



infrared tabulation of spectral data

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preface

During the past three decades the parallel development of both the theory of infrared spectroscopy and the collection and interpretation of an immense amount of infrared data has allowed chemists to correlate changes in the group frequency of a chromophore with the steric and electronic effects imposed on that chromophore by the rest of the molecule. It was inevitable, however, as such correlations became more generalized, that much of the detailed information contained in a spectrum would be lost when these generalizations were used as interpretive aids.

Indeed, while broad generalizations have considerable pedagogical value, the practical chemist must rely on more specific examples upon which to draw his analogies. In general, this necessitates a foray into the various collections of published spectra or to the original literature. While retrieval of the infrared spectrum of a specific compound is usually straightforward, collecting sufficient examples to provide adequate analogies to the problem in hand can be both a time-consuming and frustrating task. In order that such undertakings may be simplified in the future, we have collected and tabulated the data presented in this book.

So that the reader may make their own generalization concerning a specific problem we briefly describe, at the beginning of each chapter, those steric, electronic, and solute-solvent interactions which bring about changes in the characteristic group frequencies. The tables which follow the brief discussions then show changes in the group frequency as the electronic and steric environment around the group are varied. We have attempted to maintain a consistent order in which these variations are presented from chapter to chapter.

A glance at the chapter covering ketones, page 175, which is the most extensive chapter in the book, shows how these variations have been arranged. Initially the aliphatic side chains of the acyclic system are extended first on one side of the chromophore and then on the other; this is followed by branching of the side chains and then substitution of electronegative groups (halogens, carbon, nitrogen, oxygen, and so on). Aliphatic and then aromatic unsaturation follows, after which these same permutations are applied to the cyclic systems. Finally, specific classes of ketones, such as α - and β -diketones and diazoketones, are covered.

Since solute-solvent interactions and hydrogen bonding can cause significant changes in the group frequency we have included, where appropriate, a discussion of these effects in the introductions to the chapters. In addition, at the beginning of each table, we have shown how various solvents change the group frequency for the simplest members of the series. We have, where possible, given the solvent in which the spectrum was measured and the original literature reference. In those few cases when

no mention was made of the solvent, *sng* (solvent not given) is indicated.

The intensities of the absorption bands in the tables are strong unless shown as medium (m) or weak (w); shoulders are indicated by an asterisk (*). When group frequencies for two different functional groups are included in the tables, the frequencies relating to the chapter in which the example is given are shown first, followed by the remaining absorptions in decreasing wavenumber.

We have included all of those organic functional groups which have characteristic group frequencies. Starting with X-H single-bond vibrations (including main group hydrides) we continue with C-C vibrations, followed by C-N, C-O, N-N, and N-O vibrations. Since the organic chemist now uses a wide variety of inorganic and organometallic intermediates, we have included chapters on thionyl and phosphoryl compounds, as well as main group and transition metal compounds.

In addition, we have included the complete spectra of some sixty common organic solvents and impurities since the absorptions arising from these contaminants frequently confuse the interpretation of a spectrum.

Finally, we would like to thank all of our colleagues who have encouraged and helped us in this endeavor, as well as Dan Hightower and Penny Pounder for the artwork and Marci Hazard and Avril Orloff for the typing and layout.

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