A Study of the Infra-Red Absorption Spectra of Some Alkyl Substituted Carbostyrils

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Characteristic absorption bands, originating in the out-of-plane hydrogen deformation vibrations of an aromatic ring, appear in the infra-red spectrum between 1225 and 650 reciprocal centimeters ($cm.^{-1}$). Through the judicious use of the known correlations between such band positions and types of aromatic substitution, the organic chemist can show, in a surprisingly large number of cases, what product or products were formed from reactions yielding isomeric compounds.

For hetercyclic aromatics, such as quinoline, the correlations are much less reliable chiefly because of a lack of spectra from which to make deductions. Bellamy[1] discusses admirably the correlations for some pyridine and quinoline compounds and notes that the benzene correlations hold for a number of quinoline compounds when each ring is considered separately.

The present study was undertaken for the following reasons—

1. To obtain some infra-red spectra of 2-quinolones since references are practically non-existent in the literature.[2]

2. To correlate observed absorption bands in the 1000 to 650 $cm.^{-1}$ region with structure.

3. To illustrate the use of the infra-red spectra for determination of the compound isolated from a reaction which could be of two different isomeric species.

Conclusions

We conclude from this study that the unknown compound studied by infra-red absorption spectra is *most likely* to be 1,4,7-trimethylcarbostyril. The following evidence is cited for this conclusion:

1. Steric effects favor a ring closure para to the methyl group in the compound N-methyl-m-acetoacettoluide; a study of Hirschfield models supports this view.

2. The few papers which discuss the synthesis of comparable quinoline compounds state that the major product of the possible 1,4,7 and 1,4,5-quinoline isomers is the 1,4,7-isomer.

3. The absence of a medium strong to strong band in the infra-red spectrum both for the known 1,4,6-trimethylcarbostyril and the unknown plus the presence of a 700 band in 8-hydroxyquinoline, beta-picoline and many other compounds containing three free hydrogen atoms indicates that only two free hydrogen atoms are available in the unknown compound. (This statement is made with reservations until it becomes possible to carry out confirmatory work on comparable quinolines or carbostyrils containing three free hydrogens in the carbocyclic ring.)

4. The striking similarities between the spectra of the known 1,4,6-trimethylcarbostyril and the unknown compound in the regions 1100-1000; 900-840 and near 805 cm.$^{-1}$ offers additional good evidence for favoring the 1,4,7-trimethylcarbostyril isomer.

It is preferable, of course, to obtain final proof for any proposed structure by a synthetic method. This proof has not been found feasible as yet.

Literature Cited

1. BELLAMY, L. J. 1954. The Infra-red Spectra of Complex Molecules. John Wiley and Sons, Inc., New York.

2. WITKOP, B., J. B. PATRICK, AND M. ROSENBLUM. 1951. Ring effects in autoxidation. J. Am. Chem. Soc. **73**: 2641.