Interpreting Infrared and Nuclear Magnetic Resonance Spectra of Simple Organic Compounds for the Beginner

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A great deal of information may be gleaned from an infrared or nuclear magnetic resonance spectrum by an experienced chemist. A beginner, however, sees only a piece of paper with a multitude of peaks. How is it possible to "decode" the complicated spectrum?

We have devised flow charts which successfully assist the beginner to become proficient. The use of a flow chart is not totally revolutionary but merely attempts to incorporate in a systematic method the approach which might be followed by an experienced chemist.[1]

The charts are designed primarily for the beginner. They are comparatively simple in that more complex spectra will not be encountered by the user. The student can use the chart to help him or her ask the correct questions and look for various features in the spectrum, and then to draw some conclusion. He or she soon learns a method of "attacking" the interpretation. The chart will be discarded, or rather a new chart will be built up in the student's own mind.

Infrared

When studying infrared spectra, account must be taken not only of the position of the peaks but also their sizes and shapes. The flow chart in Figure 1 enables this to be done. Examples can be selected to develop the student's experience of interpreting these features. The spectrum of propan-2-ol is shown in Figure 2. For this compound the sepctrum above 2700 cm^{-1} shows a broad intense peak (due to —OH stretch) and a sharp peak (due to aliphatic —CH stretch).

Students have no difficulty in answering questions 2–4 of the flow chart (Fig. 1). No information can be obtained in answer to question 5, and this is a limitation to which students' attention may be drawn.

[1] Henson, R. C., and Stumbles, A. M., *School Sci. Rev.*, **60**, 212, 446 (1979).

Table 1. Typical Student Response for Spectrum of Liquid Containing Carbon, Hydrogen, and Oxygen

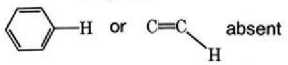
Region	Question Box	Answer	Inference
above 2700 cm^{-1}	1	yes	
	2	yes	—OH present
	3	no	 absent
	4	yes	aliphatic CH present
	5	not known (broad absorption obscures this region)	
2000–1500 cm^{-1}	6	no	C═O, aromatic, NH, alkene groups absent
1500–1100 cm^{-1}	10	yes	
	11	yes	C—O, C—N, or C—C present
	12	yes	CH_3 present
	13	yes	CH_2 or CH_3 present
below 900 cm^{-1}	14	yes	
	15	no	—CH_2— absent, aromatic, alkene or monochloro C—Cl possible

Table 1 shows a typical response in following the flow chart for this spectrum. The overall conclusion that a student will come to is that the following groups are present: OH, CH_3, and C—O or C—C. We use infrared in conjunction with other methods of identification. Students are encouraged to make use of all available information about the compound when drawing conclusions.

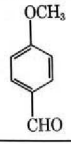
Table 2. Flow Chart Responses for NMR Spectrum of *p*-methoxybenzaldehyde

Reference peak at $\delta = 0$ identified
Molecular formula $C_8H_8O_2$
Number of hydrogens = 8
No peaks removed by D_2O
From integrated trace calculate number of hydrogens at different chemical shfits.
Note splitting pattern for each absorption.

Chemical shift	Number of hydrogens	Splitting
9.8 δ	1	singlet
7.9 δ	2	doublet
7.0 δ	2	doublet
3.8 δ	3	singlet

Region	Question Box	Answer	Inference
	1	no	—OH, —COOH, NH absent
	3	no	
Up to 6.6 δ	4	yes	
	5	1	Consider 9.8 δ peak first. One hydrogen not in region 8.0–6.6 δ so unlikely to be attached to aromatic ring. Possible CHO, —OH or —COOH group (but —OH and —COOH absent).
	6	yes	
	9	yes	ArH, OH, COOH or CHO group present (but OH, —COOH already eliminated ∴ group must be CHO). Subtracting CHO from $C_8H_8O_2$ leaves C_7H_7O.
	11	yes	Need to go round the loop again. There are 2 doublets in the region 8.0–6.6 δ of 2 hyrogen each, so these are likely to be different hydrogens attached to a benzene ring, i.e., a disubstituted ring.
	6	yes	
	9	no	
	10	no	ArH present.
	8	yes	p-disubstitution with different substituents. Subtracting C_6H_4 from C_7H_7O leaves CH_3O.
	11	no	
6.6–4.5 δ	12	no	
Above 4.5 δ	13	yes	Isolated CH_3 group. All peaks accounted for. This must be CH_3O—.

Conclusion: Groups found CH_3O—, CHO

The compound is: 

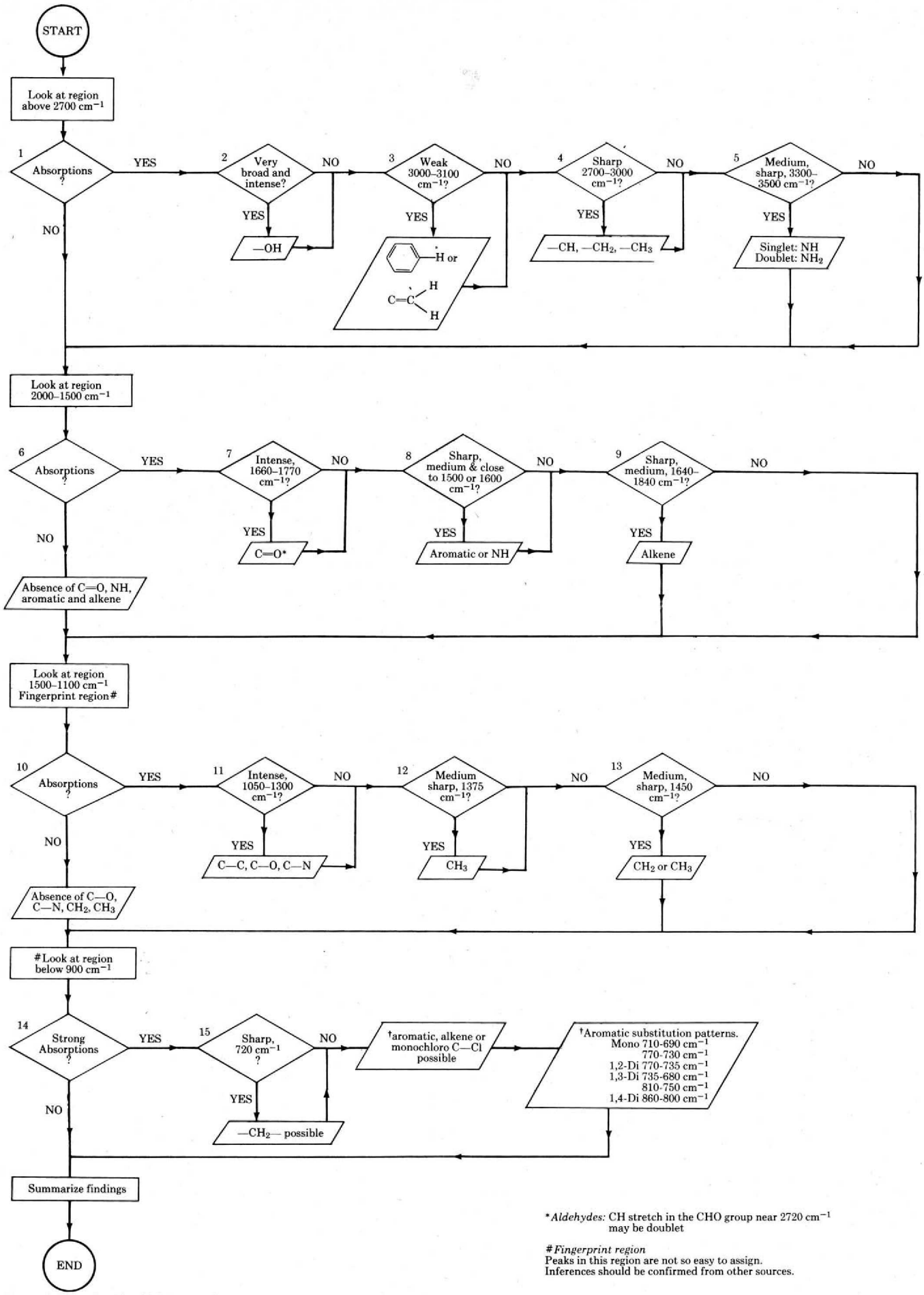


Figure 1. Flow chart for IR interpretation.

Figure 3 shows the proton NMR flow chart. This is somewhat longer and more comprehensive than the IR chart, but the approach is the same. The NMR spectrum is examined region by region starting at low field (high δ number). From the integrated intensities and splitting patterns within each region the student learns to recognize the patterns which may be attributed to definite groupings of atoms within the molecule. The exact values of chemical shifts are not used at this stage but can be used later in confirming the structure.

The flow chart does not require a detailed knowledge of chemical shift, but students are encouraged to refer to tables of chemical shifts to confirm or to modify their overall conclusions.

Figure 4 shows the NMR spectrum of *p*-methoxybenzaldehyde and Table 2 responses to the flow chart questions for this compound.

Using the Flow Charts

Both the IR and NMR charts have been used as part of our teaching for four years. Compared to the groups who had not used flow charts, those who use them are

(1) impressively quicker,
(2) more competent,
(3) more confident,
(4) and progress more quickly and more confidently with these topics than with others of comparable difficulty where flow charts have not been used.

Flow charts offer the advantages of enjoyment while using them and the opportunity to work at one's own pace. The teacher is free to spend more time dealing with individual problems.

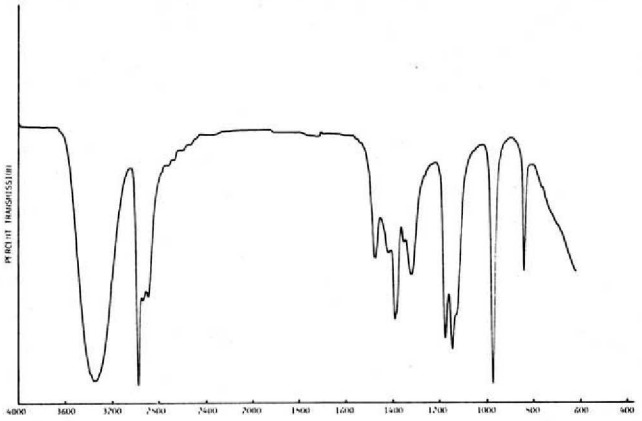


Figure 2. Spectrum of propan-2-ol.

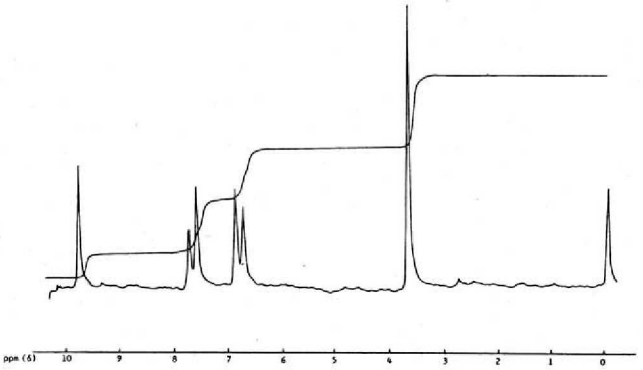


Figure 4. NMR spectrum of $C_8H_8O_2$ (no peaks removed by D_2O).

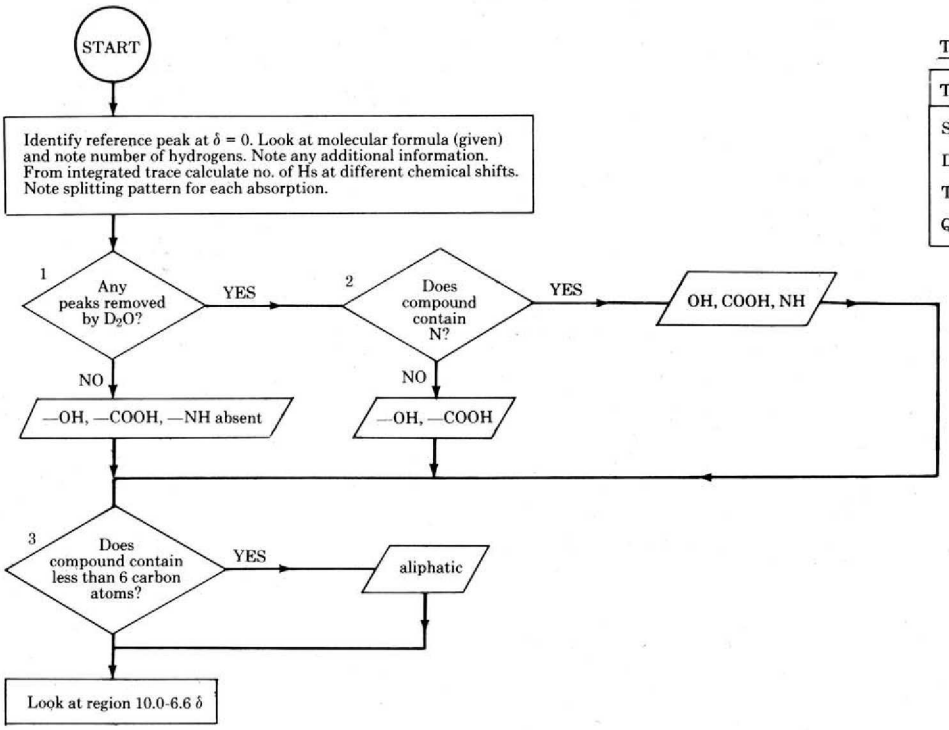
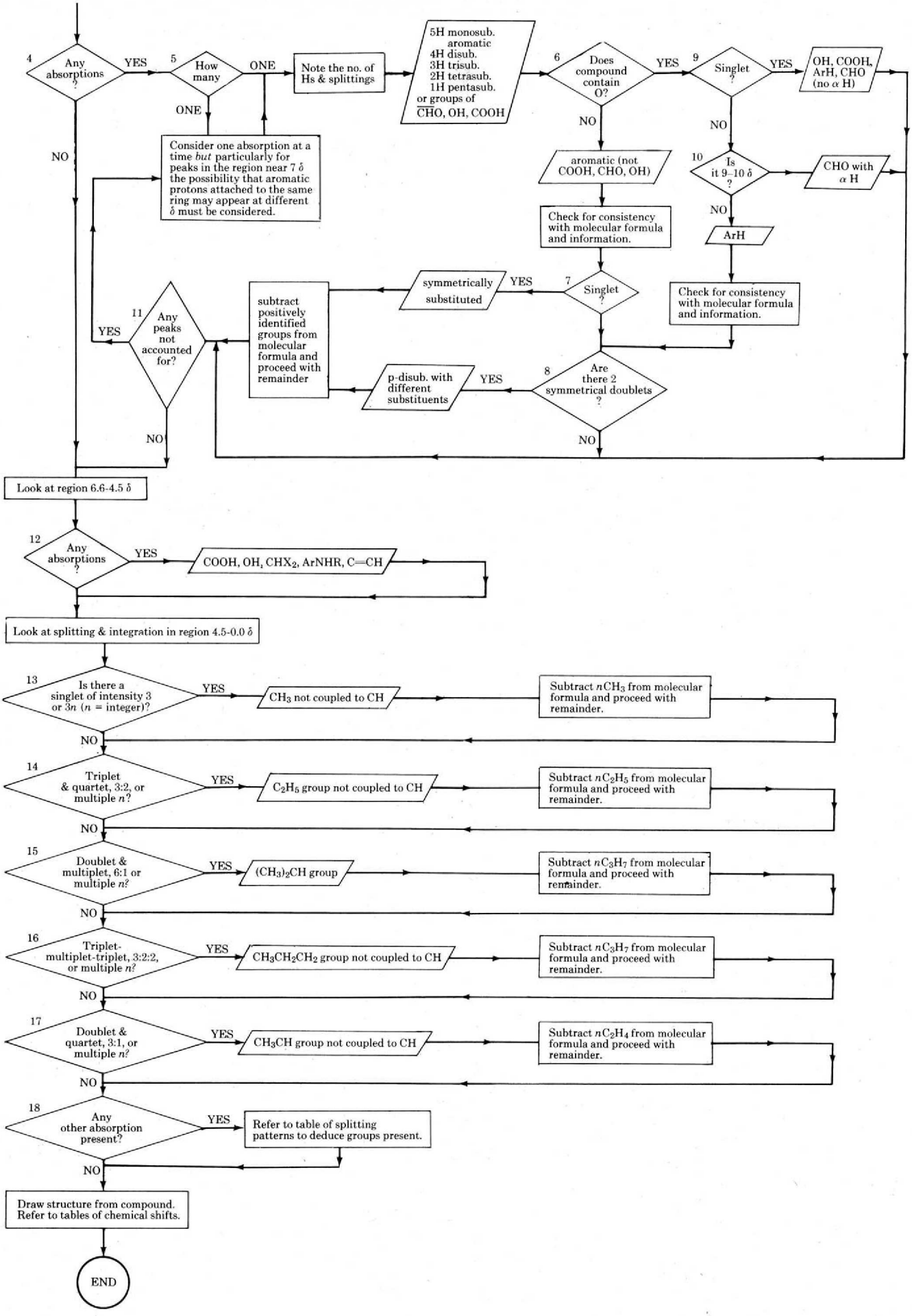


Table of Splitting Patterns

Type of Signal	Inference
Singlet	No adjacent (coupling) hydrogens
Doublet 1:1	1 adjacent hydrogen
Triplet 1:2:1	2 adjacent equivalent hydrogens
Quartet 1:3:3:1	3 adjacent equivalent hydrogens

Figure 3. Flow chart for NMR interpretation, (continued on following page).


4 Any absorptions ?
YES
5 How many
ONE
Note the no. of Hs & splittings
5H monosub. aromatic
4H disub.
3H trisub.
2H tetrasub.
1H pentasub.
or groups of CHO, OH, COOH
6 Does compound contain O?
YES
9 Singlet ?
YES
OH, COOH, ArH, CHO (no α H)
NO
ONE
Consider one absorption at a time but particularly for peaks in the region near 7 δ the possibility that aromatic protons attached to the same ring may appear at different δ must be considered.
NO
aromatic (not COOH, CHO, OH)
10 Is it 9–10 δ ?
CHO with α H
NO
Check for consistency with molecular formula and information.
ArH
Check for consistency with molecular formula and information.
7 Singlet ?
symmetrically substituted
YES
11 Any peaks not accounted for?
YES
subtract positively identified groups from molecular formula and proceed with remainder
p-disub. with different substituents
YES
8 Are there 2 symmetrical doublets ?
NO
NO
Look at region 6.6-4.5 δ
12 Any absorptions ?
YES
COOH, OH, CHX2, ArNHR, C=CH
Look at splitting & integration in region 4.5-0.0 δ
13 Is there a singlet of intensity 3 or 3n (n = integer)?
YES
CH3 not coupled to CH
Subtract nCH3 from molecular formula and proceed with remainder.
NO
14 Triplet & quartet, 3:2, or multiple n?
YES
C2H5 group not coupled to CH
Subtract nC2H5 from molecular formula and proceed with remainder.
NO
15 Doublet & multiplet, 6:1 or multiple n?
YES
(CH3)2CH group
Subtract nC3H7 from molecular formula and proceed with remainder.
NO
16 Triplet-multiplet-triplet, 3:2:2, or multiple n?
YES
CH3CH2CH2 group not coupled to CH
Subtract nC3H7 from molecular formula and proceed with remainder.
NO
17 Doublet & quartet, 3:1, or multiple n?
YES
CH3CH group not coupled to CH
Subtract nC2H4 from molecular formula and proceed with remainder.
NO
18 Any other absorption present?
YES
Refer to table of splitting patterns to deduce groups present.
NO
Draw structure from compound. Refer to tables of chemical shifts.
END