AN INDEX OF PUBLISHED INFRA-RED SPECTRA

Volume I

MINISTRY OF AVIATION

AN INDEX OF PUBLISHED INFRA-RED SPECTRA

Edited by
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Technical Information and
Library Services

VOL. I

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F O R E W O R D

Every practising infra-red spectroscopist needs to have available to him an extensive library of infra-red spectra. These are required both for comparative purposes in the identification of unknowns and for many different research applications. He also requires to know whether or not the spectrum of some particular product he is studying has appeared previously in the literature. These needs are met in part by the individual collections of spectra which every spectroscopist maintains, and many of us supplement these by the purchase of commercial collections of spectra such as those of Sadtler or of D.M.S. In the sterol field there are also atlases available which are very useful. Nevertheless it remains true that very large numbers of spectra appear in the literature which are not available elsewhere and it is becoming increasingly difficult for any individual to keep track of more than a very small proportion of them. This is particularly the case now that so many spectra are appearing in publications on pure organic chemistry as well as in papers more directly devoted to spectroscopy.

Some years ago a collaborative group consisting of infra-red spectroscopists in the British Government Defence Departments (Ministry of Aviation and the War Office) and the U.K. Atomic Energy Authority was set up to examine this and other common problems. As a direct result the group determined to produce, primarily for their own benefit, a "Beilstein" type of index of spectra which would enable any given spectrum to be traced in the literature. This would list under a formula index all the infra-red spectra available and would also give the state in which the sample was studied, the wavelength range covered, and include an indication of the optical system employed so that some estimate of the resolving power available could be made. The present two volumes, containing nearly 10,000 references, are the first fruits of this project. These include most of the spectra published up to 1957, although some gaps remain. These gaps will be filled, and data from 1957 onwards will be included in a third volume which is now in active preparation. It seemed to us that this index was likely to have a very much wider application than the limited internal use for which it was originally designed, and we have accordingly persuaded Her Majesty's Stationery Office to issue copies for sale. This has been done on my personal assurance that sufficient copies are likely to be sold to enable them to recover at least the production costs, and I hope that libraries will support this venture so that the index can go forward on a comprehensive basis with further volumes being issued from time to time.

In fairness to the many contributors to these volumes I should state that my own part in all this has been limited to the initiation of the project, and to uttering loud cries of encouragement from time to time. All the real work has been done by the faithful band whose names are listed on the following page. A particular debt is due to Mrs. M.B.B. Thomas, of the Ministry of Aviation, Technical Information and Library Services, who with some assistance from Mr. E.R. Adams has been responsible for the whole of the editorial work.

The index which follows is largely self explanatory but a few points need to be mentioned. (1) The ranges covered are expressed in either wavelengths or wavenumbers as in the original paper. The requirements for the inclusion of a spectrum have simply been that either a fairly extensive range should have been covered at normal rock-salt resolution, or a more limited range at higher resolution. (2) The state in which the sample was studied is indicated by the abbreviations: g. (gas), l. (liquid), s. (solid), soln (solution). (3) Compounds with the same formulae are listed alphabetically under this. (4) Where a number of references to a single compound are given the arrangement is chronological. The division within any single year is alphabetical by journals. (5) Inorganic compounds are listed separately in Pt. II.

It has also been necessary to make some provision for those spectra which relate to organic compounds of unknown composition which cannot adequately be described by formulae. These are listed separately in alphabetical order by name in Pt. I(b).

Although this index is still incomplete we have decided to issue the first parts at this stage, partly because even an incomplete index including nearly 10,000 references is worth having, and partly because the period beyond 1957 is already covered to a limited extent by the detailed formula indices which are included in the volumes of "Spectrographic Abstracts" which have been produced by the same group and are also printed by H.M.S.O. It is in any case hoped that the third volume will not be overlong in preparation.

L.J. BELLAMY

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P A R T I (a)

O R G A N I C C O M P O U N D S

M O L E C U L A R F O R M U L A I N D E X

(C - C_9; C_{10} onwards is contained in Vol.II)

Elements are arranged in the order: C, H, D, O, N, Cl, Br, I, F, S, P.
The remaining symbols are placed alphabetically.

C O N T E N T S

Reference	State	Range	Optics	Remarks
$CHDO_2$				
FORMIC ACID-d_1				
J.Chem.Phys.,1938,6,540	g.	10,000-650cm^{-1}	-	
J.Chem.Phys.,1940,8,447	g.	10,000-600cm^{-1}	-	30 & 160°C
FORMIC ACID-d_1 (H.COOD)				
Phys.Rev.,1940,58,208	g.	3000-2200cm^{-1}	-	
FORMIC ACID-d_1 (D.COOH)				
Phys.Rev.,1940,58,208	g.	3000-2200cm^{-1}	-	
$(CHDO_2)_2$				
FORMIC ACID-d_1, DIMER				
J.Chem.Phys.,1938,6,540	g.	10,000-650cm^{-1}	-	
CHD_3				
METHANE-d_3				
J.Chem.Phys.,1937,5,1	g.	3000-1000cm^{-1}	NaCl	
Trans.Faraday Soc.,1956,52(10),1304	g.	3-15μ	grating	high resolution 7200 & 2400 lines/in.
Canad.J.Chem.,1957,35(3),226	g.	4-11μ	LiF, NaCl	
CHD_3O				
METHANOL-d_3				
J.Chem.Phys.,1942,10,693	g.	4000-750cm^{-1}	NaCl, CaF_2, KBr	
J.Chem.Phys.,1943,11,97	-	3000-500cm^{-1}	-	
CHOF				
FORMYL FLUORIDE				
J.Chem.Phys.,1956,25(2),337	g.	2-25μ	NaCl, KBr	
" " " " " "	s.	2-25μ	NaCl, KBr	

Reference	State	Range	Optics	Remarks
CHO_2K				
POTASSIUM FORMATE				
Ann.Phys.,1942,17,5	s.	1600-600cm^{-1}	-	
CHO_2Li				
LITHIUM FORMATE				
Ann.Phys.,1942,17,5	s.	1600-600cm^{-1}	-	
CHO_2Na				
SODIUM FORMATE				
Ann.Phys.,1942,17,5	s.	1600-600cm^{-1}	-	
J.Chem.Phys.,1952,20(10),1663	s.	3400-750cm^{-1}	-	polarized light
$CHClBr_2$				
CHLORODIBROMOMETHANE				
J.Phys.Radium,1937,8,130	-	1450-525cm^{-1}	-	
J.Chem.Phys.,1942,10,116	l.	3000-200cm^{-1}	prism/grating	
J.Chem.Phys.,1952,20(12),1949	l.	3150-600cm^{-1}	NaCl	
$CHCl_3$				
CHLOROFORM				
W.W. Coblentz: "Investigations of infra-red spectra". Carnegie Institution Publication 35, Pt.1. Washington,1905	l.	8000-800cm^{-1}	NaCl	
Z.Physik.,1924,30,200	g.	10,000-3700cm^{-1}	quartz	
" " " "	l.	10,000-3700cm^{-1}	quartz	
Z.phys.Chem.,1925,117,97	l.	9000-2500cm^{-1}	-	
Compt.rend.,1931,193,928	l.	13,500-9000cm^{-1}	-	also mixed with other organic solvents
J.Amer.Chem.Soc.,1935,57,1464	soln	6000-5800cm^{-1}	glass	in CCl_4

Compt.rend.,1936,202,747	l.	12,000-3700cm^{-1}	-	
Z.wiss.Phot.,1936,35,153	-	13,000-4500cm^{-1}	-	
J.Phys.Radium,1937,8,130	l.	1450-525cm^{-1}	NaCl	
Nuovo cim.,1937,14,361	l.	1700-1200cm^{-1}	-	
Compt.rend.,1938,206,1371	soln	10,000-4000cm^{-1}	-	in CS_2
Compt.rend.,1938,207,1196	l.	590-150cm^{-1}	-	
J.Chem.Phys.,1942,10,116	l.	3000-200cm^{-1}	prism/grating	
Phys.Rev.,1945,68,99	g.	5000-670cm^{-1}	-	
" " " " "	l.	5000-670cm^{-1}	-	
Proc.Roy.Soc.(A),1945,184,3	l.	1500-500cm^{-1}	-	
Trans.Faraday Soc.,1945,41,184	l.	3400-500cm^{-1}	-	
J.Amer.Chem.Soc.,1948,70(1),194	l.	2300-1300cm^{-1}	-	dried over P_2O_5 & distilled, PE 12A spectrometer
Randall et al.: "Infra-red determination of organic structures". D.Van Nostrand Co.,Inc. N.Y.,1949	l.	3-12μ	NaCl	15μ cell
" " " " " "	l.	3-13μ	NaCl	40μ cell
J.Amer.Chem.Soc.,1950,72(6),2778	l.	2-15μ	-	
J.Amer.Chem.Soc.,1951,73(3),1431	g.	1-15μ	NaCl	
" " " " " "	l.	1-15μ	NaCl	
J.Chem.Phys.,1953,21(8),1368	g.	5955-5925cm^{-1}	grating	very high resolution

$CHBrF_2$

BROMODIFLUOROMETHANE

J.Chem.Phys.,1955,23(4),726	g.	4000-600cm^{-1}	NaCl	

$CHBr_3$

BROMOFORM

Astrophys.J.,1928,67,185	l.	12,500-3300cm^{-1}	grating	10,000 lines/in.
Z.wiss.Phot.,1936,35,153	l.	13,000-4500cm^{-1}	-	
J.Phys.Radium.,1937,8,130	l.	1450-525cm^{-1}	NaCl	
Nuovo cim.,1937,14,361	l.	1700-1200cm^{-1}	-	
Compt.rend.,1938,206,1371	-	10,000-4000cm^{-1}	-	

Reference	State	Range	Optics	Remarks
$CHBr_3$ (contd)				
BROMOFORM (contd)				
Compt.rend.,1938,207,1196	l.	590-150cm^{-1}	-	
Phys.Rev.,1945,68,99	g.	5000-670cm^{-1}	-	
" " " " "	l.	5000-670cm^{-1}	-	
CHI_3				
IODOFORM				
W.W. Coblentz: "Investigations of infra-red spectra". Carnegie Institution Publication 35, Pt.1. Washington,1905	s.	4000-700cm^{-1}	NaCl	
Astrophys.J.,1928,67,185	soln	12,500-3300cm^{-1}	grating	10,000 lines/in.
J.Phys.Radium,1937,8,130	s.	1450-525cm^{-1}	NaCl	
Compt.rend.,1938,206,1371	-	10,000-4000cm^{-1}	-	
J.Chem.Phys.,1956,24(6),1186	s.	5000-400cm^{-1}	CaF_2, NaCl, KBr	polarized radiation
CHF_3				
FLUOROFORM				
J.Chem.Phys.,1948,16(1),30	g.	1.2-2.4μ	-	
J.Chem.Phys.,1953,21(6),1077	s.	2.2-20μ	LiF, NaCl, KBr	
J.Chem.Phys.,1953,21(8),1368	g.	5985-5935cm^{-1}	grating	very high resolution
CHF_5				
PENTAFLUOROETHANE				
J.Chem.Phys.,1955,23(2),329	g.	2-38μ	LiF, NaCl, KBr, KRS-5	
" " " " " "	l.	2-38μ	LiF, NaCl, KBr, KRS-5	
$(CH_2)_n$				
POLYETHYLENE				
Proc.Roy.Soc.(A),1940,175,208	s.	3900-2600cm^{-1}	NaCl, 1m concave grating	in CCl_4, 2050 lines/in.

POLYETHYLENE, MARLEX 50				
J.Chem.Phys.,1957,26(6),1391	s.	5800-1800cm^{-1}	LiF	
" " " " "	s.	5000-700cm^{-1}	NaCl	
J.Chem.Phys.,1937,5,1	g.	3000-1000cm^{-1}	NaCl	
Canad.J.Chem.,1957,35(3),226	g.	4-11μ	LiF, NaCl	
CH_2D_2O				
METHANOL-d_2				
J.Chem.Phys.,1938,6,563	g.	4000-400cm^{-1}	grating	Hardy spectrometer
J.Chem.Phys.,1942,10,693	g.	4000-800cm^{-1}	CaF_2, NaCl, KBr	
CH_2D_3N				
METHYLAMINE-d_3				
J.Chem.Phys.,1957,26(3),690	g.	3400-400cm^{-1}	LiF, NaCl, KBr, grating	various pressures
CH_2O				
FORMALDEHYDE				
Phys.Rev.,1929,33,640	g.	12,000-2700cm^{-1}	quartz	two 60° prisms
Compt.rend.,1932,195,307	g.	10,000-1667cm^{-1}	NaCl	
Phys.Rev.,1932,39,957	g.	10,000-1400cm^{-1}	prism, grating	
Ann.Phys.,1934,1,533	g.	7500-1250cm^{-1}	NaCl	Hilger D42 spectrometer
J.Chem.Phys.,1937,5,822	g.	10,000-650cm^{-1}	prism	
" " " " "	g.	1375-1000cm^{-1}	grating	
J.Chem.Phys.,1938,6,311	g.	5000-800cm^{-1}	prisms, gratings	
Ind.Eng.Chem.(Anal.Ed.),1943,15,659	l.	2000-1000cm^{-1}	-	
Barnes et al.: "Infra-red spectroscopy". Reinhold Corp. N.Y.,1944	l.	1800-1200cm^{-1}	NaCl	5μ cell
J.Opt.Soc.Amer.,1944,34,521	g.	3025-2725cm^{-1}	-	
" " " " " "	g.	1400-980cm^{-1}	-	
Phys.Rev.,1947,71,531	g.	1000-500cm^{-1}	-	
Analyt.Chem.,1956,28(8),1218	g.	2-15μ	NaCl	
Trans.Faraday Soc.,1956,52(1),13	s.	3500-800cm^{-1}	LiF, CaF_2, NaCl	PE 12C spectrometer

Reference	State	Range	Optics	Remarks
CH_2ONAg				
SILVER FORMAMIDE				
Compt.rend.,1946,222,136	-	2000-1200cm^{-1}	-	
Compt.rend.,1946,222,1293	-	2000-1250cm^{-1}	-	
CH_2O_2				
FORMIC ACID				
Z.Physik.,1932,74,466	g.	6700-3700cm^{-1}	CaF	20 & 101°C
" " " "	l.	6700-3700cm^{-1}	CaF	20 & 101°C
J.Chem.Phys.,1934,2,306	s.	2000-1540cm^{-1}	CaF_2	90% in H_2O, Hilger spectrometer
Z.Physik,1934,87,192	l.	12,500-3800cm^{-1}	-	
J.Chem.Phys.,1937,5,839	l.	11,000-9000cm^{-1}	glass	Littrow
J.Chem.Phys.,1937,5,852	g.	10,200-10,100cm^{-1}	grating (1st order)	OH harmonic
Z.Physik,1937,105,175	l.	10,000-4000cm^{-1}	quartz	
J.Chem.Phys.,1938,6,531	g.	10,000-800cm^{-1}	-	25 & 139°C
Phys.Rev.,1940,58,208	g.	3000-2200cm^{-1}	-	
Randall et al.: "Infra-red determination of organic structures". D.Van Nostrand Co.,Inc. N.Y.,1949	l.	3-10μ	NaCl	5μ cell
Analyt.Chem.,1956,28(8),1218	g.	2-15μ	NaCl	
J.Chem.Phys.,1956,25(3),478	g.	1800-1250cm^{-1}	NaCl	
J.Chem.Soc.,1956,(2),225	s.	3500-650cm^{-1}	NaCl	
" " " " "	s.	3500-650cm^{-1}	NaCl	
$CH_2O_2N_6$				
5-NITRAMINOTETRAZOLE				
J.Org.Chem.,1957,22(3),278	s.	2-15μ	-	Nujol mull
$CH_2O_4N_4$				
METHYLENEDINITRAMINE				
J.Amer.Chem.Soc.,1954,76(12),3249	s.	4000-650cm^{-1}	CaF_2, NaCl	Nujol mull, Perkin-Elmer spectrometer

CH_2N_2

CYANAMIDE

Ind.Eng.Chem.(Anal.Ed.),1943,15,659	l.	1800-1400cm^{-1}	-	
Barnes et al.: "Infra-red spectroscopy". Reinhold Corp. N.Y.,1944	l.	1800-1400cm^{-1}	NaCl	

DIAZOMETHANE

J.Chem.Phys.,1951,19(4),406	g.	3400-400cm^{-1}	quartz, LiF, NaCl, KBr	10, 50, 100 & 300mm pressure
Trans.Faraday Soc.,1954,50(12),1270	g.	3145-3040cm^{-1}	grating	7200 lines/in.
" " " " " " "	g.	2130-2060cm^{-1}	grating	7200 lines/in.
Analyt.Chem.,1956,28(8),1218	g.	2-15μ	NaCl	
J.Chem.Phys.,1956,25(1),50	g.	2-15μ	KBr, CsBr, grating	7500, 4500 & 3600 lines/in.

CH_2N_4

TETRAZOLE

Chem.Ber.,1956,89(12),2887	s.	2-15μ	NaCl	KBr disc

CH_2ClBr

CHLOROBROMOMETHANE

J.Phys.Radium,1937,8,130	l.	1450-520cm^{-1}	-	

CH_2ClF

CHLOROFLUOROMETHANE

J.Chem.Phys.,1942,10,116	g.	3000-200cm^{-1}	prism/grating	

CH_2Cl_2

METHYLENE DICHLORIDE

Astrophys.J.,1928,67,185	l.	12,500-3300cm^{-1}	grating	10,000 lines/in.
Compt.rend.,1936,202,747	g.	12,000-3700cm^{-1}	-	
J.Phys.Radium,1937,8,130	l.	1450-525cm^{-1}	NaCl	
Compt.rend.,1938,207,1196	g.	590-150cm^{-1}	-	

Reference	State	Range	Optics	Remarks
CH_2Cl_2 (contd)				
METHYLENE DICHLORIDE (contd)				
Proc.Roy.Soc.(A),1938,165,43	l.	4500-700cm^{-1}	CaF, NaCl	Hilger D83 spectrometer
J.Phys.Radium,1939,10,143	l.	500-165cm^{-1}	-	
J.Chem.Phys.,1942,10,116	-	3000-200cm^{-1}	prism/grating	
J.Amer.Chem.Soc.,1951,73(7),3300	-	5-11μ	-	
J.Chem.Phys.,1953,21(2),360	g.	2980-706cm^{-1}	CaF_2, NaCl, KBr	
" " " " "	l.	4660-707cm^{-1}	CaF_2, NaCl, KBr	
CH_2BrI				
BROMOIODOMETHANE				
Astrophys.J.,1928,67,185	l.	12,500-3300cm^{-1}	grating	10,000 lines/in.
J.Chem.Phys.,1942,10,116	l.	3000-200cm^{-1}	prism/grating	
CH_2Br_2				
METHYLENE DIBROMIDE				
Astrophys.J.,1928,67,185	l.	12,500-3300cm^{-1}	grating	10,000 lines/in.
J.Phys.Radium,1937,8,130	l.	1450-525cm^{-1}	NaCl	
Compt.rend.,1938,207,1196	g.	590-150cm^{-1}	-	
J.Phys.Radium,1939,10,143	l.	500-165cm^{-1}	-	
Z.Physik,1941,117,589	g.	6700-667cm^{-1}	quartz, NaCl	Paschen spectrometer
J.Chem.Phys.,1942,10,116	l.	3600-200cm^{-1}	prism/grating	
CH_2I_2				
METHYLENE DIIODIDE				
Astrophys.J.,1928,67,185	l.	12,500-3300cm^{-1}	grating	10,000 lines/in.
J.Phys.Radium,1937,8,130	l.	1450-525cm^{-1}	NaCl	
Compt.rend.,1938,207,1196	l.	590-150cm^{-1}	-	
J.Phys.Radium,1939,10,143	l.	500-165cm^{-1}	-	
J.Chem.Phys.,1942,10,116	l.	3000-200cm^{-1}	prism/grating	

CH_2F_2

METHYLENE DIFLUORIDE

J.Chem.Phys.,1942,10,116	s.	3000-200cm^{-1}	prism/grating	

$-CH_3$

METHYL RADICAL

Proc.Roy.Soc.(A),1945,184,3	s.	3200-500cm^{-1}	-	

CH_3D

METHANE-d_1

J.Chem.Phys.,1935,3,668	g.	3200-1000cm^{-1}	grating	Barber & Hardy spectrometer
J.Chem.Phys.,1937,5,1	g.	3000-1000cm^{-1}	NaCl	
Proc.Roy.Soc.(A),1938-9,169,428	g.	13,000-8400cm^{-1}	-	
Canad.J.Chem.,1957,35(3),226	g.	4-10μ	LiF, NaCl	

CH_3DO

METHANOL-d_1

J.Chem.Phys.,1938,6,563	g.	4000-400cm^{-1}	grating	
Randall et al.: "Infra-red determination of organic structures". D.Van Nostrand Co.,Inc. N.Y.,1949	l.	2-10μ	NaCl	15μ cell

CH_3D_2N

METHYLAMINE-d_2

J.Chem.Phys.,1957,26(3),690	g.	3400-400cm^{-1}	LiF, NaCl, KBr, grating	various pressures

CH_3D_3NCl

METHYL AMMONIUM CHLORIDE-d_3 (N-SUBSTITUTED) (α-PHASE)

J.Chem.Phys.,1953,21(4),734	s.	3500-450cm^{-1}	SiO_2, LiF, CaF_2, NaCl, KBr, KRS-5	single crystal; (1) radiation || c-axis, (2) random orientation

Reference	State	Range	Optics	Remarks
CH_3D_3NCl (contd)				
METHYL AMMONIUM CHLORIDE-d_3 (N-SUBSTITUTED) (β-PHASE)				
J.Chem.Phys.,1953,21(4),734	s.	3500-450cm^{-1}	SiO_2, LiF, CaF_2, NaCl, KBr, KRS-5	random orientation
METHYL AMMONIUM CHLORIDE-d_3 (N-SUBSTITUTED) (γ-PHASE)				
J.Chem.Phys.,1953,21(4),734	s.	3500-450cm^{-1}	SiO_2, LiF, CaF_2, NaCl, KBr, KRS-5	random orientation
CH_3ON				
FORMAMIDE				
Bull.Soc.chim.,1941,8,601	-	1700-500cm^{-1}	-	
CH_3OCl_2SP				
METHYL PHOSPHORODICHLORIDOTHIONATE				
Canad.J.Chem.,1956,34(11),1611	l.	2-26μ	NaCl, KBr	
CH_3OCl_2P				
METHYL PHOSPHONYL DICHLORIDE				
Canad.J.Chem.,1956,34(11),1611	l.	2-26μ	NaCl, KBr	
CH_3O_2N				
NITROMETHANE				
W.W. Coblentz: "Investigations of infra-red spectra". Carnegie Institution Publication 35, Pt.1. Washington,1905	l.	4000-700cm^{-1}	NaCl	
Phys.Rev.,1930,35,605	l.	10,000-1250cm^{-1}	quartz	Hilger spectrometer
Bull.Soc.roum.Phys.,1941,42,73	g.	4000-1000cm^{-1}	-	