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TECHNICAL NOTE No. 5

SPECTROSCOPIC STUDIES: PART 2, THE INFRA-RED SPECTRA AND STRUCTURE OF METHOXYACETONITRILE AND METHYL-CHLOROMETHYLETHER

R. G. Jones and W. J. Orville-Thomas

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List of Technical Notes

TN-1 : Force Constants in Boron Trihalides. June, 1963.

TN-2 : Infra-red Dispersion Studies : Part 1, Dichloro-, Dibromo-, and Diiodomethane. June, 1963.

TN-3 : Vibrational Frequencies and Electronegativities. June, 1963.

TN-4 : Spectroscopic Studies : Part 1, The Infra-red Spectrum and Structure of Sodium Nitromethane.

TN-5 : Spectroscopic Studies : Part 2, The Infra-red Spectra and Structure of Methoxyacetonitrile and Methyl-Chloromethylether.

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The infra-red spectra of methoxyacetonitrile and methyl-chloromethyl-ether have been studied in solution and in the vapour and liquid states.

In the vapour state the band contours prove that the molecules are most stable when they have a slightly twisted trans conformation.

Methoxyacetonitrile (a) and methyl- chloro- methyl-ether (b) differ only in that the nitrile group of one is replaced by a chlorine atom.

(a) $CH_3.O.CH_2.CN$ (b) $CH_3.O.CH_2.Cl$

Since the nitrile group and the chlorine atom have approximately the same electronegativity and mass it is reasonable to expect that the vibrational frequencies of the $CH_3.O.CH_2-$ group will change but little in going from (a) to (b).

In both molecules rotation about the $(CH_3)O — C(H_2X)$ bond is possible. (Fig. 3.) In their most stable states the molecules will have particular conformations corresponding to certain definite values for the moments of inertia. A study of the band contours, obtained from vapour phase spectra, then, should give a reliable indication as to the most stable conformation.

Methyl chloromethyl ether, together with the corresponding thio-ether, has been studied by Hayashi.[2] The Raman spectra of (a) and (b) have been recorded.[2,3],

EXPERIMENTAL.

Methoxyacetonitrile was prepared by addition of excess dimethyl sulphate to the product of reaction between potassium cyanide and formalin solution at temperatures below 10°C. The oily liquid with a pyridine-like smell was extracted with ether. The ether layer was dried, the ether removed and the residue distilled at atmospheric pressure. The observed boiling point was 121°C. (Literature[4] 119°Cat 736 m.m.).

Methyl-chloromethyl-ether was prepared by the reaction between methanol formalin and hydrogen chloride, as described by Marvel and Porter[5]. The observed boiling point was 58.5°C at atmospheric pressure, to be compared with 55-60°C reported by Marvel and Porter.

The spectra were recorded on a Grubb Parsons G.S. 2A double beam infrared spectrometer calibrated with ammonia gas.

A pyrex glass vapour cell which allowed a temperature variation over the range 20°C to 200°C was used to the record the vapour spectra. Matched metal cells (4.72m.m. and 9.78m.m. in length) were used to record solution spectra in chloroform, carbon tetrachloride and carbon disulphide solvents. The spectra of capillary and 0.1 m.m. thick, liquid films were also obtained.

The spectra are reproduced in figs. 1 and 2 and the frequencies given in tables 1 and 2.

The Stable Conformations

The type of contour obtained for vibrational bands (i.e. the PQR structure) and the P-R sub-band separation depend critically upon the moments of inertia of the molecule. These, in turn, depend upon the conformation of the molecule (fig. 3.) As one part of the molecule rotates with respect to the other the absolute and relative magnitudes of the the three principal moments of inertia change continuosly: consequently the band contours and separations also change.

Molecular dimensions have not been determined for methoxyacetonitrile or for methyl-chloromethylether. Hence, from a study of similar molecules the parameters given in table 3 were chosen. With these values moments of inertia were calculated for each of the conformations given in fig. 3. (see table 4.).

The moments of inertia indicate that the molecules approximate to symmetric rotors especially for conformations near to (V). Using the theory developed by Gerhard and Dennison[6] the P-R separations have been calculated, for parallel type bands, from the expression,

$$\Delta\nu\,(P,R) = \frac{S}{\pi}\left(\frac{kT}{I}\right)^{1/2}$$

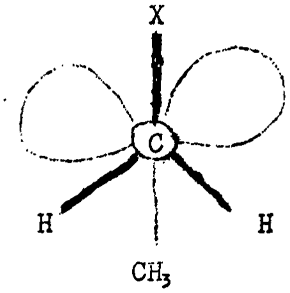
where $S = \frac{0.721}{(\beta + 4)^{1.13}}$, $\beta = (I - I_A)/I_A$,

and $I = (I_B + I_c)/2.$

The values obtained are given in table 5, and expressed diagrammatically in fig. 4. The P-R separations found experimentally for parallel-type bands (or type A bands as described by Badger and Zumwalt[7]) are given in table 6.

From a comparison of the observed and calculated P-R separations it is evident that, in both cases, the stable conformations are very close to model (V). That is the 'heavy' atom skeleton is almost planar-trans in form. This conclusion differs from that of Hayashi[2] who favours a gauche conformation fig. 3, II) for methyl chloromethyl-ether in the vapour state.

If the oxygen lone-pairs forming atomic dipoles are taken into account the terminal groups are seen to be staggered about the C-O bond.



In terms of bond-bond and bond-lone-pair repulsions this represents a most reasonable model.

Vibrational Assignment.

All the fundamental modes of vibration are infra-red active. The vibrations can be conveniently divided for discussion into two groups, viz. (i) the methyl and methylene vibrations, and (ii) those associated with the COCX skeleton.

(i) CH Vibrations.

Tables 1 and 2 contain the assignments for these molecules made on the basis of vapour phase band contours and comparisons with related molecules.

The ranges within which the various types of methyl vibrations occur are well-known and there is little uncertainty in the assignments made in tables 1 and 2.

The assignment of frequencies to the methylene bond-stretching modes is straightforward but this is not the case with the various deformation modes since they tend to vary over large spectral regions. For example the CH_2-rocking frequency occurring at 1176 cm^{-1} in CH_2F_2 is found at 714 cm^{-1} in CH_2I_2, a decrease of some 39%. In a recent study[11] relations have been found between the methylene deformation frequencies in CH_2XY molecules and the electronegativity product $\chi(X)\chi(Y)$. These correlations have been used to predict 'group electronegativities of 3.76(CH_3.O) and 3.20(CN) corresponding to frequency values centred near to 1470, 1340, 1250 and 1,000 cm^{-1} respectively for the bending, wagging, twisting, and rocking CH_2 vibrations. The observed values are in good accord with these predictions (tables 1 and 2).

The vapour spectra of the compounds are not identical in the region between 1,400 cm^{-1}. and 1,300 cm^{-1}. Two absorption bands, one, weak, with an 'A, B' contour at 1,397 cm^{-1}. and the other, stronger in intensity with an almost perfect 'A' type contour at 1324 cm^{-1}, were observed in the spectrum of methyl chloromethylether. One complex band was observed in the spectrum of methoxyactonitrile centred at 1364 cm^{-1}. The difference between the two spectra is explicable in terms of Fermi resonance between the two vibrational modes (symmetric CH_3 bending and wagging CH_2) which belong to the same symmetry class. Evidence for this is the almost equal difference in frequency between these two absorption bands in (b) and the one complex band in (a).

(b) $CH_3.O.CH_2.Cl$	1400	36 cm,$^{-1}$
(a) $CH_3.O.CH_2.CN$	1364	40 cm.$^{-1}$
(b) $CH_3.O.CH_2.Cl$	1324	

It is rather surptising that Fermi resonance is operative in (b) and not (a). The first overtone of the carbon-chloring stretching vibration should occur close to 1360 cm^{-1}, in the vapour spectrum of (b) and the interaction of this binary transition with the superimposed fundamentals might be the factor that results in difference in the two spectra.

(ii) Skeletal vibrations.

Three bands are expected to arise from the skeletal stretching vibrations in methyl chloromethyl ether. Two of these are best regarded as an asymmetric and symmetric stretching mode of the COC grouping, ν_a(COC) and ν_s(COC) whilst the third, ν(CCl), is primarily localized within the CCl bend. In methoxyacetonitrile there are four stretching modes, ν_a(COC), ν_s(COC), and two others which can be approximately described as ν(CC) and ν(CN).

The ν(CN) fundamental occurs near 2250 cm^{-1}, in all phases, with the very low intensity characteristic of β-oxygenated nitriles.

The assignment of the vibrations of the COCX chain in these molecules was facilitated by a direct comparison of the vapour spectra. Three absorption bands, of strong to medium intensity, were found in the region 1150 to 800cm^{-1}, in the spectrum of methoxyacetonitrile. The strong absorption with an almost pure B type contour, at 1132 cm^{-1}, is assigned to the ν_a(COC) stretching vibration. The frequency of the carbon-oxygen stretching vibration in gaseous methanol is 1030 cm^{-1}. If it is assumed that the coupling between the symmetric and asymmetric modes of vibration of the COC chain results in a splitting of degenerate energy levels to give energy level pairs equally spaced on either side of the unperturbed ν(CO) vibrational level, it can be predicted that the frequency of the symmetric stretching vibration of the COC chain will be near

$$1030 - (1130 - 1030) = 930 \text{ cm.}^{-1}$$

Two absorption bands, with hybrid contours, at 932 cm^{-1}, and 890 cm^{-1}, were observed in the vapour spectrum of methoxyacetonitrile. The higher frequency band is therefore assigned to ν_s(COC) and the other to ν(CC). This assignment is supported by the fact that replacement of the nitrile group by chlorine results in the disappearance of the 890 cm^{-1}, band, but does not significantly perturb the spectrum above 900 cm^{-1}. This is to be expected because the chlorine atom does not differ much in mass of electronegativity from the nitrile group.

It has been shown that for molecules exhibiting rotational isomerism certain group frequencies are characteristic of particular isomeric conformations. For example in trans-monochlorinated hydrocarbons ν(CCl) varies from 726(n-propyl) to 616^{-1}, in tert.amyl chloride, whilst the gauche frequencies range between 645 and 560 cm^{-1} for the same series.[12] In the spectrum of methyl chloromethyl ether only one ν(CCl) band centred at 646 cm^{-1} was detected. This comparatively high value underlines the correctness of choosing a trans-conformation. The absence of a second ν(CCl) band indicates that the gauche isomer is present to a very small extent, if at all.

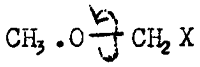
The bond-bending fundamentals of the skeleton lie below the range studied. The vibrations can be approximately described for $CH_3.O.CH_2.Cl$ as COC bending - b(COC), b(OCCl), both in the plane of the skeleton framework, and an out-of plane vibration which could be described as b(OC) or b(CCl): for $CH_3.O.CH_2.CN$ one has b(COC), b(OCC), b(CCN) all in-plane and either b(OC) or b(CN) out-of-plane.

The corresponding frequencies are expected to be below 500 cm^{-1} as is clearly shown by table 7.

Three weak bands at 838, 709, and 586 c.m.$^{-1}$ were observed in the spectrum of liquid methoxyacetonitrile. These can be assigned as overtone or combination bands in a number of ways. The interpretation of other combination bands observed in the higher frequency region is made more plausible if these frequencies are assigned as follows:-

b(COC) ~ b(OCC) = 425 c.m.$^{-1}$,
b(CCN), in plane = 360 cm.$^{-1}$
b(CCN), out of plane = 230 c.m.$^{-1}$

The torsional modes of methyl groups about a C-O bond have been assigned tentatively[9] to bands at 160 and 230 c.m.$^{-1}$ The torsional mode



$CH_3.O-CH_2X$

would therefore be expected to have an even lower frequency.

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TABLE 1: INFRA-RED SPECTRUM OF METHOXYACETONITRILE ( )

LIQUID			SOLUTIONS		VAPOUR	ASSIGNMENT.
(Raman)	Capillary	0.75mm	CCl_4 (0.5cm)	CS_2 (0.5cm.)		
		4447				3008+1450 = 4458
		4404				2946+1460 = 4406
		4356				3008+1370 = 4373
		4269				3008+1287 = 4295
		4201				3008+1196 = 4204
		4064				2916+1158 = 4074
		3949				2837+1115 = 3952
		3640				2256+1380 = 3636
		3563				2257+1289 = 3546
		3132				2257+ 886 = 3143
					3018	
3009	3008		3007	3002	3010	CH_2 Asymmetric Stretch
					3000	
2980				2963		CH_2 Symmetric Stretch
	2946		2940		2950	
2933			2936	2932	2931	CH_3 Asymmetric Stretch
					2908	
2914	2916		2902	2893	2897	CH_3 Asymmetric Stretch
					2889	
2872						
			2849	2843	2831	CH_3 Symmetric Stretch
2832	2837		2832	2824	2822	
		2656				1289+1370 = 2659
	2627	2629				1460+1158 = 2618
		2603		2595		14[illegible]0+1158 = 2613
	2463	2464				1289+1196 = 2485
	2442	2444				1289+1158 = 2447
	2389	2390				2x1196 = 2392
	2302	2301				2x1158 = 2316
2243	2256				2251	CN Stretching

TABLE 1. (Cont.)

LIQUID			SOLUTIONS		VAPOUR	ASSIGNMENT.
(Raman)	Capillary	0.75mm.	CCl_4 (0.5 cm)	CS_2 (0.5 cm)		
	2207	2206				2x1115 = 2230
	2105	2105			2136	1115+1014 = 2129
	2064	2061		2078	2060	886+1196 = 2082
	2023	2021		2025		886+1158 = 2044
	1757	1758	1758	1760		2x886 = 1772
	1631	1631				1290+360 = 1650
					1474	CH_2 Bending
	1466				1467	CH_3 Asymmetric Bending
	1458		1461		1460	
1455			1455		1456	
1435	1439		1437		1441	CH_3 Asymmetric Bending
	1380		1378		1376	
	1374				1370	CH_3 Symmetric Bending
1363			1367		1364	
	1359		1354		1359	CH_2 Wagging
				1351	1349	
					1294	
1285	1289		1284	1282	1288	CH_2 Twisting
					1279	
	1242					1014+(240) = 1254
					1207	
1185	1196		1188	1192	1200	CH_3 Rocking.
					1193	
	1158		1158	1156	1161	CH_3 Rocking.
1112	1115		1117	1117	1136	COC Asymmetric Stretch
					1128	
					1023	
	1014			1012	1017	CH_2 Rocking.
					1009	
	990					1360-(360) = 1000
	961			965		2256-1289 = 967
955						

TABLE I (Cont.)

LIQUID			SOLUTIONS		VAPOUR	ASSIGNMENT
(Raman)	Capillary	0.75mm.	CCl_4 (0.5cm.)	CS_2 (0.5cm)		
914	915		919	917	937 922 924	COC Symmetric stretching
882	886		885		899 890 882	C-C Stretch
	844	838				2x420 = 840
	704	709		695		2x350 = 700
	586	586				350+240 = 590
404	(425)					COC Bending
352	(360)					CCO Bending
242	(230)					CCN Bending

TABLE 2: INFRA-RED SPECTRUM OF METHYL CHLOROMETHYL ETHER.

LIQUID			SOLUTION		VAPOUR	ASSIGNEMENT
Raman	Capillary	0.1mm.	CCl_4	CS_2		
		4459				2295+1470 = 4465
		4413				2958+1470 = 4428
		4284				2903+1397 = 4300
		4207				2903+1320 = 4223
		4091				2837+1278 = 4115
		4028				2837+1193 = 4030
		3961				2837+1120 = 3957
3027	2995		2994	3030	3013	CH_2 Asymmetric Stretch
2980	2958		2948	2940	2930	CH_2 Symmetric Stretch
2950	2943		2932	2926	2946	CH_3 Asymmetric Stretch
2912	2903		2397	2362	2901	CH_3 Asymmetric Stretch
2837	2837		2830	2824	2844	CH_3 Symmetric Stretch.
	2778		2770	2305		1460+1320 = 2780
		2632				2x1320 = = 2640
		2606				1460+1156 = 2616
2464		2464				1470+996 = 2466
		2438				1320+1120 = 2440
		2389				2x1193 = 2386
		2311				1397+920 = 2317
		2238				1320+920 = 2240
		2193				1278+920 = 2198
	2108	2113				1193+920 = 2113
	2032	2036				920+1120 = 2040
		1345				2x920 = 1840
		1776				2903-1120 = 1783
		1650				1320+350 = 1650
		1576				2995-1397 = 1598
					1476	CH_2 Bending
1470	1470				1470	
	1467					
1460			1461		1458	CH_3 Asymmetric Bending
	1453				1451	CH_3 Asymmetric Bending

TABLE 2: (Cont.)

LIQUID			SOLUTION		VAPOUR	ASSIGNMENT
Raman	Capillary	0.1	CCl_4	CS_2		
1435 1398	1440 1397		1446 1396		1440 1408 1400 1392	CH_3 Symmetric Bending
1321	1320		1317	1315	1331 1324 1317	CH_2 Wagging
1279	1273			1273	1286 1278 1270	CH_2 Twisting
1231					1236	1397-160 = 1237
					1206 1198 1190	CH_3 Rocking
1147	1156		1156	1153 1138	1156 1148 1138	CH_3 Rocking
1128	1120		1131	1129	1138 1128 1121	COC Asymmetric Stretch
					1092	1450-350 = 1100
	1042		1043	1043	1064 1054	1397-350 = 1047
998	996			990	1008 1000 993	CH_2 Rocking
920	920		925	917	943 937 932	COC Symmetric Stretch
		805				350+466 = 816

TABLE 2: (Cont.)

LIQUID			SOLUTION		VAPOUR	ASSIGNMENT
Raman	Capillary	0.1mm.	CCl_4	CS_2		
					686	
					679	
651	646			640	677	C-Cl Stretch
					670	
455	466					COC Bending
357	(35C,					OCCl Bending
177	(160)					CH_3 O Torsion
107						CH_3O CH_2Cl Torsion

TABLE 3. DIMENSIONS OF $CH_3.O.CH_2.X$ MOLECULES.

MOLECULE	C-O	COC	OCX	C-C(I)	C≡N(I)	C-Cl(II)
$CH_3.O.CH_2.CN$	1.42	110°	111°	1.47	1.16	-
$CH_3.O.CH_2.Cl$	1.42	110°	112°	-	-	1.74

TABLE 4. CALCULATED MOMENTS OF INERTIA AND ROTATIONAL CONSTANTS OF $CH_3.O.CH_2.X$ MOLECULES.

(a) $CH_3.O.CH_2.CN$

Conformation	I_A	A	I_B	B	I_C	C
I	53	0.53	166	0.17	219	0.13
II	41	0.68	224	0.13	270	0.10
III	28	0.99	157	0.18	175	0.16
IV	38	0.75	266	0.11	343	0.08
V	17	1.65	321	0.09	338	0.08

(b) $CH_3.O.CH_2.Cl$

Conformation	I_A	A	I_B	B	I_C	C
I	63	0.45	161	0.17	224	0.13
II	51	0.55	205	0.14	244	0.12
III	23	1.20	147	0.19	161	0.18
IV	59	0.47	242	0.12	329	0.09
V	14	2.02	304	0.09	318	0.09

TABLE 5: CALCULATED P,R SEPARATIONS OF PARALLEL-TYPE BANDS ($\Delta\nu$).

(a) $CH_3.O.CH_2.CN$

CONFORMATIONS	I	II	III	IV	V
$\Delta\nu$ (P,R) cm^{-1}	1 1	17.9	21.5	16.1	13.9

(b) $CH_3.O.CH_2.Cl$

CONFORMATIONS	I	II	III	IV	V
$\Delta\nu$ (P,R) cm^{-1}	20.4	18.0	20.9	15.5	13.5

TABLE6: OBSERVED P.R SEPARATIONS OF PARALLEL-TYPE BANDS.

$CH_3.O.CH_2.CN$		$CH_3.O.CH_2.Cl$	
1349	15±1	1408	16±1
1359		1400	
1364		1392	
1279	15±1	1331	14±1
1288		1324	
1294		1317	
1193	14±1	1286	16±1
1200		1278	
1207		1270	
1123	13±1	1156	18±1
1128		1148	
1136		1138	
1009	14±1	112[illegible]	17±1
1017		1128	
1023		1138	
924	13±1	686	16±1
932		679	
937		677	
		670	

TABLE 7: FREQUENCIES OF SKELETAL VIBRATIONS.

MOLECULE	b(COC)	b(OCC)	b(XCC)	Ref.
$CH_3.O.CH_3$	414	-	-	9
$CH_3.O.CHO$	325	-	-	10
$CH_3.O.CO.CH_3$	303	429	-	10
$CH_3.CH_2.OH$	-	427	-	13
$CN.CH_2.CN$	-	-	582	14
$CH_3.CH_2.CN$	-	-	531	15
$CH_3.CH_2.F$	-	-	415	16
$HO.CH_2.CN$	-	410	-	17

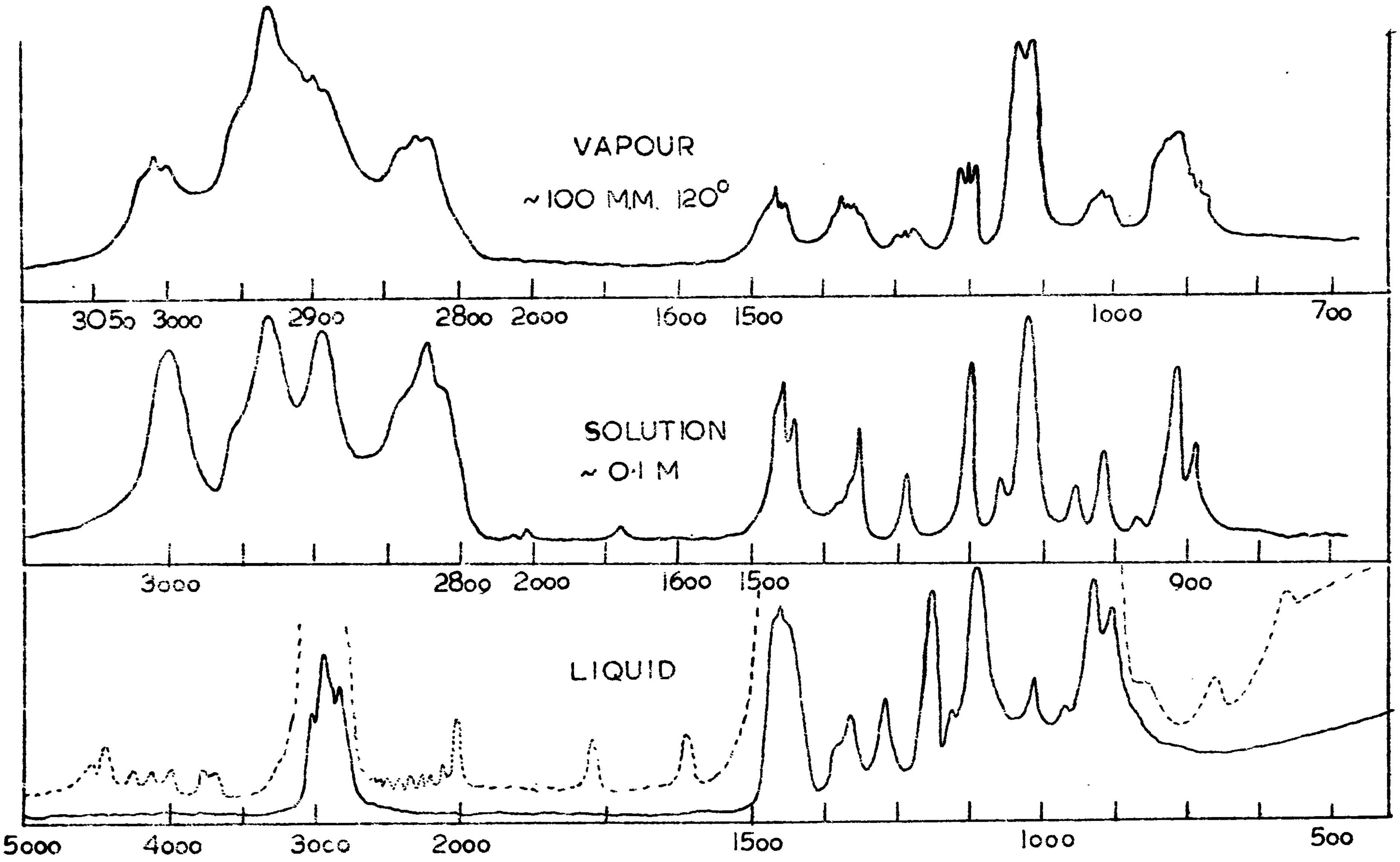


FIG. 1 CH_3OCH_2CN

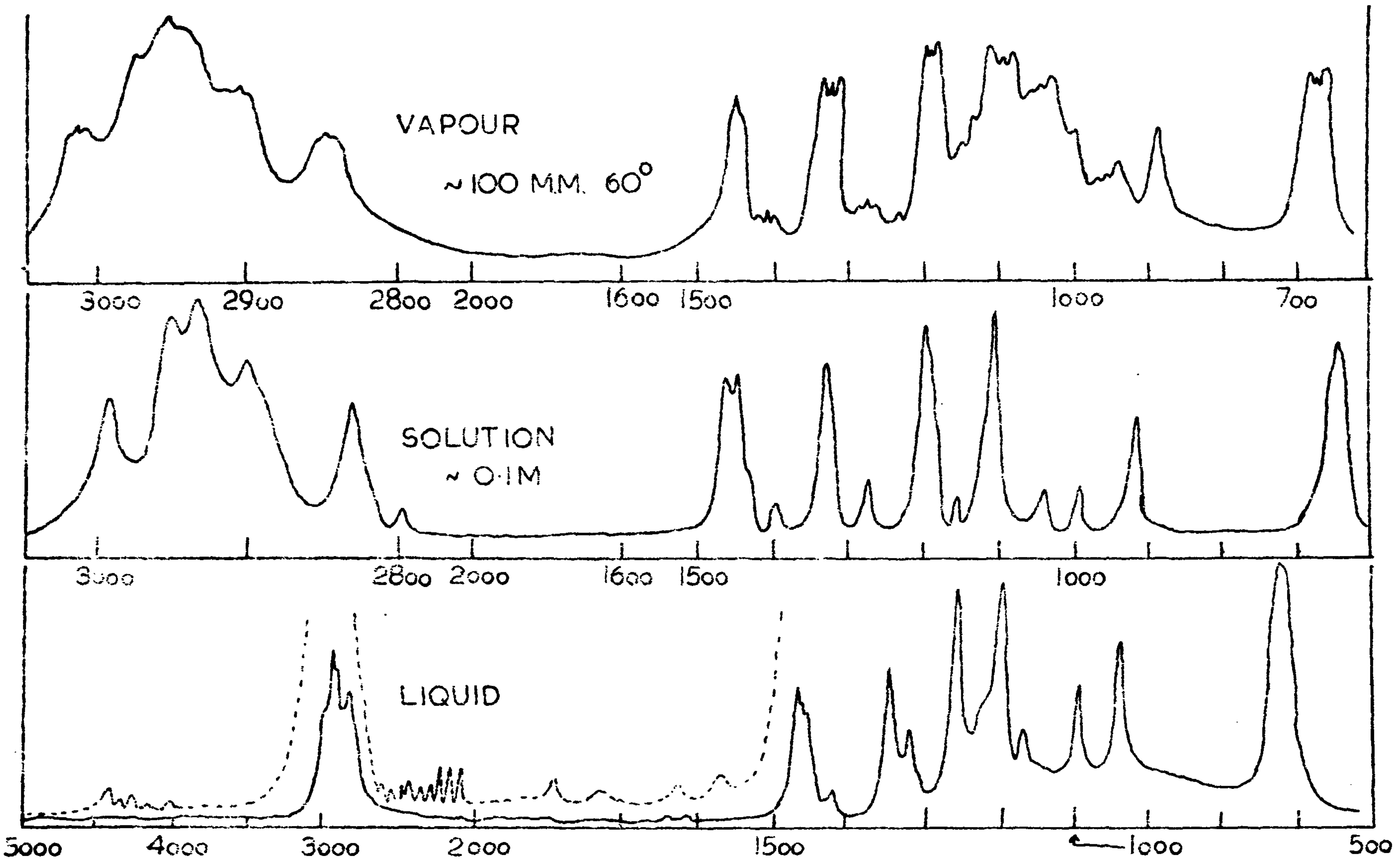


FIG 2 CH_3OCH_2Cl

FIG. 3 CONFORMATIONS OF CH_3OCH_2X MOLECULES.

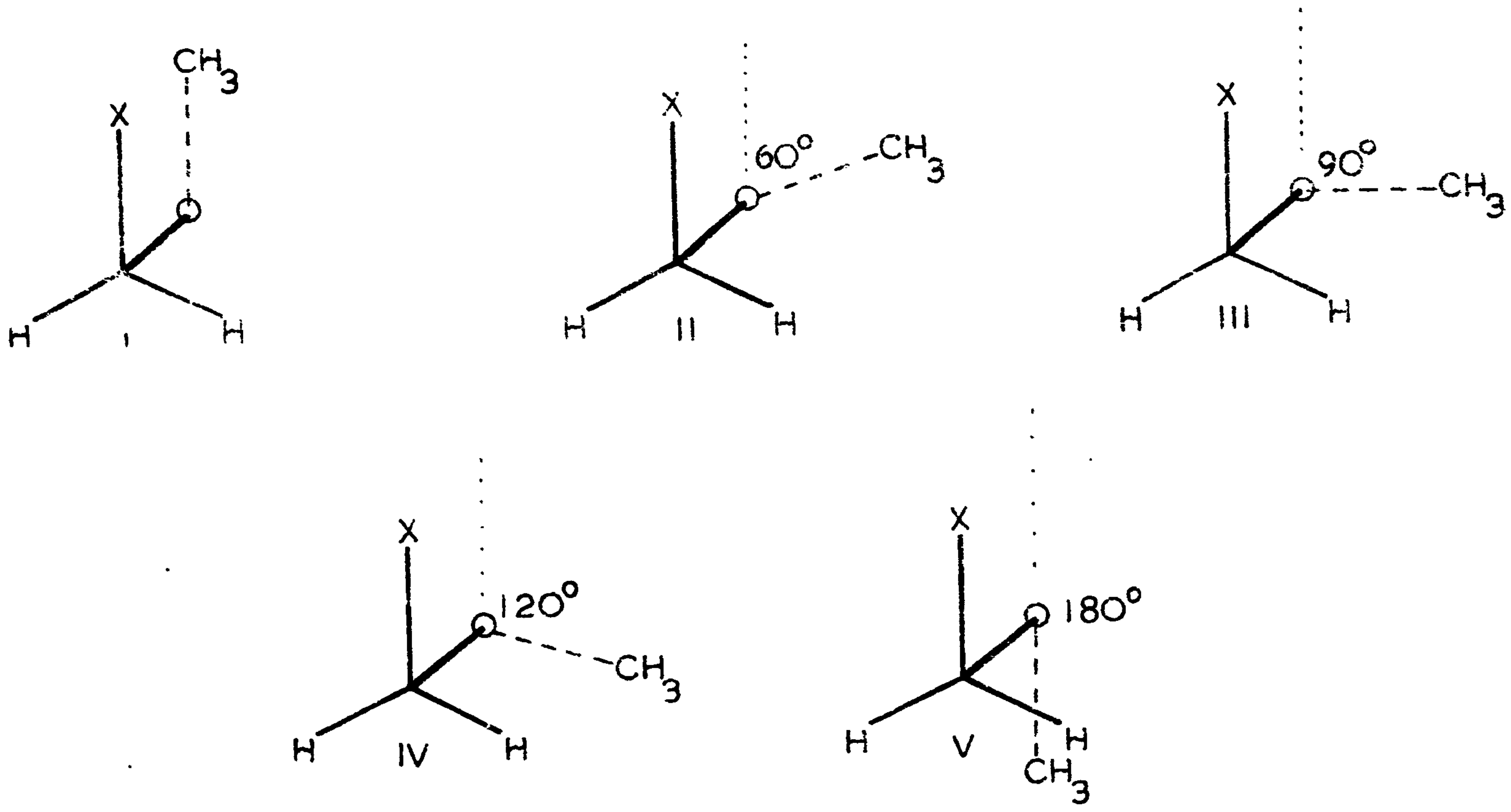


FIG. 4A CH_3OCH_2CN

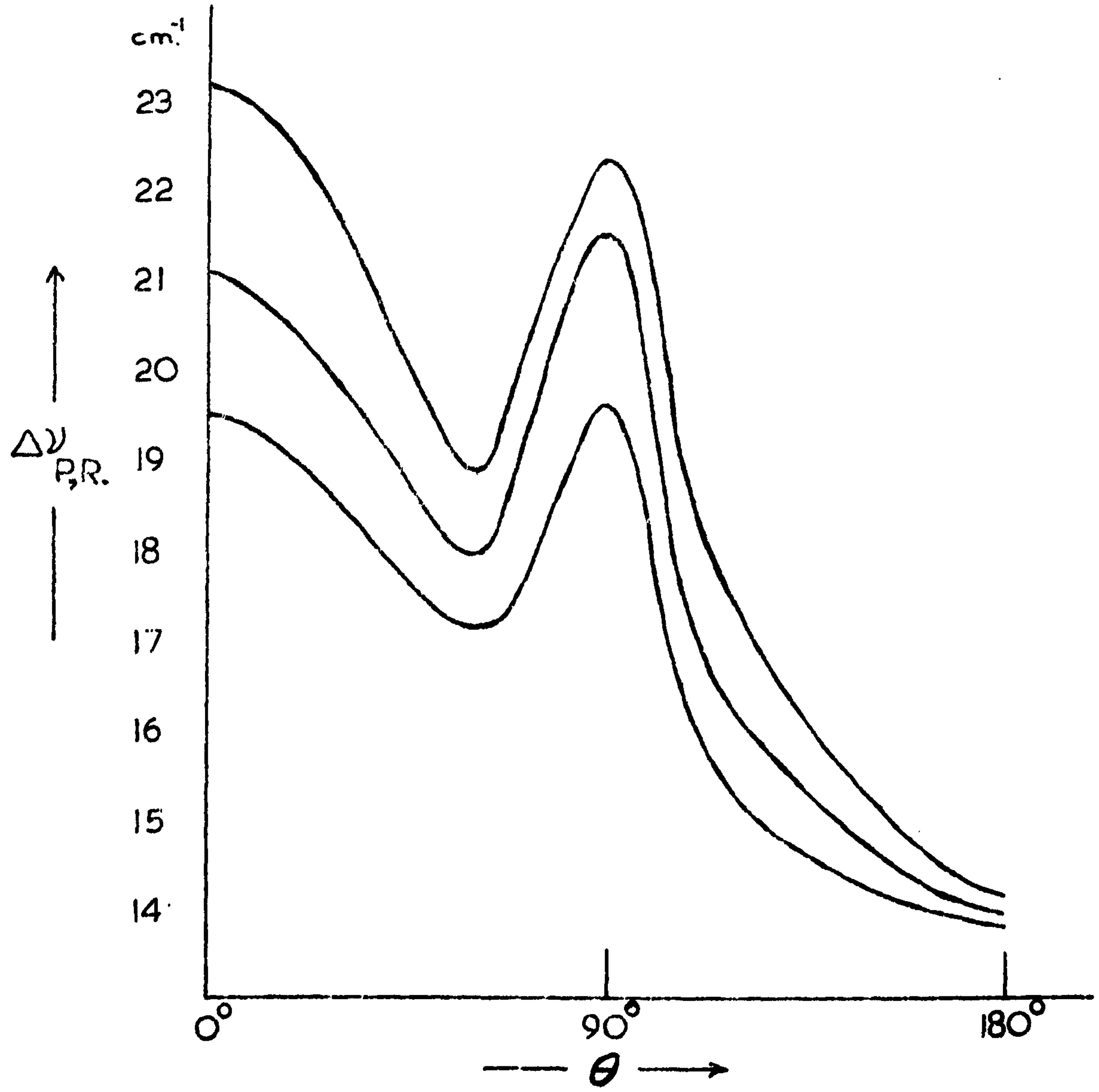
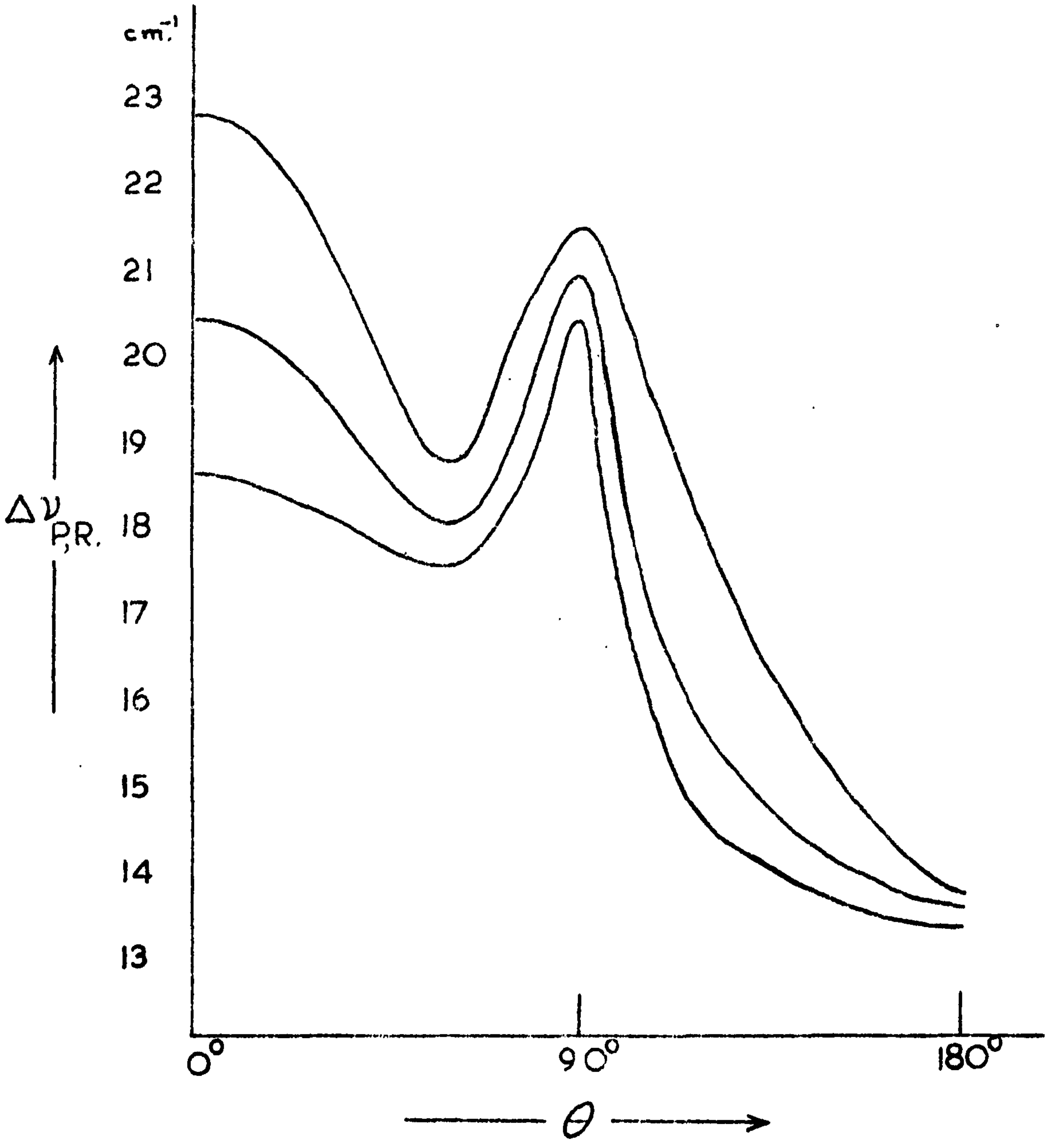


FIG 4B $CH_3 \cdot OCH_2Cl$



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SPECTROSCOPIC STUDIES: PART 2, THE INFRA-RED SPECTRA AND STRUCTURE OF METHOXYACETONITRILE AND METHYL CHLOROMETHYL ETHER.

R. G. JONES AND W. J. ORVILLE-THOMAS.

ABSTRACT: The infra-red spectra of methoxyacetonitrile and methyl chloromethyl ether have been studied in solution and in the vapour and liquid states.

In the vapour state the band contours prove that the molecules are most stable when they have a slightly twisted *trans* conformation.

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