiocholanic acid, Figure 19 to 22.



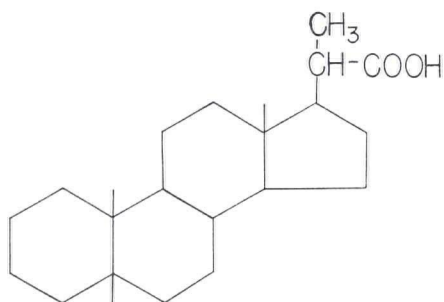
Cholic Acid

Figure 19



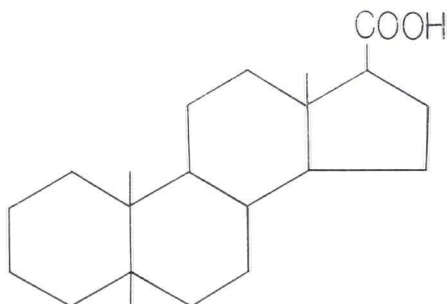
Norcholic Acid

Figure 20



Bisnorcholic Acid

Figure 21



Etiocholic Acid

Figure 22

These stem compounds make it possible to name systematically most of the steroids encountered. They are not sufficient to systematically name the sapogenins and other steroids with complex side chains, however, these compounds are seldom named systematically and we will limit ourselves to trivial names in these cases.

Steroids differ from one another due to the different stems discussed above and substitution for hydrogen atoms on the steroid nucleus by various atoms and radicals. The most common of these are shown in Table I. Since in many of the positions there are two hydrogen atoms of different configuration (one α and one β) the atom or radical replacing a given hydrogen may be either of the α or β configuration and this configuration must be specified inasmuch as the properties of the molecule depend upon this parameter. The position configuration of the substitution or substitutions are designated by placing the number of the position first and the α or β configuration and the nomenclature designation last.

Table I

SUBSTITUTION	SYMBOL or FORMULA	NOMENCLATURE
Cyanide	-C≡N	Cyano or Carbonitrile
Hydroxy	-OH	-ol
Ketone	=O	-one (or Keto in cholanic acid series) or oxo
Nitro	-NO ₂	-nitro
Methyl	-CH ₃	-methyl
Ethyl	-CH ₂ CH ₃	-ethyl
Ethynyl	-C≡CH	-ethynyl
Epoxy or oxido	-O-	-epoxy or oxido
Chlorine	-Cl	-chloro
Bromine	-Br	-bromo
Iodine	-I	-iodo
Fluorine	-F	-fluoro

- 1) Deoxy signifies that there is no oxygen at a certain position, this prefix is used with trivial names only.
- 2) Nor denotes the loss of one carbon from a chain, bisnor two carbons.

Thus we have 3(β)-ol, 3(α)-ol, 3-one, etc. Any number of substitutions may take place in a given steroid. Multiple substitutions by a single atom or radical are indicated by series designation of the positions of substitution and their configuration followed by the prefixes di, tri, tetr, etc., and then the nomenclature designation. For example, Figure 23, would be 5 α -androstan-3(β),7(α),12(α)-triol-17-one.

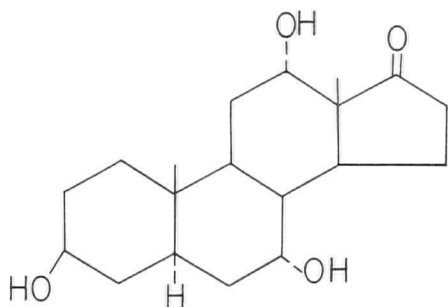


Figure 23

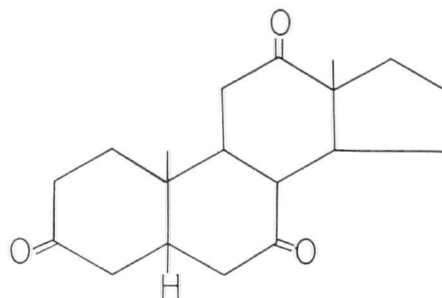


Figure 24

Figure 24 would be 5 β -androstan-3,7,12-trione. Of course, we could classify the steroid, Figure 23, as a trihydroxymonoketone and Figure 24 as a triketone. Since cis-trans isomerism is not involved in ketone substitution no α or β designation is made or is possible.

An important exception to the order of placement of the substitution products and their designations is seen in the series of compounds derived from the stems

POWDER DATA

cholanic, nor-cholanic, bisnorcholanic and etiocholanic acids. In naming such steroids the position number of the substituting atoms or radicals and their full names precede the stem name, thus, Figure 25 is 3(*a*),7(*a*),12(*a*)-trihydroxycholanic acid, Figure 26 is 3(*a*),7(*a*)-dihydroxybisnorcholanic acid and Figure 27 is 3(β)-hydroxy-12-keto-etiocholanic acid.

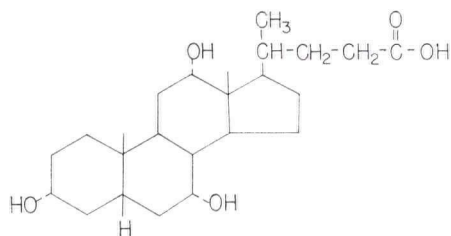


Figure 25

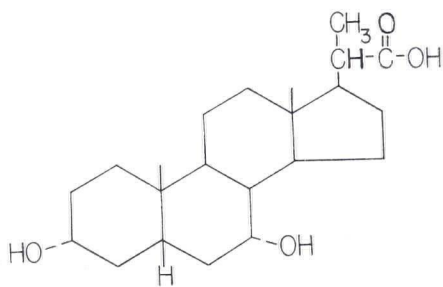


Figure 26

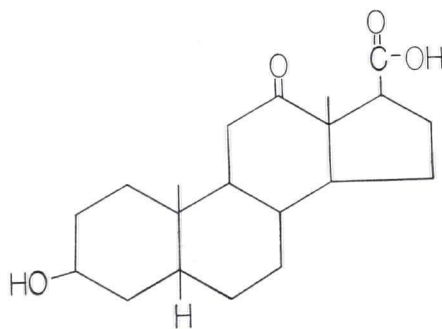


Figure 27

The prefix *epi* is encountered at times. This designation is used to indicate that the configuration of the hydroxyl in the compound is oriented in the opposite manner with respect to the orientation in the natural or typical steroid.

Steroids differ by the amount of unsaturation of the molecule. If two hydrogen atoms are removed between adjacent carbon atoms a double bond is introduced and the molecule is said to be unsaturated due to the fact that various reagents may add across the double bond without replacing hydrogen atoms. For designating the position of unsaturation we run into some confusion inasmuch as several systems have been used. In one system the Greek Δ followed by a small superscript is used. Thus, the steroid in Figure 28 would be Δ^5 . It is obvious that saying Δ^5 does not indicate whether the double bond is between 5 and 6 or 5 and 4, however, the system dictates that the double bond is between the superscript and the next highest position. However, what would one do if a double bond was to be designated between 8 and 14? Here the second number would be placed as a superscript in parenthesis. Thus, the steroid in Figure 29 is $\Delta^{8(14)}$. The stem name is amended by substitution of an

e in place of the final a in the stem. Thus, the steroid in Figure 30 would be cholestan-3(β)-ol and Figure 31 Δ^5 -cholesten-3(β)-ol. If more than one double bond is involved the final n in the stem is replaced by dien, trien, etc., and another superscript is added after the Δ following a comma. Thus, the steroid in Figure 32 is $\Delta^{5,7}$ -cholestadien-3(β)-ol.

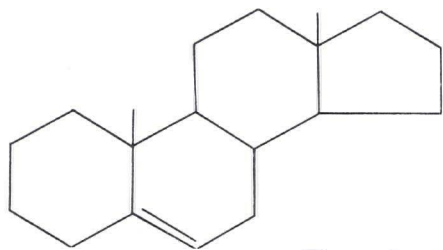


Figure 28

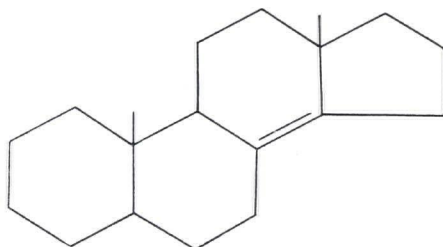


Figure 29

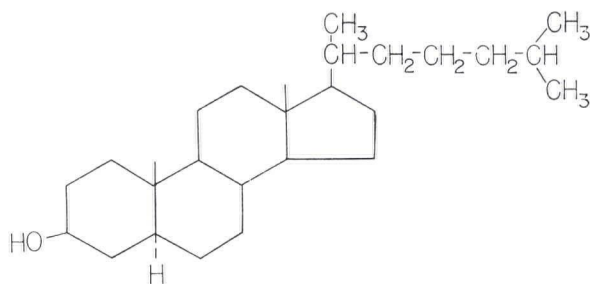


Figure 30

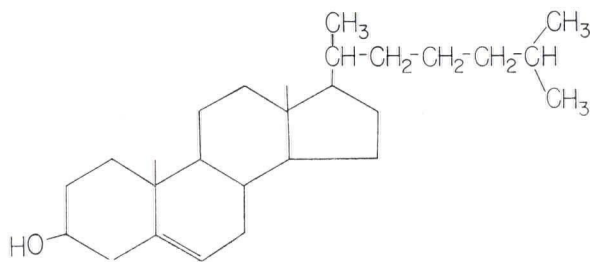


Figure 31

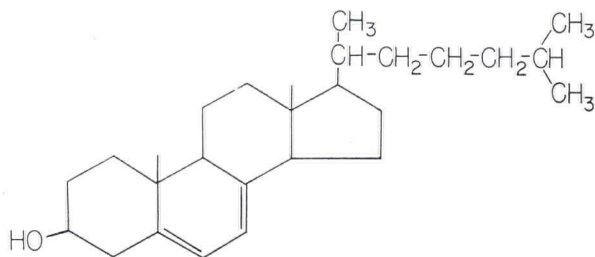


Figure 32

POWDER DATA

Some authors add a final e at the end of the stem designation thus cholesten=cholestene, dien=diene, trien=triene, etc. Some authors omit the Δ and place the number followed by a dash in front of the stem, thus, the steroid shown in Figure 33 can be named, Δ 4-androsten-3,17-dione or 4-androsten-3,17-dione.

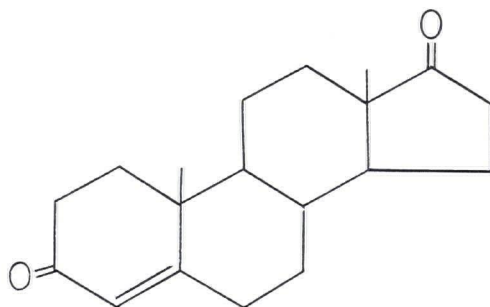


Figure 33

In another method the prefix dehydro is used to signify unsaturation. This prefix is usually preceded by a number indicating the position of unsaturation and is followed by the trivial or common name of the steroid. The steroid in Figure 34, would be called 7-dehydrocholesterol. The use of this prefix is confusing inasmuch as it is also used to indicate the elimination of two hydrogens from a hydroxyl with formation of a ketone (oxidation). An example is shown in Figure 35, where we have 11-dehydrocorticosterone. Obviously this designation should be abandoned.

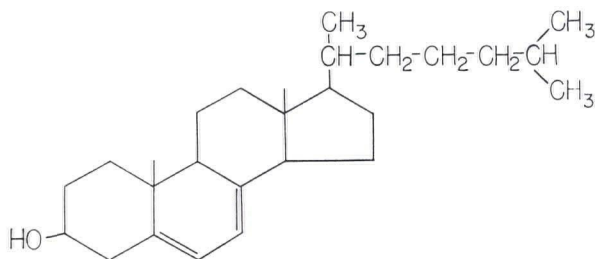


Figure 34

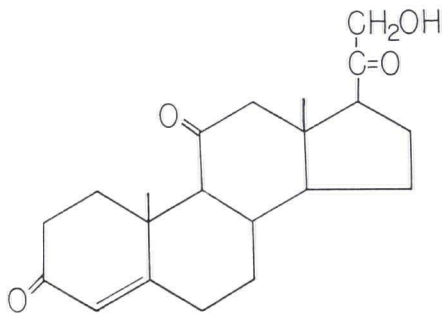


Figure 35

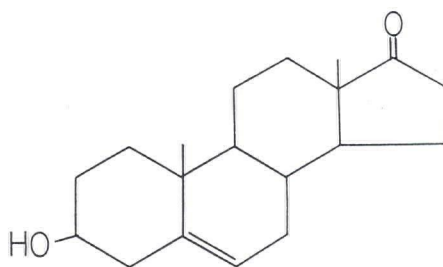


Figure 36

Still another system of designating unsaturation is illustrated by the steroid in Figure 36. We would call this steroid androst-5-en-3(β)-ol-17-one. In this system the stem minus the suffix -ane is followed by the position number of the unsaturation and this in turn is followed by -en. In the case of multiple unsaturation more than one position number is used followed by diene, triene, etc. Steroids derivatives such as esters, ethers, and acetals are named by writing the structural designation of the parent compound first and following this by the position number or numbers of the derivative and then the name of the derivative or derivatives. The derivatives shown in Figure 37 and 38 are examples:

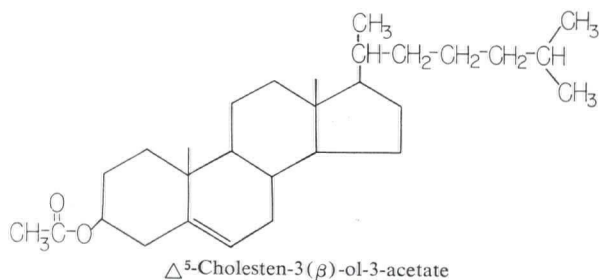


Figure 37

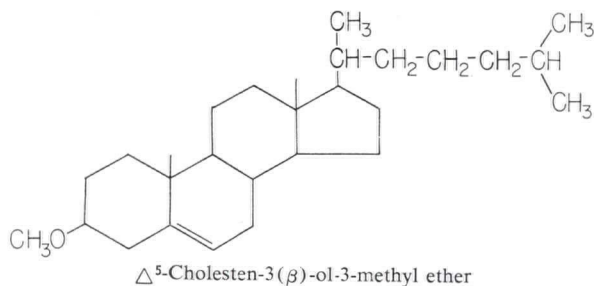


Figure 38

In an alternate type of nomenclature, Figure 37 is called 3(β)-acetoxy- Δ^5 -cholesten. The methyl esters of cholanic, norcholanic, bisnorcholanic, and etiocholanic acid are named by placing the word methyl first followed by the stem name with the ending -ic replaced by ate. Ethyl and higher esters would be named similarly. An example would be methyl cholante.

ACKNOWLEDGEMENT

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POWDER DATA

Diffraction Methods, a joint project of the American Society for Testing Materials, American Crystallographic Association, and the British Institute of Physics. The photographs were reproduced with the cooperation of the Department of Photography, Henry Ford Hospital.

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Table II

Index To Steroid X-ray Diffraction Powder Data

Pattern Number	Name	Molecular Formula	Melting Point (Corr.) °C
<i>Steroid hydrocarbons</i>			
1	Δ^2 -Cholestene ^a	C ₂₇ H ₄₆	66-67.5
2	Δ^5 -Cholestene	C ₂₇ H ₄₆	85.5-86.5
<i>Halogen steroids</i>			
3	5 α , 6 β -Dibromocholestan-3 β -ol ^a	C ₂₇ H ₄₆ O•Br ₂	112.5-115
<i>Monohydric alcohols</i>			
4	Δ^7 -Cholesten-3 β -ol	C ₂₇ H ₄₆ O	122.5-124.5
5	Δ^5 -Cholesten-3 β -ol-3-formate	C ₂₈ H ₄₆ O ₂	96.5-98
6	Δ^5 -Cholesten-3 β -ol-p-toluene sulfonate ^c	C ₃₄ H ₅₂ O ₃ S	132-135.5
7	Coprostan-3 β -ol	C ₂₇ H ₄₈ O	110-111.5
8	$\Delta^{5,7}$ -Cholestadien-3 β -ol-3-acetate (7-Dehydrocholesterol acetate)	C ₂₉ H ₄₆ O ₂	128.5-129.5
9	5 α , 6 α -Oxido-cholestan-3 β -ol ^c	C ₂₇ H ₄₆ O ₂	143—
10	5 α , 6 α -Oxido-cholestan-3 β -ol ^a	C ₂₇ H ₄₆ O ₂	143-144
<i>Dihydric alcohols</i>			
11	5 α -Pregnan-3 β , 20 α -diol	C ₂₁ H ₃₆ O ₂	216-218
12	5 α -Pregnan-3 β , 20 β -diol	C ₂₁ H ₃₆ O ₂	196-198
<i>Trihydric alcohols</i>			
13	Cholestan-3 β , 5 α , 6 β -triol	C ₂₇ H ₄₈ O ₃	238.5-241
<i>Monoketones</i>			
14	Δ^5 -Cholesten-3-one	C ₂₇ H ₄₄ O	125-127
<i>Diketones</i>			
15	$\Delta^{1,4}$ -Androstadien-3, 17-dione	C ₁₉ H ₂₄ O ₂	135.5-137.5
16	$\Delta^{4,16}$ -Pregnadien-3, 20-dione (16-Dehydroprogesterone)	C ₂₁ H ₂₈ O ₂	188-189
17	$\Delta^{4,16}$ -Pregnadien-3, 20-dione-6 α -methyl ^c	C ₂₂ H ₃₀ O ₂	181-182
18	$\Delta^{4,16}$ -Pregnadien-3, 20-dione-6 α -methyl	C ₂₂ H ₃₀ O ₂	181.5-183
19	$\Delta^{11,5\beta}$ -Pregnen-3, 20-dione	C ₂₁ H ₃₀ O ₂	135-137
20	Δ^4 -Pregnen-3, 20-dione-16 α -methyl (16-Methyl progesterone)	C ₂₂ H ₃₂ O ₂	136.5-138.5
<i>Triketones</i>			
21	Δ^4 -Pregnen-3, 11, 20-trione	C ₂₁ H ₂₈ O ₃	173.5-176
22	5 α -Pregnan-3, 11, 20-trione	C ₂₁ H ₂₀ O ₃	220-223
<i>Monohydroxy-monoketones</i>			
23	5 α -Androstan-3 α -ol-17-one-acetate (Androsterone acetate)	C ₂₁ H ₃₂ O ₃	164.5-166.5
24	5 α -Androstan-3 α -ol-17-one-benzoate (Androsterone benzoate)	C ₂₆ H ₃₄ O ₃	177.5-179.5
25	5 α -Androstan-17 β -ol-3-one-17 α -methyl	C ₂₀ H ₃₂ O ₂	195-197.5
26	Cholestan-3 β -ol-6-one ^c (6-Ketocholestanol)	C ₂₇ H ₄₆ O ₂	145.5-147
27	Cholestan-3 β -ol-6-one (6-Ketocholestanol)	C ₂₇ H ₄₆ O ₂	142.5-144.5
28	Δ^5 -Cholesten-3 β -ol-7-one-3-acetate	C ₂₉ H ₄₆ O ₃	160-161.5
29	$\Delta^{16,5\beta}$ -Pregnen-3 β -ol-20-one ^a (16-Dehydropregnanolone)	C ₂₁ H ₃₂ O ₂	183-186.5
30	5 α -Pregnan-20 β -ol-3-one	C ₂₁ H ₃₄ O ₂	196-198.5
<i>Dihydroxy-monoketones</i>			
31	5 α -Pregnan-3 β , 17 α -diol-20-one	C ₂₁ H ₃₄ O ₃	261-262.5
32	5 β -Pregnan-3 α , 6 α -diol-20-one	C ₂₁ H ₃₄ O ₃	192.5-194
33	Δ^5 -Pregnen-3 β , 17 α -diol-20-one-3-acetate	C ₂₃ H ₃₄ O ₄	236-240

POWDER DATA

Table II — (Continued)

Pattern Number	Name	Molecular Formula	Melting Point (Corr.) °C
<i>Monohydroxy-diketones</i>			
34	Δ^4 -Pregnen-11 α -ol-3, 20-dione ^c (11 α -Hydroxy progesterone)	C ₂₁ H ₃₀ O ₃	164-165
35	Δ^4 -Pregnen-11 α -ol-3, 20-dione (11 α -Hydroxy progesterone)	C ₂₁ H ₃₀ O ₃	164-166
36	Δ^4 -Pregnen-17 α -ol-3, 20-dione-17-acetate (17 α -Hydroxy progesterone acetate)	C ₂₃ H ₃₂ O ₄	248-248.5
<i>Dihydroxy-triketones</i>			
37	5 α -Pregnan-17 α , 21-diol-3, 11, 20-trione-21-acetate ^c	C ₂₃ H ₃₂ O ₆	227-230
38	5 α -Pregnan-17 α , 21-diol-3, 11, 20-trione-21-acetate	C ₂₃ H ₃₂ O ₆	232-236
<i>Trihydroxy-diketones</i>			
39	5 β -Pregnan-3 α , 17 α , 21-triol-11, 20-dione-21-acetate	C ₂₃ H ₃₄ O ₆	215-217.5
<i>Carboalkoxy acids</i>			
40	3 α , 7 β -Dihydroxycholanolic acid (Ursodeoxycholic acid)	C ₂₄ H ₄₀ O ₄	198-200
41	3 α , 12 α -Dihydroxy- Δ^8 -(14)-cholenic acid (Apochoolic acid)	C ₂₄ H ₃₈ O ₄	173-176.5
42	3 α , 6 α , 7 α -Trihydroxycholanolic acid (Hyochoolic acid)	C ₂₄ H ₄₀ O ₅	179-182
<i>Sapogenins and sapogenin derivatives</i>			
43	Kryptogenin	C ₂₇ H ₄₂ O ₄	180.5-182.5
<i>Digitalis glycosides</i>			
44	$\Delta^{20(22)}$ -3, 14, 21-Trihydroxycholenic acid lactone (Digitoxigenin)	C ₂₃ H ₃₄ O ₄	250-252
<i>Pseudo steroids</i>			
45	3, 4-Bis(p-methoxyphenyl)-3-hexene ^b (Diethylstilbestrol dimethyl ether)	C ₂₀ H ₂₄ O ₂	123.5-125
46	3, 4-Bis(p-dipalmitoxyphenyl)-3-hexene (Diethylstilbestrol dipalmitate)	C ₅₀ H ₈₀ O ₄	86-87.5

^aRecrystallized from acetone^bRecrystallized from petroleum ether^cUnrecrystallized

Table III

1		2		3	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
12.36	0.41	15.16	0.06	10.65	0.15
9.83	0.08	10.49	0.30	10.22	0.56
8.39	0.02	7.95	0.04	8.71	0.20
7.50	0.11	6.85	0.08	7.53	0.38
7.03	0.08	6.18	0.15	7.08	0.08
6.63	0.11	5.80	0.03	6.76	0.02
6.03	0.05	5.49	1.00	6.42	0.02
5.59	1.00	5.22	0.01	6.15	0.20
5.39	0.15	4.68	0.20	5.81	0.15
5.17	0.20	4.33	0.08	5.47	0.47
4.77	0.08	3.99	0.11	5.05	1.00
4.31	0.11	3.82	0.01	4.83	0.08
4.14	0.03	3.69	0.02	4.63	0.03
4.01	0.27	3.54	0.06	4.47	0.03
3.79	0.08	3.40	0.01	4.35	0.01
3.71	0.02	3.25	0.01	4.22	0.33
3.51	0.08	3.18	0.01	4.10	0.10
3.27	0.04	3.09	0.01	4.00	0.05
3.20	0.02	2.96	0.02	3.88	0.11
3.12	0.01	2.77	0.03	3.60	0.11
2.98	0.02	2.52	0.02	3.53	0.20
2.92	0.01	2.47	0.02	3.45	0.15
2.84	0.01	2.38	0.01	3.37	0.18
2.75	0.01	2.34	0.01	3.28	0.08
2.68	0.01	2.28	0.04	3.20	0.05
2.60	0.07	2.18	0.02	3.08	0.08
2.51	0.05	2.05	0.02	3.00	0.24
2.46	0.01			2.91	0.05
2.40	0.07			2.81	0.07
2.28	0.08			2.75	0.11
2.19	0.07			2.69	0.03
2.13	0.07			2.63	0.05
2.07	0.02			2.57	0.05
2.00	0.07			2.50	0.05
1.94	0.05			2.44	0.11
				2.40	0.07
4		5			
d,A	I/I ₁	d,A	I/I ₁		
10.69	0.50	14.03	0.13		
8.96	0.20	12.11	0.02		
7.82	0.15	9.21	0.01		
7.07	0.10	7.25	0.20		
5.71	0.20	6.44	0.03		
5.55	0.27	5.89	1.00		
5.33	0.07	5.61	0.67		
5.06	0.05	5.25	0.36		
4.92	1.00	5.04	0.49		
4.64	0.07	4.80	0.27		
4.48	0.07	4.68	0.36		
4.25	0.01	4.43	0.04		
3.91	0.24	4.24	0.11		
3.62	0.02	4.06	0.13		
3.47	0.15	3.89	0.09		
3.08	0.07	3.79	0.04		
2.64	0.01	3.65	0.07		
2.56	0.01	3.51	0.07		
2.48	0.01	3.30	0.04		
2.24	0.02	3.20	0.01		
2.18	0.01	3.12	0.01		
2.11	0.02	3.02	0.13		
2.05	0.01	2.93	0.09		
		2.82	0.02		
		2.59	0.03		
		2.54	0.01		
		2.47	0.02		
		2.38	0.02		
		2.30	0.01		
		2.23	0.02		
		2.15	0.02		
		2.11	0.03		
		2.01	0.04		

POWDER DATA

6		7		8	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
13.15	0.15	12.19	0.27	16.58	0.15
11.38	0.15	10.65	0.02	6.08	0.40
9.64	0.20	8.01	0.17	5.58	1.00
8.03	0.01	7.00	0.09	5.22	0.04
7.46	0.50	6.61	0.13	5.02	0.05
6.38	0.07	6.07	1.00	4.76	0.08
6.02	0.80	5.85	0.01	4.58	0.63
5.71	0.88	5.59	0.67	4.35	0.04
5.43	0.44	5.28	0.17	4.14	0.03
5.23	1.00	4.85	0.36	4.03	0.04
4.96	0.15	4.63	0.20	3.87	0.04
4.79	0.15	4.26	0.09	3.76	0.08
4.54	0.20	3.98	0.17	3.66	0.06
4.35	0.27	3.84	0.02	3.53	0.04
4.18	0.20	3.61	0.02	3.39	0.04
4.02	0.20	3.43	0.03	3.06	0.11
3.86	0.01	3.33	0.02	3.00	0.01
3.72	0.27	3.12	0.01	2.91	0.06
3.59	0.15	3.04	0.01	2.84	0.01
3.35	0.07	2.87	0.01	2.75	0.06
3.29	0.10	2.80	0.02	2.55	0.01
3.21	0.10	2.68	0.02	2.49	0.03
3.11	0.02	2.57	0.01	2.29	0.06
3.04	0.02	2.48	0.01	2.17	0.01
3.00	0.15	2.43	0.01	2.09	0.01
2.82	0.13	2.22	0.02	2.04	0.02
2.73	0.03			1.96	0.02
2.57	0.10			1.89	0.01
2.42	0.02				
2.37	0.10				
2.31	0.07				
2.23	0.15				
2.16	0.10				
2.11	0.07				
2.04	0.07				
1.99	0.07				

9		10		11	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
14.30	0.15	11.90	0.11	13.33	0.01
11.22	0.10	8.91	0.05	11.74	0.05
7.15	0.03	8.06	0.05	10.43	0.01
6.77	0.10	7.67	0.02	9.23	0.05
6.22	0.08	6.90	0.05	8.56	0.04
6.03	0.27	6.54	0.08	8.09	0.05
5.84	0.10	6.22	0.08	6.72	0.04
5.51	1.00	6.01	0.28	6.40	0.05
5.18	0.50	5.69	1.00	6.14	0.04
4.88	0.18	5.48	0.15	5.74	1.00
4.58	0.07	5.24	0.20	5.35	0.08
4.36	0.03	5.00	0.56	4.78	0.73
4.19	0.07	4.33	0.11	4.57	0.05
4.08	0.15	4.17	0.08	4.27	0.15
3.92	0.10	3.85	0.08	4.09	0.08
3.72	0.20	3.71	0.03	3.78	0.08
3.56	0.01	3.57	0.03	3.66	0.01
3.34	0.01	3.35	0.08	3.54	0.05
3.25	0.05	3.25	0.01	3.22	0.11
3.15	0.01	3.13	0.02	3.11	0.04
2.96	0.01	3.00	0.08	3.03	0.01
2.83	0.07	2.83	0.05	2.89	0.02
2.76	0.01	2.65	0.01	2.76	0.02
2.57	0.01	2.58	0.01	2.66	0.01
2.38	0.01	2.45	0.02	2.58	0.01
2.24	0.02	2.40	0.02	2.52	0.04
2.20	0.05	2.35	0.03	2.44	0.01
		2.20	0.03	2.38	0.01
		2.16	0.01	2.29	0.10
				2.19	0.01
				2.14	0.01
				2.07	0.01
				2.01	0.01

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12		13		14	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
12.28	0.11	11.77	0.07	9.75	0.37
8.98	0.08	9.98	0.05	7.33	0.50
6.15	0.40	8.84	0.05	5.58	0.44
5.45	1.00	8.15	0.02	5.40	0.10
5.10	0.08	7.49	0.11	5.02	1.00
4.72	0.06	6.60	0.01	4.87	0.15
4.46	0.03	6.02	1.00	4.44	0.13
4.34	0.30	5.59	0.02	4.25	0.01
4.00	0.07	5.39	0.02	3.96	0.10
3.88	0.03	5.01	0.41	3.70	0.13
3.79	0.01	4.20	0.10	3.55	0.03
3.40	0.08	4.02	0.04	3.48	0.15
3.31	0.01	3.86	0.04	3.35	0.01
3.18	0.11	3.68	0.04	3.11	0.03
3.07	0.13	3.51	0.04	3.06	0.02
2.98	0.03	3.38	0.05	2.96	0.03
2.87	0.05	3.09	0.04	2.85	0.02
2.81	0.04	3.02	0.01	2.79	0.01
2.75	0.06	2.94	0.01	2.68	0.03
2.64	0.01	2.88	0.01	2.22	0.03
2.55	0.04	2.75	0.02	2.09	0.02
2.50	0.05	2.62	0.02	1.99	0.03
2.42	0.03	2.54	0.03		
2.30	0.06	2.40	0.01		
2.18	0.06	2.25	0.01	d,A	I/I ₁
2.14	0.05	2.20	0.04	8.55	0.10
2.08	0.05	2.08	0.01	8.15	0.05
2.03	0.04	2.01	0.01	6.81	0.04
1.99	0.04	1.97	0.01	6.33	0.04
1.96	0.05			5.81	0.07
1.90	0.04			5.59	1.00
1.87	0.04			5.23	0.27
				4.85	0.15
				4.63	0.20
				4.36	0.11
				4.22	0.20
				3.98	0.11
				3.87	0.08
				3.79	0.01
				3.58	0.02
				3.43	0.18
				3.24	0.01
				3.16	0.05
				3.06	0.01
				2.98	0.05
				2.87	0.01
				2.80	0.11
				2.72	0.02
				2.66	0.01
				2.60	0.02
				2.53	0.05
				2.48	0.01
				2.44	0.01
				2.39	0.05
				2.30	0.05
				2.18	0.04
				2.14	0.04
				1.98	0.04
				1.91	0.03
				1.86	0.01
				1.73	0.04

POWDER DATA

16		17		18	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
11.87	0.17	11.95	0.01	12.45	0.13
6.22	0.36	10.65	0.11	10.85	0.11
5.91	0.36	8.63	0.11	6.73	0.04
5.66	1.00	6.37	0.27	6.15	0.15
5.49	0.20	5.99	0.05	5.91	0.02
5.07	0.04	5.79	0.27	5.66	0.05
4.72	0.01	5.57	0.05	5.34	1.00
4.58	0.09	5.39	1.00	4.94	0.01
4.25	0.67	5.25	0.04	4.75	0.03
4.07	0.27	4.93	0.34	4.62	0.18
3.80	0.09	4.53	0.15	4.32	0.13
3.63	0.20	4.40	0.11	4.12	0.04
3.31	0.17	4.26	0.03	4.02	0.13
3.21	0.17	4.10	0.05	3.74	0.15
3.07	0.04	3.98	0.08	3.49	0.15
2.98	0.02	3.87	0.05	3.39	0.05
2.89	0.01	3.75	0.05	3.21	0.03
2.74	0.02	3.58	0.03	3.02	0.20
2.65	0.02	3.48	0.04	2.93	0.11
2.54	0.01	3.39	0.11	2.87	0.02
2.43	0.02	3.06	0.02	2.78	0.04
2.38	0.04	2.99	0.11	2.71	0.02
2.27	0.02	2.92	0.05	2.66	0.01
2.20	0.01	2.84	0.04	2.52	0.04
2.16	0.02	2.77	0.03	2.46	0.05
2.13	0.02	2.72	0.01	2.41	0.01
2.08	0.02	2.68	0.01	2.37	0.01
2.00	0.02	2.63	0.04	2.32	0.08
		2.54	0.05	2.27	0.03
		2.34	0.08	2.22	0.01
		2.23	0.04	2.17	0.01
		2.18	0.05	2.12	0.05
		2.13	0.05	2.08	0.04
		2.10	0.04	2.04	0.01
		2.06	0.02	2.01	0.01
		1.99	0.05	1.98	0.05

19	
d,A	I/I ₁
6.63	0.15
6.33	1.00
5.93	0.11
5.66	0.56
5.11	0.47
4.80	0.01
4.47	0.38
3.89	0.05
3.58	0.15
3.50	0.08
3.39	0.11
3.28	0.02
3.21	0.02
3.15	0.08
2.97	0.13
2.91	0.08
2.83	0.08
2.75	0.06
2.69	0.09
2.63	0.03
2.55	0.02
2.42	0.08
2.38	0.01
2.30	0.06
2.23	0.08
2.19	0.01
2.15	0.05
2.11	0.09
1.95	0.11

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20		21		22	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
10.34	0.27	11.15	0.15	11.48	0.08
6.86	0.10	8.44	0.20	8.34	0.03
6.30	0.20	6.45	0.32	6.86	0.01
6.13	1.00	6.01	1.00	6.26	0.40
5.89	0.10	5.44	0.75	5.99	0.04
5.66	0.07	5.15	0.10	5.74	0.06
5.40	0.75	5.00	0.23	5.57	1.00
5.05	0.63	4.80	0.20	5.10	0.30
4.77	0.27	4.49	0.27	4.82	0.04
4.47	0.15	4.19	0.23	4.56	0.03
4.17	0.37	3.99	0.07	4.37	0.06
3.90	0.01	3.84	0.10	4.17	0.08
3.70	0.03	3.70	0.05	4.02	0.05
3.65	0.15	3.50	0.15	3.90	0.01
3.53	0.03	3.34	0.01	3.79	0.02
3.44	0.15	3.18	0.15	3.67	0.06
3.31	0.15	3.09	0.13	3.54	0.01
3.20	0.02	3.01	0.20	3.43	0.04
3.14	0.01	2.94	0.09	3.33	0.05
3.06	0.07	2.86	0.07	3.24	0.02
2.96	0.03	2.78	0.13	3.16	0.25
2.74	0.10	2.66	0.09	3.07	0.08
2.66	0.07	2.62	0.07	2.98	0.04
2.60	0.05	2.56	0.03	2.88	0.02
2.55	0.10	2.51	0.09	2.83	0.08
2.40	0.03	2.42	0.01	2.78	0.02
2.31	0.02	2.36	0.03	2.72	0.02
2.25	0.02	2.32	0.02	2.67	0.01
2.19	0.13	2.27	0.05	2.56	0.04
2.11	0.01	2.08	0.03	2.51	0.03
2.03	0.02	2.05	0.02	2.40	0.09
1.93	0.01	1.99	0.02	2.34	0.02
1.87	0.01	1.90	0.03	2.30	0.01
		1.87	0.05	2.26	0.01
				2.18	0.04

POWDER DATA

23		24		25	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
11.36	0.11	11.05	0.15	11.07	0.08
7.88	0.15	9.56	0.10	6.26	0.47
6.93	0.01	7.20	0.07	5.97	0.66
6.16	1.00	6.30	0.88	5.46	0.38
5.76	0.27	5.81	0.50	4.94	1.00
5.51	0.02	5.50	1.00	4.73	0.11
5.33	0.87	5.23	0.20	4.61	0.20
5.04	0.20	4.77	0.18	4.12	0.15
4.49	0.15	4.58	0.01	3.88	0.01
4.15	0.20	4.40	0.37	3.70	0.05
3.93	0.08	4.25	0.07	3.56	0.13
3.76	0.08	4.21	0.27	3.45	0.01
3.63	0.03	4.12	0.15	3.07	0.13
3.47	0.13	3.98	0.20	2.98	0.11
3.32	0.08	3.67	0.07	2.92	0.01
3.22	0.11	3.48	0.13	2.86	0.08
3.09	0.02	3.37	0.02	2.78	0.01
2.98	0.03	3.29	0.03	2.70	0.08
2.86	0.08	3.16	0.15	2.53	0.05
2.70	0.02	3.06	0.01	2.48	0.15
2.62	0.04	2.91	0.03	2.40	0.05
2.58	0.03	2.75	0.07	2.36	0.01
2.53	0.04	2.59	0.03	2.30	0.01
2.47	0.02	2.49	0.02	2.25	0.04
2.42	0.01	2.45	0.03	2.19	0.08
2.37	0.08	2.35	0.10	2.14	0.01
2.32	0.08	2.24	0.05	2.07	0.13
2.22	0.07	2.19	0.02		
2.13	0.03	2.15	0.01		
2.01	0.02	2.12	0.02		
1.99	0.01	2.07	0.03		
1.95	0.01	1.96	0.02		
1.91	0.03	1.93	0.02		
1.88	0.04	1.90	0.01		
1.82	0.03	1.83	0.03		
1.79	0.04				
				d,A	I/I ₁
				10.78	1.00
				9.66	0.04
				8.51	0.04
				7.50	0.11
				6.89	0.11
				6.53	0.02
				6.19	0.05
				5.74	0.04
				5.17	0.91
				4.77	0.73
				4.53	0.20
				4.39	0.01
				4.26	0.07
				4.13	0.02
				3.93	0.05
				3.79	0.15
				3.67	0.11
				3.36	0.04
				3.21	0.04
				3.13	0.05
				3.06	0.07
				2.98	0.03
				2.87	0.04
				2.79	0.04
				2.67	0.02
				2.50	0.03
				2.41	0.04
				2.32	0.01
				2.23	0.04
				2.16	0.04
				2.08	0.03
				1.99	0.02

26

d,A	I/I ₁
10.34	0.15
8.85	0.20
7.03	0.10
5.91	0.27
5.61	1.00
5.28	0.03
5.07	0.24
4.54	0.01
4.43	0.15
4.25	0.01
4.09	0.02
3.89	0.07
3.75	0.10
3.34	0.07
3.03	0.01
2.93	0.01
2.80	0.01

27

d,A	I/I ₁
8.55	0.01
7.94	0.04
7.47	0.02
6.17	0.09
5.89	0.49
5.57	0.36
5.19	1.00
4.81	0.27
4.20	0.02
4.01	0.24
3.83	0.01
3.70	0.04
3.41	0.02
3.18	0.02
2.97	0.02

PARSONS, WONG, BEHER AND BAKER

29		30		31	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
10.78	0.11	11.71	0.11	12.24	0.11
7.76	0.05	10.92	0.08	6.72	0.01
7.37	0.08	6.19	0.38	6.00	1.00
6.42	0.11	5.93	0.24	5.75	0.20
6.12	1.00	5.50	1.00	5.15	0.41
5.77	0.01	5.23	0.11	4.94	0.05
5.50	0.56	5.01	0.15	4.58	0.34
5.31	0.38	4.81	0.01	4.05	0.05
4.90	0.07	4.61	0.05	3.81	0.02
4.77	0.08	4.45	0.20	3.70	0.02
4.52	0.01	4.29	0.28	3.59	0.08
4.37	0.11	4.14	0.03	3.33	0.01
4.17	0.05	3.92	0.01	3.15	0.04
4.00	0.03	3.82	0.11	3.04	0.15
3.83	0.33	3.55	0.08	2.85	0.08
3.68	0.02	3.37	0.13	2.76	0.03
3.47	0.08	3.30	0.10	2.69	0.02
3.28	0.10	3.10	0.08	2.57	0.05
3.13	0.01	2.97	0.01	2.47	0.08
3.06	0.03	2.90	0.03	2.38	0.01
2.91	0.01	2.80	0.01	2.33	0.01
2.80	0.10	2.75	0.01	2.29	0.02
2.64	0.08	2.71	0.04	2.26	0.01
2.56	0.02	2.66	0.04	2.15	0.01
2.45	0.01	2.61	0.04	2.08	0.08
2.37	0.01	2.54	0.03	2.05	0.03
2.31	0.05	2.41	0.05	1.99	0.03
2.25	0.03	2.31	0.05	1.95	0.04
2.19	0.15	2.24	0.03	1.89	0.01
2.08	0.01	2.20	0.01	1.84	0.02
2.04	0.01	2.15	0.03		
1.99	0.01	2.07	0.05		
1.96	0.01	2.00	0.04		
1.88	0.01	1.96	0.01		
1.82	0.04	1.90	0.03		

POWDER DATA

32		33		34	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
8.27	0.15	13.56	0.08	7.37	0.28
6.89	0.37	6.93	0.04	7.03	0.02
6.51	1.00	6.08	0.27	6.51	0.20
5.61	0.88	5.91	0.15	6.24	1.00
5.36	0.03	5.53	1.00	5.72	0.20
5.14	0.88	5.11	0.27	5.54	0.38
4.62	0.32	4.88	0.41	5.32	0.02
4.50	0.15	4.73	0.01	4.73	0.33
4.21	0.20	4.55	0.55	4.55	0.20
3.93	0.07	4.05	0.03	4.37	0.03
3.85	0.03	3.70	0.11	4.19	0.47
3.75	0.03	3.58	0.08	4.01	0.05
3.51	0.10	3.44	0.11	3.88	0.05
3.43	0.03	3.29	0.10	3.76	0.05
3.34	0.09	3.14	0.11	3.66	0.11
3.27	0.09	3.08	0.03	3.37	0.20
3.16	0.15	2.97	0.27	3.25	0.11
3.06	0.05	2.88	0.11	3.15	0.15
3.00	0.05	2.76	0.08	2.96	0.08
2.90	0.02	2.69	0.05	2.75	0.05
2.81	0.15	2.65	0.02	2.71	0.08
2.70	0.07	2.59	0.01	2.64	0.05
2.63	0.02	2.51	0.11	2.56	0.11
2.57	0.05	2.41	0.01	2.47	0.02
2.49	0.03	2.37	0.05	2.39	0.01
2.42	0.01	2.31	0.04	2.28	0.03
2.38	0.02	2.26	0.05	2.21	0.03
2.32	0.05	2.20	0.08	2.17	0.03
2.25	0.03	2.14	0.11	2.12	0.05
2.18	0.03	2.08	0.01	2.06	0.03
2.11	0.10	2.04	0.05	2.00	0.02
2.07	0.01	2.00	0.07	1.94	0.01
2.03	0.03	1.96	0.08	1.92	0.01
2.00	0.02	1.92	0.05	1.85	0.03
1.92	0.07				

PARSONS, WONG, BEHER AND BAKER

35		36		37	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
11.33	0.13	9.61	0.28	14.98	0.15
8.76	0.55	7.94	0.11	13.28	0.02
7.08	0.27	7.14	0.08	8.80	0.08
6.28	0.15	6.58	0.24	7.58	0.08
5.85	0.02	6.37	0.47	6.44	0.01
5.64	0.73	6.05	0.01	5.89	1.00
4.94	0.08	5.64	1.00	5.59	0.75
4.72	0.11	5.44	0.56	5.02	0.20
4.50	1.00	5.19	0.08	4.74	0.11
4.39	0.05	4.96	0.11	4.51	0.08
4.08	0.18	4.74	0.15	4.34	0.38
3.82	0.05	4.37	0.11	4.16	0.10
3.67	0.03	4.19	0.20	3.99	0.08
3.57	0.03	4.04	0.10	3.87	0.08
3.38	0.03	3.89	0.08	3.72	0.02
3.30	0.05	3.76	0.03	3.59	0.03
3.21	0.02	3.66	0.10	3.45	0.08
3.07	0.01	3.59	0.01	3.37	0.03
2.97	0.05	3.39	0.20	3.27	0.04
2.91	0.08	3.30	0.01	3.18	0.04
2.77	0.05	3.18	0.15	3.07	0.04
2.60	0.11	3.04	0.05	2.99	0.02
2.52	0.02	2.99	0.03	2.88	0.08
2.45	0.04	2.92	0.05	2.79	0.08
2.41	0.01	2.71	0.03	2.69	0.03
2.35	0.05	2.64	0.05	2.63	0.05
2.25	0.03	2.60	0.01	2.56	0.02
2.21	0.05	2.54	0.01	2.48	0.01
2.15	0.08	2.47	0.08	2.37	0.01
2.09	0.02	2.36	0.10	2.33	0.05
2.06	0.05	2.29	0.01	2.24	0.04
		2.23	0.01	2.17	0.01
		2.19	0.01	2.12	0.01
		2.16	0.08	1.98	0.04
				1.94	0.01
				1.91	0.02

POWDER DATA

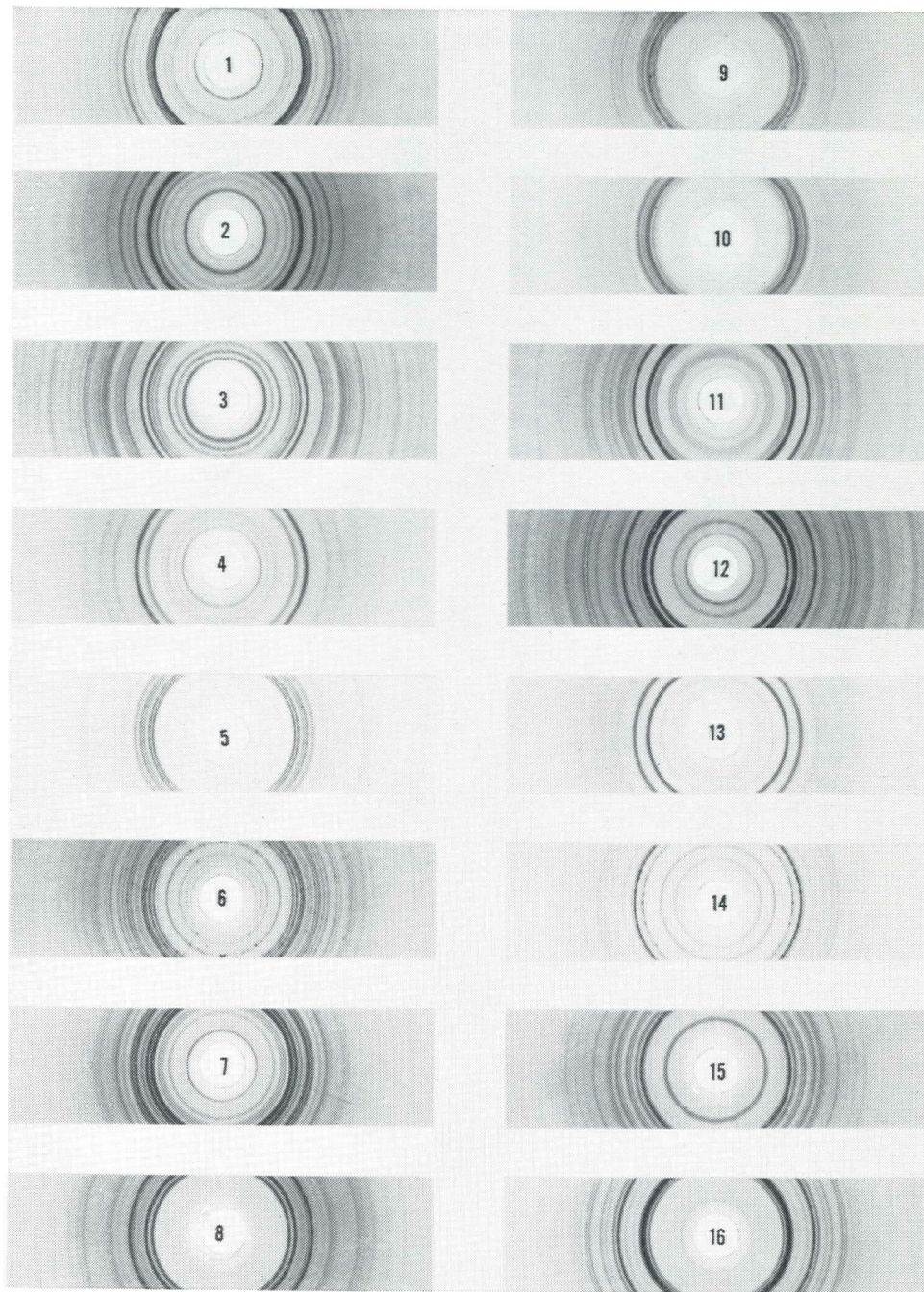
38		39		40	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
15.50	0.11	7.57	0.75	13.29	0.09
10.11	0.01	7.11	0.08	12.36	0.04
8.80	0.15	6.74	0.11	9.51	0.67
8.15	0.11	6.42	0.88	7.56	0.20
6.66	0.05	5.72	1.00	6.73	0.17
6.01	1.00	5.34	0.11	6.53	0.20
5.70	0.08	5.17	0.47	5.95	0.49
5.54	0.38	4.88	0.02	5.66	1.00
5.00	0.28	4.63	0.20	5.40	0.09
4.87	0.56	4.37	0.47	5.11	0.36
4.71	0.20	4.17	0.11	4.93	0.07
4.43	0.08	3.90	0.08	4.78	0.20
4.12	0.33	3.78	0.20	4.59	0.17
3.93	0.11	3.65	0.01	4.45	0.07
3.80	0.11	3.56	0.04	4.32	0.13
3.68	0.08	3.49	0.04	4.20	0.07
3.58	0.01	3.38	0.08	4.00	0.24
3.48	0.04	3.30	0.04	3.89	0.07
3.28	0.08	3.21	0.15	3.63	0.36
3.17	0.11	3.03	0.10	3.52	0.13
3.00	0.20	2.91	0.15	3.41	0.03
2.92	0.20	2.83	0.05	3.28	0.03
2.75	0.08	2.67	0.10	3.12	0.09
2.69	0.05	2.60	0.04	3.00	0.01
2.63	0.04	2.53	0.02	2.95	0.01
2.56	0.01	2.49	0.05	2.82	0.17
2.48	0.04	2.38	0.04	2.67	0.09
2.34	0.11	2.32	0.04	2.60	0.09
2.28	0.03	2.24	0.04	2.49	0.04
2.24	0.08	2.19	0.08	2.42	0.02
2.19	0.04	2.15	0.11	2.31	0.04
2.14	0.03	2.09	0.11	2.25	0.04
2.11	0.04	2.01	0.08	2.21	0.04
2.04	0.11	2.00	0.04	2.13	0.11
		1.91	0.08	2.07	0.07

PARSONS, WONG, BEHER AND BAKER

41		42		43	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
11.05	0.11	14.90	0.04	13.72	0.11
9.72	0.02	10.87	0.43	11.21	0.15
8.71	0.41	9.23	0.58	7.60	0.28
7.17	0.03	7.70	0.04	6.64	0.75
6.61	0.04	6.31	0.06	5.78	0.15
6.22	1.00	5.91	0.67	5.47	0.33
5.97	0.01	5.76	1.00	5.13	1.00
5.68	0.07	5.58	0.20	4.27	0.94
5.49	0.08	5.43	0.20	3.89	0.28
5.11	0.24	5.25	0.36	3.77	0.05
4.86	0.02	4.91	0.84	3.70	0.05
4.65	0.02	4.68	0.02	3.58	0.05
4.34	0.05	4.53	0.36	3.49	0.08
4.22	0.05	4.42	0.02	3.32	0.05
3.96	0.11	4.23	0.13	3.27	0.03
3.76	0.15	4.11	0.20	3.18	0.08
3.66	0.02	3.73	0.13	2.97	0.10
3.57	0.01	3.60	0.04	2.91	0.10
3.44	0.02	3.43	0.20	2.67	0.08
3.33	0.01	3.23	0.01	2.63	0.05
3.24	0.04	3.14	0.09	2.54	0.08
3.18	0.04	3.06	0.09	2.50	0.05
3.03	0.01	2.87	0.01	2.37	0.10
2.90	0.04	2.73	0.02	2.33	0.01
2.84	0.04	2.69	0.06	2.27	0.05
2.77	0.01	2.54	0.04	2.22	0.08
2.58	0.03	2.49	0.09	2.17	0.07
2.51	0.02	2.39	0.04	2.14	0.03
2.43	0.03	2.33	0.06	2.10	0.05
2.31	0.01	2.21	0.09	2.06	0.02
2.25	0.05	2.16	0.04	2.03	0.02
2.16	0.05	2.06	0.13		
2.10	0.01				
2.04	0.01				
1.97	0.01				
1.92	0.02				

POWDER DATA

44		45		46	
d,A	I/I ₁	d,A	I/I ₁	d,A	I/I ₁
9.21	0.01	8.51	0.50	9.71	0.41
7.90	0.15	7.28	0.08	9.03	0.02
6.81	0.20	6.35	0.50	7.83	0.02
6.53	0.04	6.11	0.01	6.63	0.01
6.18	0.11	5.79	0.75	6.03	0.34
5.70	1.00	5.20	0.75	5.85	0.02
5.36	0.20	4.90	0.01	5.56	0.04
5.01	0.06	4.48	1.00	4.86	0.15
4.85	0.08	4.27	0.20	4.72	0.01
4.51	0.13	4.10	0.27	4.10	1.00
4.12	0.03	3.99	0.27	3.80	0.20
4.03	0.04	3.82	0.20	3.66	0.02
3.75	0.03	3.66	0.24	3.54	0.15
3.63	0.08	3.56	0.10	3.36	0.01
3.45	0.30	3.45	0.32	3.21	0.01
3.28	0.02	3.25	0.27	3.01	0.05
3.21	0.03	3.05	0.20	2.94	0.01
3.08	0.06	2.88	0.10	2.86	0.02
2.86	0.03	2.83	0.10	2.64	0.01
2.80	0.04	2.74	0.07	2.45	0.05
2.71	0.01	2.66	0.01	2.31	0.02
2.65	0.08	2.60	0.02	2.24	0.02
2.53	0.06	2.56	0.07	2.16	0.02
2.38	0.01	2.46	0.01	2.11	0.02
2.34	0.03	2.40	0.01	2.06	0.01
2.30	0.01	2.36	0.01	1.99	0.04
2.23	0.07	2.27	0.11		
2.17	0.01	2.20	0.02		
2.11	0.03	2.08	0.20		
2.07	0.04	2.04	0.02		
2.02	0.01	1.94	0.01		
1.96	0.04	1.91	0.03		
1.88	0.04	1.88	0.01		
		1.78	0.07		



POWDER DATA

