[Contribution from the Division of Pure Chemistry of the National Research Council of Canada and the Sloan-Kettering Institute for Cancer Research]

CHARACTERISTIC GROUP FREQUENCIES IN THE INFRARED SPECTRA OF STEROIDS[1]

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The infrared absorption spectra of steroids have been studied in several laboratories, and some forty papers have been published on this subject since 1946. From comparisons of the spectra of steroids of known structure it has been found possible to relate absorption bands at certain frequencies with specific molecular structure, and these correlations are now being used extensively in the identification of steroids and related natural products.

Correlations between infrared spectra and steroid structure established prior to 1949 have been reviewed by Jones and Dobriner (26) but since that time many additional correlations have been published in the literature. In our own laboratories we have also accumulated several new characteristic steroid group frequencies which have not hitherto been reported. The object of this article is to tabulate all this material in a form convenient for easy reference.

The characteristic group frequencies are classified in the accompanying table in terms of the type of vibration involved. These vibrations are arranged under sections A–O, and within each section a sequence of diminishing frequency is followed. For most of the group vibrations references are given to papers which deal specifically with steroid spectra, but in a few cases, such as the C—H stretching vibrations, where the steroid spectra have not been studied very extensively, some more general references are included. The steroid numbering

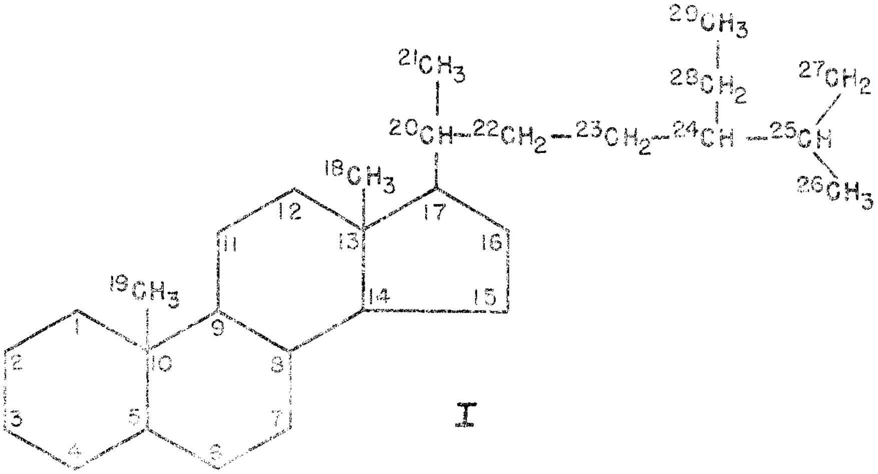

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TABLE I

Characteristic Group Frequencies in the Infrared Spectra of Steroids

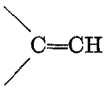
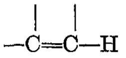
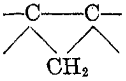
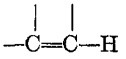
Frequency (cm.$^{-1}$)	Structure	References[a]
	A. O—H Stretching Bands	
3625–3600	Non-associated hydroxyl group.	9, 14, 15, 21, 31, 37, 39, *40*, 45
3550–2700	Associated hydroxyl group. In steroid alcohols this band usually occurs between 3550 and 3300 cm.$^{-1}$ but lower values occur occasionally, as in dimeric forms of carboxylic acids (47).	9, 14, 15, 21, 31, 37 39, 45, *47*
	B. C—H Stretching Bands	
3340–3300	$-C \equiv C-H$ group in 17-ethinyl steroids.	9, 22, 31, 32
3100–3000	Aromatic C—H bonds in steroid estrogens, benzoate esters etc.	9, 31
3085	 $C=CH_2$ group in 17-vinyl steroids.	9, 22, 31, 32
3055–3050	 $-\overset{\mid}{C}=\overset{\mid}{C}-H$ in Δ^{14}-double bond.	2, 21
3052–3030	 $-C-C-$ in 3,5-cyclosteroids.	5, 38
3040–3010	 $-\overset{\mid}{C}=\overset{\mid}{C}-H$ in six membered ring double bond systems.	2, 19
2970–2850	CH_3— and —CH_2— groups. This region has not yet been studied systematically in steroids. In aliphatic hydrocarbons methyl groups absorb at 2962 and 2872 cm.$^{-1}$ and methylene groups at 2926 and 2853 cm.$^{-1}$. The positions of these bands are changed and the intensities diminished when the methyl and methylene groups are adjacent to carbonyl groups or linked to oxygen atoms (See reference *13*).	*3*, 9, *12*, *13*, *42*
	C. O—D Stretching Bands	
2630–2620	Non-associated O—D group[b(3)].	53
2600–2400	Associated O—D group in deuterated 3-hydroxy and 17-hydroxy steroids[b(3)].	53

TABLE I—*Continued*

Frequency (cm.⁻¹)	Structure	References[a]
	D. C—D Stretching Bands	
2275 2235	—$OCOCD_3$ ester group in steroid d_3-acetates. These bands are very weak and may be confused with overtone vibrations.	25
2255 2220	CD_3—CO— group in 21-d_3-20-ketones.	25
2215 2145 2105	—CD_2—CO—CD_2— group in 2,4-d_4-3-ketones.	25
2215 2140	—CD_2—CO— group in 16-d_2-17-ketones.	25
	E. C≡C Stretching Bands	
2280–2080	This band has not been detected in 17-ethinyl steriods.	*51*, 53
	F. C═O Stretching Bands in Carbon Disulfide and Carbon Tetrachloride Solution	
1793–1786	δ-Lactone group in 20-spiro-(3′-oxa-4′-oxo-cyclopentano-)steroids (*cardanolides*)[b(2)].	53
1786–1780[c, e]	Unsaturated γ-lactone group in $\Delta^{20(22)}$-cardenolides[b(2)].	53
1781–1777	γ-Lactone group in 20-spiro-(2′-oxa-3′-oxo-cyclopentano-)steroids.	29
1770	Naphtholic 3-acetate ester.	26, 29
1769–1765	Δ^{16}-Ene-17-ol acetate ester[b(6)].	53
1767–1764	Phenolic 3-acetate and phenolic 3-propionate esters.	26, 29, 36
1764	16,16-Dibromo-17-ketone.	26
1762	21-Benzal-$\Delta^{17(20)}$-ene-20-ol acetate ester.	31
1758[d]	2-Chloro-4-bromo-3-ketone[b](1).	53
1758–1756[d]	2,4-Dibromo-3-ketone.	29, 35, 36
1758–1754[e]	21-Acetoxy-20-ketone.	26, 29, 31
1758–1754	$\Delta^{3,5}$-Diene-3-ol acetate ester.	26, 29
1758–1753	Δ^{2}-Ene-3-ol acetate ester[b(3)].	53
1758–1748	Monomeric carboxylic acid group.	*8*, *11*, 29, *47*
1757–1755[f]	Unsaturated δ-lactone group in $\Delta^{20(22)}$-cardenolides.	9
1756[e]	17aβ-Acetoxy-17-keto-D-homo steroid[b(1)].	53
1756–1749	$\Delta^{17(20)}$-Ene-20-ol acetate ester.	31, 50
1755–1752	$\Delta^{20(21)}$-Ene-20-ol acetate ester.	50
1755–1752[e]	12β-Acetoxy-11-ketone[b(2)].	53
1754	$\Delta^{3,5}$-Diene-3-ol propionate ester.	26, 37
1754–1752	Δ^{14}-17-Ketone	26, 29, 36, 37
1753–1752[e]	11β-Acetoxy-12-ketone[b(2)].	53
1753–1748[e]	11α-Acetoxy-12-ketone[b(2)].	53
1752[e]	21-Propionoxy-20-ketone[b(1)].	53
1752[e]	12α-Acetoxy-11-ketone[b(2)].	53

TABLE I—*Continued*

F. C=O Stretching Bands in Carbon Disulfide and Carbon Tetrachloride Solution—*Cont.*

Frequency (cm.$^{-1}$)	Structure	References^a
1752–1748^e	11,17-Diketone.	26, 28, 29
1749	$\Delta^{9(11)}$-Ene-11-ol acetate ester$^{b(3)}$.	53
1749	16-Ketone.	36
1749	17β-Hydroxy-16-ketone$^{b(1)}$.	53
1749	20,21-Diacetate	31
1749–1746^e	6α-Acetoxy Δ^4-3-ketone$^{b(2)}$.	53
1746	Phenolic 3-benzoate and naphtholic 3-benzoate esters$^{b(3)}$.	53
1745^e	2ξ-Carbomethoxy-Δ^4-3-ketone$^{b(1)}$.	53
1745^e	2ξ-Acetoxy-Δ^4-3-ketone$^{b(1)}$.	53
1745–1743^e	6β-Acetoxy-Δ^4-3-ketone$^{b(4)}$.	53
1745–1741	17-Ketone.	26, 29, 36, 37
1744–1742	δ-Lactone group in 4-oxa-3-ketones$^{b(4)}$.	53
1743	δ-Lactone group in 16-oxo-17-oxa-D-homo steroids$^{b(3)}$.	53
1742	δ-Lactone group in 17-oxo-17a-oxa-D-homo steroids.	29
1742–1736^e	17β-Acetoxy-20-ketone.	31
1742	2-Bromo-2-chloro-3-ketone$^{b(1)}$.	53
1742–1739	Methyl esters of cholanic, norcholanic and bisnorcholanic acids.	29, 36, 37
1742–1739^e	12-Ketoetiocholanic acid methyl ester.	26, 29
1742–1737	17-Acetate ester.	26, 29, 36, 37
1742–1737	17-Propionate ester.	26, 29
1739–1736	17α-Hydroxy-20 ξ-acetate ester.	31
1739–1735	Methyl esters of etiocholanic and etioallocholanic acids.	29
1739–1735	3-Propionate ester.	29
1739–1735	17-Hexahydrobenzoate ester.	29
1739–1733	3-Acetate ester.	29, 36, 37
1738^d	2-Chloro-3-ketone$^{b(1)}$.	53
1737^e	17aα-Acetoxy-17-keto-D-homo steroid$^{b(2)}$.	53
1737–1735	2,2-Dibromo-3-ketone.	26, 29, 35, 36
1736^e	17α-Acetoxy-20-ketone$^{b(2)}$.	53
1736^e	4-Carbomethoxy-Δ^4-3-ketone$^{b(1)}$.	53
1736–1733	20-Acetate ester.	26, 29, 31
1736–1724^f	21-Acetoxy-20-ketone.	26, 29
1735	11α-Bromo-12-ketone.	35
1735–1733^d	2-Bromo-3-ketone.	26, 29, 35, 36
1735–1733^d	4-Bromo-3-ketone.	26, 29, 35, 36
1730^f	21-Propionoxy-20-ketone$^{b(1)}$.	53
1730–1727^f	12β-Acetoxy-11-ketone$^{b(2)}$.	53
1730–1726^f	11α-Acetoxy-12-ketone$^{b(2)}$.	53
1729^f	17aβ-Acetoxy-17-keto-D-homo steroid$^{b(1)}$.	53
1729–1725	3-Formate ester.	31
1726	11,12-Diketone	26, 28, 29
1724^d	2-Iodo-3-ketone.	35, 36
1724–1717	3-, and 17-Benzoate esters.	26, 29
1723^f	12-Ketoetiocholanic acid methyl ester.	26, 28, 29

TABLE I—*Continued*

Frequency (cm.$^{-1}$)	Structure	References[a]
F. C=O Stretching Bands in Carbon Disulfide and Carbon Tetrachloride Solution—*Cont.*		
1723–1718	3,6-Diketone.	28, 29
1722	25-Ketone[b(1)].	53
1722	5-Methyl-3,6-diketone[b(1)].	53
1720[f]	12α-Acetoxy-11-ketone[b(2)].	53
1720–1710[f]	11β-Acetoxy-12-ketone[b(2)].	53
1719[f]	17α-Acetoxy-20-ketone[b(2)].	53
1719	17α-Hydroxy-bisnorcholanic acid methyl ester.	31
1719–1713	3-Ketone.	26, 29, 36, 37
1719–1713[f]	11,17-Diketone.	26, 28, 29
1719–1713	7-Ketone.	26, 28, 29, 36, 37
1718	20β-Hydroxy-12α-acetate ester.	31
1718	10-Aldehyde[b(1)].	53
1717[e]	Δ^{16}-12,20-diketone.	41
1717–1716	24-Ketone[b(2)].	53
1716[f]	17aα-Acetoxy-17-keto-D-homo steroid[b(2)].	53
1716	Δ^{15}-17-Ketone.	26, 29, 36, 37
1716[f]	17β-Acetoxy-20-ketone.	31
1714–1713	6-Ketone of allo series.	29
1714–1709	12α-Bromo-11-ketone.	35
1713–1711	3,9-Epoxy-11-ketone.	28, 48
1712–1706	12-Ketone.	26, 28, 29, 36
1712	4-Ketone[b(1)].	53
1710–1707[e]	17α- and 17β-hydroxy-20-ketones.	31
1710–1706	20-Ketone.	26, 29, 31, 36, 37
1710–1704	11-Ketone.	28, 36, 48
1710–1700	Dimeric carboxylic acid group.	*8*, *11*, 26, 29, *47*
1708	17a-Keto-D-homo steroid[b(3)].	53
1708–1706	6-Ketone of normal series.	29
1707–1704	22-Ketone.	48
1706	11β-Bromo-12-ketone.	35
1706–1704	12β-Hydroxy-11-ketone.	48
1705	17α-Bromo-20-ketone.	31, 35
1705–1703	$\Delta^{8(14)}$-15-ketone[b(1)].	53
1702[d]	2,4-Dibromo-Δ^{1}-3-ketone[b(1)].	53
1700[f]	2ξ-Acetoxy-Δ^{4}-3-ketone[b(1)].	53
1697	2-Bromo-Δ^{1}-3-ketone.	26, 29
1697[d]	2-Bromo-Δ^{4}-3-ketone.	26, 29, 36
1697–1690[f]	17α- and 17β-Hydroxy-20-ketone.	31
1695–1689	3,5-Cyclo-6-ketone (*i-steroid 6-ketone*).	39, 53
1692	Δ^{4}-3,6-Diketone.	29, 53
1688[f]	6β-Acetoxy-Δ^{4}-3-ketone[b(4)].	53
1686–1685[f]	6α-Acetoxy-Δ^{4}-3-ketone[b(2)].	53
1686–1681[d]	2-Iodo-Δ^{4}-3-ketone[b(1)].	53
1685	16,17-Methylene-20-ketone.	31
1685	6ξ-Bromo-Δ^{4}-3-ketone[b(1)].	53
1684	21-Benzal-20-ketone.	26
1684–1680	Δ^{1}-3-Ketone.	26, 29, 32

TABLE I—*Continued*

Frequency (cm.$^{-1}$)	Structure	References[a]
F. C=O Stretching Bands in Carbon Disulfide and Carbon Tetrachloride Solution—*Cont.*		
1684–1680	$\Delta^{9(11)}$-12-Ketone.	26, 28, 29, 32
1682–1674	Δ^{5}-7-Ketone[b].	48, 53
1681–1677	Δ^{4}-3-Ketone.	26, 29, 36, 37
1678[f]	Δ^{16}-12,20-Diketone.	41
1678[f]	2ξ-Carbomethoxy-Δ^{4}-3-ketone[b(1)].	53
1678[f]	4-Carbomethoxy-Δ^{4}-3-ketone[b(1)].	53
1671–1663	$\Delta^{1,4}$-Diene-3-ketone.	26, 29, 32, 36
1670–1666	Δ^{16}-20-ketone.	26, 29, 32, 37
1669–1666	$\Delta^{4,6}$-Diene-3-ketone.	26, 29, 32, 36
1667	Δ^{8}-7-Ketone[b(1)].	53
1667	4-Aza-3-ketone[b(1)].	53
1666	2-Bromo-$\Delta^{1,4}$-diene-3-ketone[b(1)].	53
1663	$\Delta^{3,5}$-Diene-7-ketone.	26, 28, 29
1660	$\Delta^{8(9)}$-11-Ketone[b(1)].	53
1658	N-Acetyl-4-aza steroid[b(1)].	53
G. C=O Stretching Bands in Chloroform Solution		
1790[c, e]	Unsaturated γ-lactone group in $\Delta^{20(22)}$-cardenolides[b(3)].	53
1790[c, e]	Unsaturated γ-lactone group in $\Delta^{16,20(22)}$-cardadienolide[b(1)].	53
1762	Naphtholic 3-acetate ester[b(1)].	53
1753	Phenolic 3-acetate ester[b(1)].	53
1752[d]	2,4-Dibromo-3-ketone[b(3)].	53
1750–1747[f]	Unsaturated γ-lactone group in $\Delta^{20(22)}$-cardenolides.	9
1750–1745[e]	21-Acetoxy-20-ketone.	31
1748	Unsaturated γ-lactone group of $\Delta^{16,20(22)}$-cardadienolide[b(1)].	53
1742	17β-Hydroxy-16-ketone[b(2)].	53
1742–1738[e]	11,17-Diketone[b(4)].	53
1739–1736	20,21-Diacetate.	31
1737–1733	17-Ketone.	37
1733–1730[e]	17β-Acetoxy-20-ketone[b(1)].	53
1732–1728	Methyl esters of cholanic, norcholanic, bisnorcholanic, etiocholanic, and etioallocholanic acids.	37
1732–1725	2,2-Dibromo-3-ketone[b(8)].	53
1729[d]	4-Bromo-3-ketone[b(1)].	53
1728–1726	17β-Propionate ester[b(2)].	53
1728–1719	3-Acetate[b(15)] and 3-propionate[b(2)] esters.	53
1727–1720[f]	21-Acetoxy-20-ketone.	31
1725–1722[d]	2-Bromo-3-ketone[b(3)].	53
1722–1720	17β-Acetate ester[b(3)].	53
1722–1719	20-Acetate ester.	31
1722–1716	21-Bromo-20-ketone.	31, 35
1720	17α-Acetate ester[b(1)].	53
1719	Diunsaturated δ-lactone group in $\Delta^{20,22}$-bufadienolides[b(3)].	53

TABLE I—*Continued*

Frequency (cm.^{-1})	Structure	References[a]
	G. C=O Stretching Bands in Chloroform Solution—*Cont.*	
1714[f]	17β-Acetoxy-20-ketone[b(1)].	53
1713–1710	3-Benzoate and 17-benzoate esters[b(6)].	53
1711	25-Ketone.	48
1711–1707[f]	11,17-Diketone[b(6)].	53
1710–1700[e]	17α-Hydroxy-20-ketone.	31
1709–1700	3-Ketone.	31
1709	24-Ketone.	48
1707	7-Ketone.	48
1707–1698	20-Ketone.	31, 37
1705–1698	11-Ketone.	31, 48
1705–1698	12-Ketone.	48, 53
1700	22-Ketone.	48
1688–1685[f]	17α-Hydroxy-20-ketone.	31
1685	2-Bromo-Δ^{1}-3-ketone[b(2)].	53
1685–1680[d]	2-Bromo-Δ^{4}-3-ketone[b(3)].	53
1676–1671	$\Delta^{9(11)}$-12-Ketone[b(1)].	53
1675	6ξ-Bromo-Δ^{4}-3-ketone[b(1)].	53
1672–1670	Δ^{1}-3-Ketone.	31
1669–1666	Δ^{5}-7-Ketone[b(3)].	53
1668–1660	Δ^{4}-3-Ketone.	31
1666–1660	$\Delta^{1,4}$-Diene-3-ketone[b(4)].	53
1662–1652	Δ^{16}-20-Ketone.	31
1656	2-Bromo-$\Delta^{1,4}$-diene-3-ketone[b(1)].	53
	H. C=C Stretching Bands[g]	
1672–1667	Δ^{5}	2, 14, 26, 32
1672–1664	Δ^{7}	2, 32
1671–1670[e]	$\Delta^{3,5}$-Diene-3-ol acetate and propionate esters.	26, 32
1666–1664	Δ^{22}[b(2)].	53
1660	Δ^{20}-Ene-20-ol acetate ester.	50
1657	Δ^{4}	2
1657–1654	Δ^{2}	19, 26, 32
1648–1646	Δ^{14}	2, 21, 26, 32
1648–1644	$\Delta^{9(11)}$	2, 53
1647	Δ^{3}	19
1644	Δ^{1}	19
1639[f]	$\Delta^{3,5}$-Diene-3-ol acetate and propionate esters.	26, 32
1639–1633	Δ^{6}	19
1638–1636[e]	Diunsaturated δ-lactone group in $\Delta^{20,22}$-bufadienolides[b(3)].	53
1630–1621	Δ^{16}	26, 32
1628–1620	Δ^{11}	19, 26, 32
1627[e]	$\Delta^{3,5}$-Diene-7-ketone.	26, 32
1625[h]	Aromatic ring in equilenin and related compounds.	32
1624–1619	Unsaturated γ-lactone group in $\Delta^{20(22)}$-cardenolides[b(3)].	53

TABLE I—*Continued*

Frequency (cm.$^{-1}$)	Structure	References[a]
	H. C═C Stretching Bands[g]—*Cont.*	
1621[e]	$\Delta^{1,4}$-Diene-3-ketone.	26, 32
1619–1616[e]	$\Delta^{4,6}$-Diene-3-ketone.	32
1619–1613	Δ^{4}-3-Ketone.	14, 16, 26, 32
1618[e]	$\Delta^{3,5}$-Diene.	26, 32
1613–1611[h]	Aromatic ring system in estrone and related compounds.	15, 32
1609–1604	Δ^{1}-3-Ketone.	26, 32
1607	$\Delta^{9(11)}$-12-ketone.	32
1606–1603[f]	$\Delta^{1,4}$-Diene-3-ketone.	26, 32
1605[i]	Aromatic ring system in equilenin and related compounds.	32
1604–1603[e]	Aromatic ring system in benzoate esters.	32
1602[f]	Diunsaturated δ-lactone group in $\Delta^{20,22}$-bufadienolides[b(2)].	53
1598[f]	$\Delta^{3,5}$-Diene-7-ketone.	26, 32
1592–1587	Δ^{16}-20-ketone.	16, 26, 31, 32
1590–1589[i]	Aromatic ring system in estrone and related compounds.	32
1587[f]	$\Delta^{4,6}$-Diene-3-ketone.	32
1586–1584[f]	Aromatic ring system of benzoate esters.	32
1578[f]	$\Delta^{3,5}$-Diene.	26, 32
1573[i]	Aromatic ring system in equilenin and related compounds.	32
1503–1490[i, k]	Aromatic ring system in estrone and related compounds.	15, 24
	I. C—H Scissoring Bands of Methylene Groups[l]	
1475–1464	Weak band attributed tentatively in unperturbed cyclic methylene groups.	24
1470–1462	Strong band in unperturbed linear side chain methylene groups.	24
1464–1446	Strong band in unperturbed cyclic methylene groups.[m]	24
1445–1432	—CH_2—C═C—. The intensity of this band depends on the location of the double bond; it is very weak in Δ^{7} and Δ^{14} steroids.	24
1440–1430	Unassigned band in some, but not all acetate esters.	24
1438–1426	4-, 6-, 7-, 11-, and 12-Ketosteroids having an unsubstituted methylene group adjacent to the carbonyl group.	24, 25
1426–1415	3-Ketosteroids having an unsubstituted methylene group at C_2 or C_4. If both C_2 and C_4 are unsubstituted the band usually shows asymmetry with an inflection on the high frequency side.[n]	24, 25
1415–1412	C_{21}-Methylene group in 21-acetoxy-20-ketones.	24
1410	C_{21}-Methylene group in 21-hydroxy-20-ketones[b(1)].	53
1410–1404	17-Ketosteroids having an unsubstituted methylene group at C_{16}.	1, 24, 25

TABLE I—*Continued*

J. C—H Bending Bands of Methyl Groups

Frequency (cm.$^{-1}$)	Structure	References[a]
1465–1455	Unsymmetrical methyl bending vibration. In steroids this band is usually masked by stronger methylene absorption.	*13*, *42*, *46*
1440–1435[e]	Carbomethoxy ester	24
1392–1374	Angular methyl group (C_{19}?).	24
1386–1374	Side chain methyl groups at C_{21}, C_{26}, C_{27}, C_{28}, and C_{29}.	24
1383–1372	Angular methyl group (C_{18}?).	24
1382–1369[e]	Acetate methyl group in 3-, 12-, 17- and 20-acyl acetates and 3-phenolic acetates.	24, 25
1374–1360	Terminal gem dimethyl group in C_{27}, C_{28}, and C_{29} steroids.	24
1370–1360[f]	Acetate methyl group in 3- and 17-acetates.	24, 25
1365–1356[f]	Carbomethoxy ester.	24
1359–1356	C_{21}-Methyl group in 20-ketosteroids.	24, 25

K. Characteristic Bands in Steroid Esters and Ethers, Tentatively Assigned to C—O Stretching Vibrations

Frequency (cm.$^{-1}$)	Structure	References[a]
1270	3-Benzoate and 17-benzoate esters.	30
1257 1243–1241 1224–1221 1212–1206	Three or four strong bands in 3-benzoate esters of estrone, equilenin and related compounds with phenolic or naphtholic 3-hydroxyl group.	30
1257 1243 1236	Three strong bands in 4α-acetoxy allo steroids.	18
1256 1251	Two strong bands in 12α-acetoxy-20β-hydroxy steroids.	31
1256–1255 1247–1243 1235–1229	Three strong bands in Δ^5-3α-acetoxy steroids.	18, 20
1256–1234	Two or three strong bands in this region in 2-acetoxy and 3-acetoxy steroids in which the acetate group is in axial conformation to the A ring. *viz.* 2α-acetoxy[g] and 3β-acetoxy normal steroids, 2β-acetoxy and 3α-acetoxy allo steroids and 3β-acetoxy-5α, 10α-steroids (*lumistanols*).	4, 6, 7, 10, 18, 30
1250–1245 1243–1230 1230–1221	Two or three bands in 2ξ,3ξ-Diacetate esters of steroid sapogenins[b](7).	53
1247 1236	Two strong bands in 4β-acetoxy allo steroids.	18
1245–1232	7-Acetate and 20-acetate esters.	30

TABLE I—*Continued*

Frequency (cm.$^{-1}$)	Structure	References[a]
K. Characteristic Bands in Steroid Esters and Ethers, Tentatively Assigned to C—O Stretching Vibrations—*Cont.*		
1244–1238[e]	17β-Acetate ester (*strong band*).	30
1242	17α-Acetate ester[b(2)]	53
1242–1240	12α-Acetate ester	30, 31
1242–1236	A single strong band in 2-acetoxy and 3-acetoxy steroids in which the acetate group is in equatorial conformation to the A ring. *viz.* 2β-acetoxy[o] and 3α-acetoxy normal steroids, 2α-acetoxy and 3β-acetoxy allo steroids and Δ^{5}-3β-acetoxy steroids.	4, 6, 7, 10, 18, 20, 30
1235–1232	12β-Acetate ester.	30
1230–1228	21-Acetoxy-20-ketone.	26, 30
1225–1223	$\Delta^{20(21)}$-Ene-20-ol acetate ester.	50
1225–1219	$\Delta^{17(20)}$-Ene-20-ol acetate ester.	30, 50
1225–1215[f]	17β-Acetate ester (*weak band*).	30
1218–1217[e]	Δ^{2}-Ene-3-ol acetate ester[b(3)].	53
1212–1206	One or two bands in $\Delta^{3,5}$-diene-3-ol-acetate ester[b(3)].	53
1206–1204[e]	Δ^{16}-Ene-17-ol acetate ester[b(6)].	53
1206–1202	Phenolic and naphtholic 3-acetate esters.	30
1190–1189[h]	3-, 7-, 12-, 17-, and 20-*p*-toluenesulfonate esters[b(13)].	53
1190–1188	3-Propionate ester.	30
1180–1178[i]	3-, 7-, 12-, 17-, and 20-*p*-toluenesulfonate esters[b].	30
1180–1175	3-Formate ester.	30
1179–1178	3-, 7-, 12-, and 17-methanesulfonate esters[b(13)].	53
1173–1168	Methyl esters of cholanic acids[b(20)].	53
1166–1163[e]	3-Methoxy derivatives of estrone[b(4)].	53
1164–1162	Methyl esters of bisnorcholanic acid[b(10)].	53
1163–1160	3-Methoxy derivatives of equilenin[b(3)].	53
1160–1155	Methyl esters of etioallocholanic acid[b(10)].	53
1159–1158[f]	Δ^{2}-Ene-3-ol acetate ester[b(3)].	53
1156–1154[f]	3-Methoxy derivatives of estrone[b(4)].	53
1123–1122[e]	$\Delta^{3,5}$-Diene-3-ol acetate ester[b(3)].	53
1112–1109[f]	$\Delta^{3,5}$-Diene-3-ol acetate ester[b(3)].	53
1103	3-Methoxy steroid.	39
1102–1100	16-Methoxy steroid[b(4)].	53
1099–1097[j]	3-, 7-, 12-, 17-, and 20-*p*-toluenesulfonate esters[b].	30
1099–1098	6-Methoxy-3-5-cyclo-steroid.	39
1098–1096[f]	Δ^{16}-Ene-17-ol acetate ester[b(6)].	53
1050–1000	At least one strong band occurs in this region in the spectra of most steroid acetates, but these have not yet been systematically studied.	53
L. Characteristic Bands in Steroid Alcohols, Tentatively Assigned to C—O Stretching Vibrations		
1060–1000	At least one strong band occurs in this region in the spectra of most hydroxy steroids but these have only been studied systematically for the 3-hydroxy compounds.	53

TABLE I—*Continued*

Frequency (cm.$^{-1}$)	Structure	References^a
	L. Charactistic Bands in Steroid Alcohols, Tentatively Assigned to C—O Stretching Vibrations—*Cont.*	
1052–1050	Δ^{5}-3β-Hydroxy steroid.	6, 7
1044–1037	3α-Hydroxy normal steroid.	6, 7, 45
1040–1037	3β-Hydroxy allo steroid.	6, 7, 45
1036–1032	3β-Hydroxy normal steroid.	6, 7
1034	3α-Hydroxy-5α,10α-steroid (*epilumistanol*).	4
1010	3β-Hydroxy-5α,10α-steroid (*lumistanol*).	4
1002–996	3α-Hydroxy allo steroid.	6, 7, 45
	M. Characteristic Bands in Unsaturated Steroids	
974–970	*trans* Δ^{22}-*steroid.*	9, 22, 23, 43, 49
840 800	Δ^{5}-Steroid.	2, 9, 14, 16
830^p 800	3β-Acetoxy-Δ^{7}-steroid.	20
828–821^p	$\Delta^{9(11)}$-Steroid.	20
825–822^p 810–808 801–800	Δ^{14}-Steroid.	20
821 800	3β-Chloro-Δ^{5}-steroid.	20
814–812 803–797	3β-Acetoxy-Δ^{5}-steroid.	9, 20
808–806 801–799	3β-Hydroxy-Δ^{5}-steroid	20
774–772 663	Δ^{2}-Steroid.	19, 53
773 671	Δ^{3}-Steroid.	19
772–771 739 729 710–704	Δ^{6}-Steroid.	19
754–742	Δ^{1}-Steroid.	19

TABLE I—*Continued*

Frequency (cm.$^{-1}$)	Structure	References[a]
N. Characteristic Bands in the Spectra of Ketosteroids; not Yet Assigned to Specific Group Vibrations.[q]		
1354–1353 1337–1335 1267–1264[r] 1250–1247[r] 1223–1219 1173–1167 1150–1146 1104–1100 829– 824 767– 764	3-Ketone of normal series.	27
1272–1271[r] 1252–1248[r] 1228–1226[r] 1176–1168 1154–1150 1127–1125 1122–1116 812– 804 760– 753	3-Ketone of allo series.	27
1272–1268 1258–1256 1166–1160 936– 934 820– 816 779– 777[r]	Δ^1-3-Ketone of allo series.	27
1332–1328 1271–1268[r] 1233–1226[r] 1194–1187[r] 958– 956 950– 940 867– 862[r] 777– 772 684– 674	Δ^4-3-Ketone.	27
1290–1289 1245–1241 932– 927 888– 887[r] 816– 814 807– 805 702– 701 687– 683	$\Delta^{1,4}$-Diene-3-ketone.	27

TABLE I—*Continued*

Frequency (cm.$^{-1}$)	Structure	References[a]
N. Characteristic Bands in the Spectra of Ketosteroids; not Yet Assigned to Specific Group Vibrations.[q]—*Cont.*		
1326–1324 1268–1264[r] 1228–1222[r] 1199–1198 967– 965 948– 945 875– 874[r] 779– 771 752	$\Delta^{4,6}$-Diene-3-ketone.	27
1318 1294 1238–1236[s] 1189–1184 1037–1035[s] 988– 987 958– 955[r] 939– 935[r] 921– 919[r] 905– 903[r] 869– 866 825– 818 813– 812 700– 698	3β-Acetoxy-Δ^{5}-7-ketone.	27
1257–1254 1245–1243 1171–1167 1101–1088 1051–1049[r] 1016–1005[r] 830– 825 823– 818 708– 704	17-Ketone of normal series.	27
1208–1200 1170–1162 1130–1117 1106–1100 1058–1047[r] 1012–1009[r] 831– 828 824– 818 712– 709	17-Ketone of allo series.	27

TABLE I—*Concluded*

Frequency (cm.$^{-1}$)	Structure	References[a]
N. Characteristic Bands in the Spectra of Ketosteroids; not Yet Assigned to Specific Group Vibrations.[q]—*Cont.*		
1289 1236–1234^r 1219^r 1195–1191 1176–1173^r 1155–1154^r	20-Ketone of normal series.	27
1292–1289 1232–1231^r 1213–1208^r 1184–1177 1156–1152^r 1075–1070 964– 951	20-Ketone of allo series.	27
O. Other Miscellaneous Bands		
1330–1322 1209–1197 897– 891 863– 859	6-Methoxy-3,5-cyclosteroids.	39
1255–1240	Phenolic 3-hydroxyl group.	15
1240–1237 1180–1173 1054–1048 981– 976 920– 916 899– 897	22a-Spirostan and derivatives (Iso-sapogenins).	10, 33, 34
1225–1220 1175–1168 1068–1064 1052–1046 987– 984 920– 915 899– 894	22b-Spirostan and derivatives (Normal sapogenins).	10, 33, 34
	(Both normal and iso-sapogenins contain several other weaker bands between 1350 and 800 cm.$^{-1}$ also characteristic of the spirostan cyclic acetal structure. In the normal compounds the 920–915 cm.$^{-1}$ band is more intense than the 899–894 cm.$^{-1}$ band while in the iso-sapogenins the 899–897 cm.$^{-1}$ band is more intense than the 920–916 cm.$^{-1}$ band.)	
1155–1145	Estrone and derivatives.	15
885– 875	Estrone, equilin and equilenin derivatives.	15
708– 703	Benzoate ester[b(5)].	53

[a] References to general papers which do not deal specifically with steroid spectra are *italicized*.

[b] New correlation based on observations in our laboratories. Figures in parentheses indicate the number of compounds examined.

[c] This band is anomalous in suggesting that two bands are associated with one carbonyl group.

[d] The position of this band is dependent on the stereochemical relationship between the C=O and C—Halogen bonds (see reference 35).

[e] The upper of two bands characterizing the group.

[f] The lower of two bands characterizing the group.

[g] These bands are most conveniently studied in chloroform solution.

[h] The upper of three bands characterizing the group.

[i] The middle of three bands characterizing the group.

[j] The lower of three bands characterizing the group.

[k] This band is obscured in chloroform solution and is best observed in carbon tetrachloride.

[l] These bands are most conveniently studied in carbon tetrachloride solution.

[m] This band may be modified in shape by contributions from methyl group absorptions in the same frequency range (see Section J of Table).

[n] This band has recently been resolved into two separate components under high resolution. It is presumed that the C_2 and C_4 methylene groups are each responsible for one of the bands.

[o] This characteristic group frequency has not yet been established experimentally but it is inferred by analogy with the known behavior of the 3-acetoxy steroids of related stereochemical conformation.

[p] This correlation is reported by the author of reference 20 as tentative only.

[q] These correlations have been established recently for simple steroids containing not more than two functional groups. The nature of the vibrations involved in these bands is not yet understood and the band specificity in more highly substituted steroids remains to be evaluated. There is evidence that some of these bands may be disturbed appreciably on the introduction of unsaturated linkages or other carbonyl groups, particularly if these substituents modify the degree of ring strain. In reference 27 are included additional weak bands not given in this Table.

[r] These bands are the more prominent and of principal importance for the characterization of the group.

[s] Acetate bands, see Section K.

system (I) and the nomenclature conform with the recommendations of the Ciba conference (52).

The band positions given in the table are for measurements made on solutions. Most investigators have worked with solutions but a few papers have appeared dealing with structure correlations based on measurements made in the solid state (14–17, 43, 44). The group frequencies reported for solid state spectra may differ from those based on measurements made in solution, particularly where vibrations involving hydroxy groups and carbonyl groups are involved. The solvents commonly employed are carbon disulfide, carbon tetrachloride, and chloroform and in most regions of the spectrum the band positions are not solvent sensitive. The carbonyl stretching vibrations however, although essentially the same in carbon tetrachloride and carbon disulfide are displaced to lower frequencies in chloroform and these are listed respectively in Sections F and G Data for carbonyl band positions in other solvents are meagre at present.

The frequency ranges given for some of the bands in the accompanying table may differ by a few wave numbers from those reported in earlier publications from these laboratories. Where such differences occur it may be inferred that the values given in this publication have been revised as a consequence of more recent information.

The infrared spectra of three hundred steroids have been published recently in atlas form (9) and the introductory section of that atlas contains a more general account of the steroid structure correlations than is given here.

CONCLUDING REMARKS

The characteristic group frequencies summarized above are too numerous for individual commentary in an article of this scope. The majority have been described previously and adequate cross-references are provided to the earlier publications. New correlations, reported here for the first time are identified by a superscript *b* in the table, followed in parentheses by the number of compounds examined. It is anticipated that more detailed and critical evaluations of these will be published at a later date.

It must be emphasized that the various group frequencies listed in this paper are not all of equally well established validity; while some are based on measurements of large numbers of compounds, others are derived from studies of one or two compounds only. This table is to be regarded primarily as a literature summary, and the original publications should be consulted whenever possible.

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SUMMARY

Four hundred and sixty infrared absorption bands characteristic of specific molecular structure in steroids are summarized in tabular form. The table includes about one hundred characteristic group frequencies identified recently in our laboratories but not previously reported.

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