# NMR Spectral Data: A Compilation of Aromatic Proton Chemical Shifts in Mono- and Di-Substituted Benzenes

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NMR chemical shifts for protons directly attached to mono- and di-substituted benzenes are compiled from the literature. Data for 1053 sets of data are presented. The data have been examined for reliability using criteria which include high spectral quality, rigorous experimental technique, and sufficient description to assure correct interpretation of results. The data, presented in tabular form, include compound name and formula, solvent employed, concentration, temperature, chemical shift, and observation frequency. Other NMR-related data are not given. An author index is included. The data and references cover the literature to June 1976.

Key words: Aromatic proton chemical shifts; mono- and di-substituted benzenes; NMR spectral data.

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## 1. Introduction and Scope

The chemical literature contains hundreds of thousands of pieces of nuclear magnetic resonance (NMR) data in numerical form, including chemical shifts, spin-spin couplings, relaxation times, etc., for a wide variety of nuclei. The nature of these data varies extremely widely, as do the methods of reporting the various spectral measurements and the (sometimes) derived NMR parameters. The latter two factors, as much as the sheer volume of numerical data, preclude any automated, omnibus approach to data storage, retrieval, and utilization. Furthermore, it has been recognized for some time that these data are of widely varying quality for a variety of reasons, including:

(1) Much of the literature data was obtained for qualitative, confirmatory purposes in the course of more purely chemical investigations. Many of these spectral determinations were performed in a relatively crude, routine manner, and often on solutions of poorly defined and/or documented natures.

(2) Even when the problems discussed in (1) were avoided, many analyses of the data were very approximate, incomplete, and even casual.

(3) In a substantial number of cases, the reporting of the raw data (e.g., observed line frequencies) is so incomplete that it is not possible to assess the quality of the data. Sometimes, high quality chemical shift data are obtained and reported completely, but the measurements are not referenced or convertible to the standard δ-scale.

For these reasons it was decided to exclude from this compilation all data which are not demonstrably of high quality and reliability. This general guideline has led to a rejection rate for the NMR literature data of well above 95 percent, and quite possibly above 98 percent.

Careful selection of data is particularly important in the compound class chosen for this compilation, viz., the aromatic proton chemical shifts for some simple substituted benzenes. In such molecules, the four or five aromatic protons constitute spin systems which are not, except in a very few instances, amenable to the simple "first-order" type of analysis with which most non-spectroscopic chemical practitioners are familiar. It is indeed these simple and very approximate analyses (often of a qualitative nature) which are applied to the vast majority of NMR spectral data obtained. Thus at the outset it was recognized that this compilation would need to be restricted to data from compounds where (a) very high quality experimental spectra and line frequency measurements were obtained, (b) rigorous analytical methods were employed, and (c) sufficient detail and documentation of the analyses were

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given or very clearly implied. With only a few exceptions, a simple, operationally useful criterion was applied: data were compiled only for cases where computer-aided spectral analyses were performed. In a very few instances, other methods were equally valid, and such cases have been considered.

Even with these limitations, a number of practical reasons dictated that a selected set of sub-classes of aromatic proton chemical shift data would be the subject of this compilation. Taking all factors into account, it was decided to limit the scope of this compilation as follows:

A. This compilation is limited to the compilation of aromatic proton chemical shifts. Thus, the shifts of non-aromatic protons in the same molecules are not included, nor are any coupling constants or other type of NMR data.

B. The compound class would be limited to mono- and di-substituted benzenes (and benzene itself) with the following additional restrictions:

(i) Polynuclear aromatic compounds were excluded, as were all cases where the benzene ring is fused to a heterocyclic ring. (The tables of this compilation include a very few such samples, but only when the compounds are very closely related to other included compounds, and all quality criteria are met.)

(ii) Protonated aromatic compounds, and other solutions containing aromatic systems strongly perturbed by ion formation are not included, because very little data on such systems has been obtained with the requisite precision. Exceptions are such included compounds as phenyllithium, phenylmagnesium halides, and a few anilinium and phosphonium salts.

(iii) Likewise, few data are included on aqueous solutions, for the reasons of lack of adequate referencing and/or analytical accuracy. In fact, very few mono- or di-substituted benzene shifts appear to have been determined in aqueous media.

Within this context, the literature was searched by a variety of means, including the following:

1. Line-by-line or page-by-page search of the major scientific journals known to contain NMR data of adequate quality.

2. Detailed manual and computer-assisted searching of the extensive listings in the Nuclear Magnetic Resonance Abstracts and Index published by the Preston Technical Abstracts Company of Niles, Illinois.

3. Scrutiny of the major texts and reference books on relevant areas of NMR spectroscopy, including available issues of such serial publications as Annual Review of NMR Spectroscopy, Progress in Nuclear Magnetic Resonance Spectroscopy, NMR—Basic Principles and Progress and the Special Periodical Reports on Nuclear Magnetic Resonance (Chemical Society of London, England).

4. Careful scrutiny of the references in more recent articles where NMR data are found, to help insure that as little as possible was missed in the older literature.

This compendium had as its goal the compilation of shifts appearing in the literature up to and including journal issues dated through the month of June 1976. In a few, relatively less important cases, unavoidable delays made the cutoff date as much as a few months earlier. Because of the analytical criteria discussed above, very little data adequate for the purposes of this compilation appeared before early 1965, when suitable computer programs became generally available.

Finally, one extensive collection of data of unquestionably good quality was obtained from Dr. S. Castellano of Carnegie-Mellon University, who kindly consented to the appearance of these data in our compilation.

## 2. Explanation of Tables

1. Entry Number: A serial listing of each data set, beginning with entry 001 for each table.

2. Molecular Formula: The elements are arranged in standard *Chemical Abstracts* order. Neither the molecular formula nor the compound name are repeated for multiple entries pertaining to the same compound.

3. Name: For each compound a common name is provided. The choice of names is based on utility rather than Chemical Abstracts or IUPAC rigor. The following examples illustrate the types of names used: *p*-fluorophenol, *p*-nitrostyrene, biphenyl, 9-iodofluorene, *o*-methoxyacetophenone, *m*-cresol acetate, etc.

In a few cases, where the positions of substituents in the molecule are of necessity designated in the usual numerical fashion, this numbering conflicts with the uniform numbering system adopted for the aromatic protons, as indicated below. This conflict is perforce left unresolved, but the operational principle is that the numbered designations of the protons for which NMR shifts are given refer explicitly to the entries in the column marked "Substituents" and to the structural formula and proton code designations given at the top of each table.

4. Substituent(s): The structure of the substituents is given in the columns marked A (mono), or A and B (ortho, meta, and para). As indicated in the structural code formula at the top of each table, substituent A is always that at C-1, with substituent B being at C-2 (ortho-disubstituted compounds), C-3 (meta) or C-4 (para), respectively. Thus all proton shifts are unambiguously designated.

In a number of cases, the complexity of the molecules was such as to render the above designation of substituents and proton designations extremely cumbersome. In such instances, a single molecular formula appears centered in the "Substituents" column. Such instances are immediately obvious, and in these, a complete molecular formula with proton designation numbers is given.

5. Proton Chemical Shifts, $\delta_H$: All shifts are reported on the conventional δ-scale, i.e., $\delta_H$ (tetramethylsilane, TMS) = 0.00 by definition, with increasing δ-values referring to shifts appearing at lower applied fields (or higher frequencies); the dimensions of the δ-scale are parts-per-million (ppm).

Shifts are reported to either 2 or 3 decimal places, according to the compiler's judgement of the accuracy with which the line frequencies were determined, the analysis performed, and the solution conditions defined. In some cases, data given in the original publication to three decimal places were rounded off to two.

Where three decimal places are given, this should be taken primarily as a judgement concerning the superior precision and reliability of the chemical shift values so reported, even for those cases where the last figure is probably subject to a ±2 or 3 implied error limit for reasons of statistical analysis and/or poorly defined concentration or temperature. Because of the latter sources of systematic error, all three-decimal place data are probably accurate to no better and ±2 in the last place, and the uncertainty is possibly as much as ±3 or even 4 in some cases. Chemical shifts given to two decimal places are believed to be accurate to at least ±1 in the second decimal place. (It was clear in at least a few cases that some of the two-decimal place data are really more precise than the authors conservatively claimed.)

6. Solvents: For space reasons, the solvents are designated in tables I-IV by code numbers which are given in both serial and alphabetical order in table V. Since solvent isotope effects, if any such exist, are certainly much smaller than other factors affecting the precision and accuracy of the reported shifts, a single solvent designation is made for an unlabelled and a deuterated solvent, e.g., code number 8 is used to refer to both acetone and acetone-$d_6$. Code number 1 is used for the several shifts obtained on what NMR practitioners normally refer to as a "neat liquid". In fact, it is the pure substance adulterated only by a variable small amount of the reference substance, usually tetramethylsilane.

Because of the well-known existence of solvent effects on chemical shifts, data for a particular compound are given in all solvents for which good quality data were found. In a few cases, two measurements at approximately the same concentration in the same solvent were reported. The very close agreement of the two or more reports in such cases gives a measure of the overall precision—and perhaps accuracy—of these data. In other cases two reports may differ by distinctly nontrivial amounts; the compiler was unable to make an objective choice between the conflicting values, even after close scrutiny of the original papers. Hence both values were reported and caution is recommended in the use of such data.

Table I contains a sizable number of reports on the chemical shift of benzene at several concentrations in several solvents, and measured at more than one spectrometer frequency. These data are useful for their own sake, but it is hoped that an intercomparison of different values obtained by different authors may also provide valuable calibration guidance for interpreting data on other compounds in these solvents.

7. Concentration: Where only a numerical value is given in this column, it refers to the percentage of the substrate in the indicated solvent. In the majority of works, the distinction between w/w, w/v or other types of percentage concentration is not made, and would probably be of dubious meaning if it were. Thus the concentration percentages should be taken as only approximate, although where more than one concentration of a substrate in a given solvent is reported in a paper, the relative concentrations are probably of good precision.

In some cases the authors gave the solute concentration as molarity, with insufficient data to convert this to a w/v or other percent concentration. In these cases, the concentration is given as e.g., 0.5 M. In the cases of the "neat liquid" samples (solvent code No. 1), concentrations are given as 100 (%) when it is clear that only a few (less than 5) percent TMS was added as the internal reference, whereas the concentration may be designated as 90 percent or 80 percent, etc., if larger amounts of tetramethylsilane were explicitly indicated. A concentration indication of 0 percent is used for those cases where chemical shifts were carefully extrapolated to "infinite dilution". In a number of instances, more than one concentration in a particular solvent is given so that the reader may assess for himself some idea of the precision with which solutions are prepared, data gathered, and analyses performed. In a very few cases, no solvent is specified, and it is presumed that the neat liquid was employed; such data are rarely included, and then only for those compounds where the spectral analysis precision is very high, and the compound of particular intrinsic interest.

8. Temperature: The measurement of probe temperatures is poorly done in many (perhaps most) otherwise carefully NMR spectroscopic investigations, for reasons both technical and historical. Where the temperature has been given by the authors, it is provided in the tables, and otherwise the general descriptor "x" is given for unspecified or inadequately specified references to temperature. In most such cases, the sample temperature will be in the range 22-38 °C. Over such a range, chemical shift variations are normally less than 0.01 ppm for the type of protons in the compounds of this compilation. While this may seem unsatisfactory to the purist, the exclusion of all data for which accurate temperature measurements are not reported would result in a compilation containing very few shifts indeed.

9. Spectrometer Frenquency: The spectrometer frequency in megahertz (MHz) is given, with the designation "60 or 100" used where an author gives the chemical shifts only as the final $\delta_H$ values, rather than the raw, observed frequencies. In such investigations, one spectrometer frequency may be used for some of the data, and another for the remainder of the data, or two spectrometers used to check the same sample. These spectrometer frequencies are given so that one can compare the value obtained when a

given sample is reported at the same or similar concentrations in the same solvent.

10. Reference: The complete literature citation is given in the list of references at the end of the compilation, along with an author index.

11. Footnotes: Attention is drawn to footnote indicators *a-e* in the data tables. These footnotes are stated only once at the end of each table while the symbols *, †, §, and ‖ refer only to the page on which they appear, with the explanatory material appearing as footnotes on that page.

## 3. Acknowledgements

A compilation of this magnitude is clearly not the work of a single individual, and it is a pleasure to acknowledge those without whom this compilation would have been smaller, later, and infinitely less reliable. Omnibus apologies are offered to those who helped but are not acknowledged explicitly. Thanks are due to Mr. G. C. Luce and Mr. L. W. Richardson who provided timely and accurate proofreading assistance. Special thanks are also due to Dr. S. Castellano of the Carnegie-Mellon University, Pittsburgh, Pennsylvania, for providing us with the excellent data on a substantial number of monosubstituted benzenes which have not been reported in the open literature.

The help provided by Mr. Seaton T. Preston, Jr., of the Preston Technical Abstracts Company, Niles, Illinois, in making available a complete set of the NMR Abstracts is greatly appreciated, for without this the coverage of the literature would have been considerably less extensive. Appreciation is also expressed to Dr. E. D. Becker, Mr. E. Leininger, and Mr. W. H. Jennings of the National Institutes of Health for providing a sizeable computer printout from the computer-stored retrieval system for the Preston Abstracts. We thank them also for locating and providing us with copies of articles from difficult-to-obtain journals.

Throughout the course of this compilation work and preparation of the report, we have enjoyed the constructive and cheerful guidance of Drs. L. H. Gevantman and S. A. Rossmassler of the Office of Standard Reference Data, National Bureau of Standards. They have been unfailingly cordial, helpful and patient.

Finally, it is obvious that a sizable compilation of data does not assemble, type, and produce itself. It is a pleasure to acknowledge the excellent work performed by Mrs. L. M. King and Mrs. L. W. Shapiro. Their performance under considerable time pressure was as graceful as it was efficient.

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

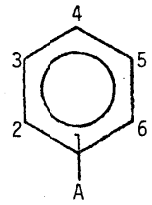


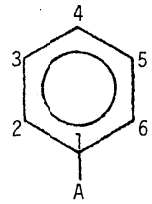

Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H{}^a$ 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 055 | $C_6H_5F$ | fluorobenzene | F | 7.047 | 7.339 | 7.130 | 22 | 10 | 38 | 60 | 58 |
| 056 | | | F | 6.947 | 7.208 | 7.014 | 25 | 0[c] | 38 | 60 | 57 |
| 057 | | | F | 6.921 | 7.183 | 6.983 | 25 | 10 | 38 | 60 | 31, 57,58 |
| 058 | | | F | 6.878 | 7.107 | 6.921 | 25 | 50 | 38 | 60 | 57 |
| 059 | | | F | 6.871 | 7.079 | 6.902 | 25 | 80 | 38 | 60 | 57 |
| 060 | | | F | 6.870 | 7.076 | 6.900 | 25 | 100 | 38 | 60 | 57 |
| 061 | | | F | 7.082 | 7.366 | 7.163 | 26 | 10 | 38 | 60 | 58 |
| 062 | | | F | 7.145 | 7.408 | 7.187 | 28 | 10 | 38 | 60 | 58 |
| 063 | | | F | 7.062 | 7.340 | 7.128 | 29 | 10 | 38 | 60 | 58 |
| 064 | $C_6H_5I$ | iodobenzene | I | 7.510 | 6.846 | 7.079 | 1 | 90 | x[d] | 100 | 52 |
| 065 | | | I | 7.520 | 6.863 | 7.099 | 1 | 100 | 36 | 60 | 27 |
| 066 | | | I | 7.707 | 7.105 | 7.330 | 2 | 0 | 52 | 60 | 11 |
| 067 | | | I | 7.643 | 7.041 | 7.253 | 4 | 0 | x | 100 | 51 |
| 068 | | | I | 7.653 | 7.045 | 7.257 | 4 | 0 | 52 | 60 | 11 |
| 069 | | | I | 7.637 | 7.029 | 7.245 | 4 | 10 | 36 | 60 | 27 |
| 070 | | | I | 7.738 | 7.172 | 7.387 | 8 | 0 | 52 | 60 | 11 |





PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

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| 056 | | | F | 6.947 | 7.208 | 7.014 | 25 | 0[c] | 38 | 60 | 57 |
| 057 | | | F | 6.921 | 7.183 | 6.983 | 25 | 10 | 38 | 60 | 31, 57,58 |
| 058 | | | F | 6.878 | 7.107 | 6.921 | 25 | 50 | 38 | 60 | 57 |
| 059 | | | F | 6.871 | 7.079 | 6.902 | 25 | 80 | 38 | 60 | 57 |
| 060 | | | F | 6.870 | 7.076 | 6.900 | 25 | 100 | 38 | 60 | 57 |
| 061 | | | F | 7.082 | 7.366 | 7.163 | 26 | 10 | 38 | 60 | 58 |
| 062 | | | F | 7.145 | 7.408 | 7.187 | 28 | 10 | 38 | 60 | 58 |
| 063 | | | F | 7.062 | 7.340 | 7.128 | 29 | 10 | 38 | 60 | 58 |
| 064 | $C_6H_5I$ | iodobenzene | I | 7.510 | 6.846 | 7.079 | 1 | 90 | x[d] | 100 | 52 |
| 065 | | | I | 7.520 | 6.863 | 7.099 | 1 | 100 | 36 | 60 | 27 |
| 066 | | | I | 7.707 | 7.105 | 7.330 | 2 | 0 | 52 | 60 | 11 |
| 067 | | | I | 7.643 | 7.041 | 7.253 | 4 | 0 | x | 100 | 51 |
| 068 | | | I | 7.653 | 7.045 | 7.257 | 4 | 0 | 52 | 60 | 11 |
| 069 | | | I | 7.637 | 7.029 | 7.245 | 4 | 10 | 36 | 60 | 27 |
| 070 | | | I | 7.738 | 7.172 | 7.387 | 8 | 0 | 52 | 60 | 11 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED

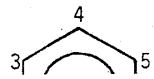



Table I

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED

BENZENES (AND IN BENZENE ITSELF)

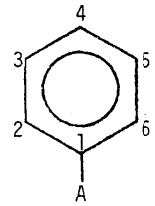



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 001 | $C_6H_5Br$ | bromobenzene | Br | 7.294 | 6.948 | 7.019 | 1 | 90 | x[d] | 100 | 52 |
| 002 | | | Br | 7.301 | 6.950 | 7.022 | 1 | 100 | 36 | 60 | 27 |
| 003 | | | Br | 7.495 | 7.237 | 7.297 | 2 | 0[e] | 52 | 60 | 10 |
| 004 | | | Br | 7.445 | 7.173 | 7.220 | 4 | 0 | 52 | 60 | 10 |
| 005 | | | Br | 7.438 | 7.174 | 7.216 | 4 | 0 | x | 100 | 51 |
| 006 | | | Br | 7.430 | 7.154 | 7.202 | 4 | 10 | 36 | 60 | 27 |
| 007 | | | Br | 7.533 | 7.312 | 7.357 | 8 | 0 | 52 | 60 | 10 |
| 008 | | | Br | 7.410 | 7.095 | 7.148 | 9 | 0 | 52 | 60 | 10 |
| 009 | | | Br | 7.467 | 7.192 | 7.242 | 10 | 0 | 52 | 60 | 10 |
| 010 | | | Br | 7.505 | 7.263 | 7.310 | 11 | 0 | 52 | 60 | 10 |
| 011 | | | Br | 7.400 | 7.092 | 7.147 | 12 | 0 | 52 | 60 | 10 |
| 012 | | | Br | 7.522 | 7.287 | 7.333 | 13 | 0 | 52 | 60 | 10 |
| 013 | | | Br | 7.495 | 7.273 | 7.327 | 14 | 0 | 52 | 60 | 10 |
| 014 | | | Br | 7.512 | 7.298 | 7.338 | 15 | 0 | 52 | 60 | 10 |
| 015 | | | Br | 7.383 | 7.068 | 7.125 | 25 | 10 | 38 | 60 | 53 |
| 016 | $C_6H_5BrMg$ | phenylmagnesium bromide | MgBr | 7.64 | 7.02 | 6.98 | 10 | 1M | 33 | 60 | 36 |
| 017 | | | MgBr | 7.64 | 7.00 | 6.98 | 10 | 1M | x | 100 | 49 |
| 018 | | | MgB | 7.656 | 7.067 | 7.000 | 10 | 10 | 36 | 60 | 95 |
| 019 | | | MgB | 7.640 | 6.952 | 6.870 | 27 | 10 | 36 | 60 | 95 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

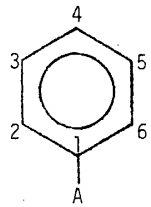
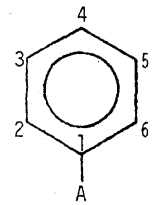



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 073 | $C_6H_5I$ | iodobenzene | I | 7.717 | 7.127 | 7.343 | 11 | 0[e] | 52 | 60 | 11 |
| 074 | | | I | 7.613 | 6.960 | 7.182 | 12 | 0 | 52 | 60 | 11 |
| 075 | | | I | 7.730 | 7.143 | 7.362 | 13 | 0 | 52 | 60 | 11 |
| 076 | | | I | 7.698 | 7.143 | 7.363 | 14 | 0 | 52 | 60 | 11 |
| 077 | | | I | 7.715 | 7.153 | 7.363 | 15 | 0 | 52 | 60 | 11 |
| 078 | | | I | 7.593 | 6.940 | 7.168 | 25 | 10 | 38 | 60 | 53 |
| 079 | $C_6H_5Li$ | phenyllithium | Li | 8.01 | 7.04 | 6.96 | 10 | 1M | x[d] | 100 | 49 |
| 080 | | | Li | 8.02 | 7.02 | 6.96 | 10 | 1.0M | 33 | 60 | 36 |
| 081 | | | Li | 8.034 | 7.052 | 6.974 | 10 | 10 | 36 | 60 | 95 |
| 082 | $C_6H_5NO$ | nitrosobenzene | NO | 7.813 | 7.548 | 7.610 | 4 | 10 | 36 | 60 | 28 |
| 083 | $C_6H_5NO_2$ | nitrobenzene | $NO_2$ | 8.106 | 7.480 | 7.642 | 1 | 90 | x | 100 | 52 |
| 084 | | | $NO_2$ | 8.106 | 7.485 | 7.648 | 1 | 100 | 36 | 60 | 28 |
| 085 | | | $NO_2$ | 8.203 | 7.550 | 7.702 | 2 | 0 | 52 | 60 | 10 |
| 086 | | | $NO_2$ | 8.207 | 7.512 | 7.633 | 4 | 0 | x | 100 | 51 |
| 087 | | | $NO_2$ | 8.203 | 7.512 | 7.633 | 4 | 0 | 52 | 60 | 10 |
| 088 | | | $NO_2$ | 8.191 | 7.520 | 7.653 | 4 | 10 | 36 | 60 | 28 |
| 089 | | | $NO_2$ | 8.238 | 7.670 | 7.820 | 8 | 0 | 52 | 60 | 10 |
| 090 | | | $NO_2$ | 8.160 | 7.561 | 7.721 | 8 | 70 | 36 | 100 | 18 |
| 091 | | | $NO_2$ | 8.158 | 7.398 | 7.520 | 9 | 0 | 52 | 60 | 10 |

Table I

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)




| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 092 | $C_6H_5NO_2$ | nitrobenzene | $NO_2$ | 8.207 | 7.545 | 7.678 | 10 | 0[e] | 52 | 60 | 10 |
| 093 | | | $NO_2$ | 8.237 | 7.630 | 7.768 | 11 | 0 | 52 | 60 | 10 |
| 094 | | | $NO_2$ | 8.148 | 7.393 | 7.520 | 12 | 0 | 52 | 60 | 10 |
| 095 | | | $NO_2$ | 8.263 | 7.662 | 7.803 | 13 | 0 | 52 | 60 | 10 |
| 096 | | | $NO_2$ | 8.222 | 7.658 | 7.807 | 14 | 0 | 52 | 60 | 10 |
| 097 | | | $NO_2$ | 8.225 | 7.660 | 7.805 | 15 | 0 | 52 | 60 | 10 |
| 098 | | | $NO_2$ | 8.090 | 7.394 | 7.535 | 25 | 10 | 38 | 60 | 76 |
| 099 | $C_6H_5N_3$ | azidobenzene | $N_3$ | 6.925 | 7.234 | 7.027 | 4 | 10 | 36 | 60 | 95 |
| 100 | $C_6H_5NaO$ | sodium phenolate | ONa | 6.435 | 6.819 | 6.101 | 28 | 10 | 36 | 60 | 95 |
| 101 | $C_6H_5NaO_2S$ | sodium benzenesulfinate | $SO_2Na$ | 7.557 | 7.330 | 7.269 | 5 | 10 | 36 | 60 | 95 |
| 102 | $C_6H_5NaO_3S$ | sodium benzenesulfonate | $SO_3Na$ | 7.675 | 7.343 | 7.330 | 5 | 10 | 36 | 60 | 95 |
| 103 | $C_6H_6$ | benzene | H | 7.150 | 7.150 | 7.150 | 1(=6) | 100 | x[d] | 60 | 32 |
| 104 | | | H | 7.159 | 7.159 | 7.159 | 1(=6) | 100 | x | 100 | 42 |
| 105 | | | H | 7.192 | 7.192 | 7.192 | 1(=6) | 100 | x | 60 | 65 |
| 106 | | | H | 7.146 | 7.146 | 7.146 | 1(=6) | 100 | 33 | 100 | 74 |
| 107 | | | H | 7.353 | 7.353 | 7.353 | 3 | 5 | 28 | 60 | 56 |
| 108 | | | H | 7.339 | 7.339 | 7.339 | 3 | 5 | x | 60 | 32 |
| 109 | | | H | 7.336 | 7.336 | 7.336 | 3 | 5 | 33 | 100 | 74 |
| 110 | | | H | 7.323 | 7.323 | 7.323 | 3 | 10 | x | 60 | 65 |

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

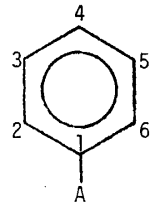



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H{}^a$ 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 111 | $C_6H_5$ | benzene | H | 7.255 | 7.255 | 7.255 | 4 | 0[e] | x[d] | 100 | 51 |
| 112 | | | H | 7.258 | 7.258 | 7.258 | 4 | 1.4 | 52 | 60 | 11 |
| 113 | | | H | 7.266 | 7.266 | 7.266 | 4 | 2 | x | 40 | 30 |
| 114 | | | H | 7.257 | 7.257 | 7.257 | 4 | 5 | x | 60 | 32 |
| 115 | | | H | 7.248 | 7.248 | 7.248 | 4 | 6 | 33 | 100 | 74 |
| 116 | | | H | 7.262 | 7.262 | 7.262 | 4 | 10 | x | 60 | 65 |
| 117 | | | H | 7.357 | 7.357 | 7.357 | 5 | 10 | x | 60 | 65 |
| 118 | | | H | 7.222 | 7.222 | 7.222 | 7 | 10 | x | 60 | 65 |
| 119 | | | H | 7.34 | 7.34 | 7.34 | 8 | 2 | 40 | 60 | 34 |
| 120 | | | H | 7.335 | 7.335 | 7.335 | 8 | 10 | x | 60 | 65 |
| 121 | | | H | 7.213 | 7.213 | 7.213 | 9 | 10 | x | 60 | 65 |
| 122 | | | H | 7.257 | 7.257 | 7.257 | 10 | 1.0M | 33 | 60 | 36 |
| 123 | | | H | 7.267 | 7.267 | 7.267 | 10 | 10 | x | 60 | 65 |
| 124 | | | H | 7.22 | 7.22 | 7.22 | 12 | 0.02M | 29 | 60 | 1 |
| 125 | | | H | 7.214 | 7.214 | 7.214 | 12 | 1.4 | 52 | 60 | 11 |
| 126 | | | H | 7.23 | 7.23 | 7.23 | 12 | 2 | 40 | 60 | 34 |
| 127 | | | H | 7.213 | 7.213 | 7.213 | 12 | 10 | x | 60 | 65 |
| 128 | | | H | 7.310 | 7.310 | 7.310 | 22 | 10 | x | 60 | 65 |
| 129 | | | H | 7.23 | 7.23 | 7.23 | 24 | 0.02M | 10 | 60 | 1 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

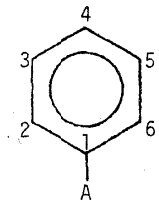



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 130 | $C_6H_6$ | benzene | H | 7.21 | 7.21 | 7.21 | 24 | 0.02M | 30 | 60 | 1 |
| 131 | | | H | 7.216 | 7.216 | 7.216 | 25 | 5 | x[d] | 60 | 32 |
| 132 | | | H | 7.213 | 7.213 | 7.213 | 25 | 10 | 38 | 60 | 53 |
| 133 | | | H | 7.34 | 7.34 | 7.34 | 26 | 2 | 40 | 60 | 34 |
| 134 | | | H | 7.352 | 7.352 | 7.352 | 26 | 10 | x | 60 | 65 |
| 135 | | | H | 7.285 | 7.285 | 7.285 | 27 | 10 | x | 60 | 65 |
| 136 | | | H | 7.360 | 7.360 | 7.360 | 28 | 10 | x | 60 | 65 |
| 137 | | | H | 7.285 | 7.285 | 7.285 | 31 | 10 | x | 60 | 65 |
| 138 | | | H | 7.341 | 7.341 | 7.341 | 32 | 10 | x | 60 | 65 |
| 139 | | | H | 7.290 | 7.290 | 7.290 | 33 | 10 | x | 60 | 65 |
| 140 | | | H | 7.318 | 7.318 | 7.318 | 34 | 10 | x | 60 | 65 |
| 141 | $C_6H_6O$ | phenol | OH | 6.733 | 7.094 | 6.815 | 4 | 10 | 36 | 60 | 28 |
| 142 | | | OH | 6.697 | 7.133 | 6.808 | 4 | 0[e] | x | 100 | 51 |
| 143 | | | OH | 6.615 | 7.020 | 6.761 | 6 | 10 | 36 | 60 | 28 |
| 144 | | | OH | 6.836 | 7.168 | 6.799 | 8 | 10 | 36 | 60 | 95 |
| 145 | | | OH | 6.838 | 7.174 | 6.803 | 8 | 1.0M | x | 100 | 9 |
| 146 | | | OH | 6.67 | 6.99 | 6.72 | 12 | 5 | x | 100 | 79 |
| 147 | | | OH | 6.816 | 7.125 | 6.767 | 37 | 10 | 36 | 60 | 95 |
| 148 | | | OH | 6.656 | 7.043 | 6.656 | 38 | 10 | 36 | 60 | 95 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

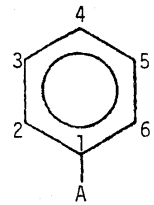



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 149 | $C_6H_5O$ | phenol | OH | 6.871* | 7.205* | 6.802* | 39* | 10 | 36 | 60 | 95 |
| 150 | | | OH | 6.673* | 7.177* | 6.609* | 40* | 10 | 36 | 60 | 95 |
| 151 | $C_6H_5S$ | thiophenol | SH | 7.10 | 7.02 | 6.95 | 12 | 5 | x[d] | 100 | 79 |
| 152 | $C_6H_7BO_2$ | phenylboronic acid | $B(OH)_2$ | 7.712 | 7.306 | 7.359 | 22 | 10 | 36 | 60 | 95 |
| 153 | $C_6H_7N$ | aniline | $NH_2$ | 6.375 | 7.033 | 6.664 | 1 | 90 | x | 100 | 52 |
| 154 | | | $NH_2$ | 6.354 | 7.009 | 6.639 | 1 | 100 | 36 | 60 | 28 |
| 155 | | | $NH_2$ | 6.647 | 7.107 | 6.693 | 2 | 0[e] | 52 | 60 | 10 |
| 156 | | | $NH_2$ | 6.520 | 7.013 | 6.610 | 4 | 0 | 52 | 60 | 10 |
| 157 | | | $NH_2$ | 6.509 | 7.006 | 6.603 | 4 | 0 | x | 100 | 51 |
| 158 | | | $NH_2$ | 6.457 | 7.008 | 6.618 | 4 | 10 | 36 | 60 | 28 |
| 159 | | | $NH_2$ | 6.356 | 7.050 | 6.692 | 6 | 17 | x | 100 | 23 |
| 160 | | | $NH_2$ | 6.637 | 7.017 | 6.553 | 8 | 0 | 52 | 60 | 10 |
| 161 | | | $NH_2$ | 6.477 | 6.985 | 6.600 | 9 | 0 | 52 | 60 | 10 |
| 162 | | | $NH_2$ | 6.542 | 6.977 | 6.530 | 10 | 0 | 52 | 60 | 10 |
| 163 | | | $NH_2$ | 6.585 | 6.990 | 6.538 | 11 | 0 | 52 | 60 | 10 |
| 164 | | | $NH_2$ | 6.480 | 6.983 | 6.595 | 12 | 0 | 52 | 60 | 10 |
| 165 | | | $NH_2$ | 6.600 | 7.000 | 6.547 | 13 | 0 | 52 | 60 | 10 |
| 166 | | | $NH_2$ | 6.637 | 7.028 | 6.577 | 14 | 0 | 52 | 60 | 10 |

*Shifts measured relative to DSS (sodium 2,2-dimethyl-2-silapentane-5-sulfonate) and converted to normal δ-scale. See Solvent Table re detail of solvents No. 39 and 40.

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

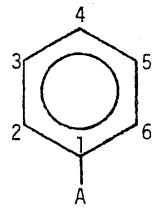



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H{}^a$ 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 167 | $C_6H_7N$ | aniline | $NH_2$ | 6.600 | 6.983 | 6.512 | 15 | 0[e] | 52 | 60 | 10 |
| 168 | $C_6H_8Ge$ | phenylgermane | $GeH_3$ | 7.44 | 7.24 | 7.28 | 4 | 0 | x[d] | 100 | 45 |
| 169 | $C_6H_8GeO$ | phenoxygermane | $OGEH_3$ | 6.67 | 6.99 | 6.72 | 12 | 5 | x | 100 | 79 |
| 170 | $C_6H_8GeS$ | thiophenoxygermane | $SGeH_3$ | 7.10 | 7.02 | 6.95 | 12 | 5 | x | 100 | 79 |
| 171 | $C_6H_8N_2$ | phenylhydrazine | $NHNH_2$ | 6.700 | 7.171 | 6.765 | 3 | 10 | 36 | 60 | 95 |
| 172 | $C_6H_8OSi$ | phenoxysilane | $OSiH_3$ | 6.76 | 7.08 | 6.82 | 12 | 5 | x | 100 | 79 |
| 173 | $C_6H_8SSi$ | thiophenoxysilane | $SSiH_3$ | 7.12 | 7.04 | 6.96 | 12 | 5 | x | 100 | 79 |
| 174 | $C_6H_8Si$ | phenylsilane | $SiH_3$ | 7.501 | 7.253 | 7.300 | 4 | 10 | 36 | 60 | 95 |
| 175 | | | $SiH_3$ | 7.52 | 7.27 | 7.32 | 4 | 0 | x | 100 | 45 |
| 176 | $C_7H_5BrO$ | benzoyl bromide | COBr | 7.877 | 7.351 | 7.555 | 1 | 100 | 36 | 60 | 95 |
| 177 | | | COBr | 8.056 | 7.468 | 7.624 | 4 | 0 | x | 100 | 51 |
| 178 | | | COBr | 8.029 | 7.466 | 7.636 | 4 | 10 | 36 | 60 | 95 |
| 179 | $C_7H_5ClO$ | benzoyl chloride | COCl | 7.928 | 7.351 | 7.537 | 1 | 90 | x | 100 | 52 |
| 180 | | | COCl | 7.930 | 7.354 | 7.504 | 1 | 100 | 36 | 60 | 95 |
| 181 | | | COCl | 8.095 | 7.477 | 7.616 | 4 | 0 | x | 100 | 51 |
| 182 | | | COCl | 8.072 | 7.471 | 7.628 | 4 | 10 | 36 | 60 | 95 |
| 183 | $C_7H_5Cl_3$ | benzotrichloride | $CCl_3$ | 7.813 | 7.186 | 7.167 | 1 | 90 | x | 100 | 52 |
| 184 | | | $CCl_3$ | 7.816 | 7.191 | 7.170 | 1 | 100 | 36 | 60 | 95 |
| 185 | | | $CCl_3$ | 7.893 | 7.381 | 7.356 | 4 | 0 | x | 100 | 51 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

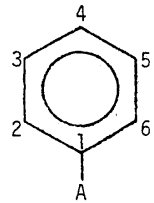



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 186 | $C_7H_5Cl_3$ | benzotrichloride | $CCl_3$ | 7.882 | 7.348 | 7.324 | 4 | 10 | 36 | 60 | 95 |
| 187 | | | $CCl_3$ | 7.87 | 7.30 | 7.31 | 4 | 33 | x[d] | 60 or 100 | 99 |
| 188 | $C_7H_5FO$ | benzoyl fluoride | COF | 7.885 | 7.394 | 7.581 | 1 | 100 | 36 | 60 | 95 |
| 189 | | | COF | 7.973 | 7.469 | 7.640 | 4 | 10 | 36 | 60 | 95 |
| 190 | $C_7H_5F_3$ | benzotrifluoride | $CF_3$ | 7.448 | 7.189 | 7.257 | 1 | 100 | 32 | 100 | 19 |
| 191 | | | $CF_3$ | 7.452 | 7.193 | 7.259 | 1 | 100 | 36 | 60 | 19 |
| 192 | | | $CF_3$ | 7.557 | 7.378 | 7.439 | 4 | 10 | 36 | 60 | 19 |
| 193 | $C_7H_5N$ | benzonitrile | CN | 7.559 | 7.387 | 7.522 | 1 | 90 | x | 100 | 52 |
| 194 | | | CN | 7.559 | 7.387 | 7.522 | 1 | 100 | 36 | 60 | 95 |
| 195 | | | CN | 7.616 | 7.437 | 7.537 | 4 | 0[e] | x | 100 | 51 |
| 196 | | | CN | 7.596 | 7.443 | 7.559 | 4 | 10 | 36 | 60 | 95 |
| 197 | | | CN | 7.614 | 7.438 | 7.570 | 8+25 | 70 | x | 90 | 54 |
| 198 | $C_7H_5NO$ | phenyl isocyanate | NCO | 6.985 | 7.216 | 7.090 | 4 | 10 | 36 | 60 | 95 |
| 199 | $C_7H_6F_2$ | benzal fluoride | $CHF_2$ | 7.204 | 7.037 | 7.068 | 6 | 15 | 30 | 100 | 22 |
| 200 | $C_7H_6O$ | benzaldehyde | CHO | 7.819 | 7.413 | 7.508 | 1 | 100 | 36 | 60 | 95 |
| 201 | | | CHO | 7.816 | 7.476 | 7.549 | 4 | 0 | x | 100 | 51 |
| 202 | | | CHO | 7.818 | 7.478 | 7.552 | 4 | 2.6 | x | 100 | 51 |
| 203 | | | CHO | 7.797 | 7.449 | 7.535 | 4 | 10 | 36 | 60 | 95 |

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

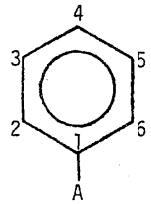



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H{}^a$ 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 204 | $C_7H_6O$ | benzaldehyde | CHO | 7.788 | 7.438 | 7.526 | 4 | 25.4 | x[d] | 100 | 51 |
| 205 | | | CHO | 7.81 | 7.45 | 7.54 | 5 | x[d] | x | 100 | 85 |
| 206 | $C_7H_6O_2$ | benzoic acid | $CO_2H$ | 8.11 | 7.44 | 7.53 | 4 | 0[e] | x | 100 | 65 |
| 207 | | | $CO_2H$ | 8.081 | 7.510 | 7.624 | 8 | 1.0M | x | 100 | 9 |
| 208 | | | $CO_2H$ | 8.059 | 7.498 | 7.612 | 8 | 10 | 36 | 60 | 95 |
| 209 | $C_7H_7NO$ | benzamide | $CONH_2$ | 7.954 | 7.443 | 7.514 | 8 | 5 | 36 | 60 | 95 |
| 210 | | | $CONH_2$ | 7.964 | 7.445 | 7.515 | 8 | 10 | 36 | 60 | 95 |
| 211 | $C_7H_8$ | toluene | $CH_3$ | 6.973 | 7.085 | 7.004 | 1(=20) | 100 | 36 | 60 | 95 |
| 212 | $C_7H_8O$ | anisole | $OCH_3$ | 6.790 | 7.138 | 6.830 | 1 | 90 | x | 100 | 52 |
| 213 | | | $OCH_3$ | 6.784 | 7.132 | 6.823 | 1 | 100 | 36 | 60 | 28 |
| 214 | | | $OCH_3$ | 6.771 | 7.162 | 6.816 | 4 | 0 | x | 100 | 51 |
| 215 | | | $OCH_3$ | 6.904 | 7.259 | 6.901 | 8 | 1.0M | x | 100 | 9 |
| 216 | | | $OCH_3$ | 6.772 | 7.149 | 6.817 | 4 | 10 | 36 | 60 | 28 |
| 217 | | | $OCH_3$ | 6.72 | 7.08 | 6.75 | 12 | 5 | x | 100 | 79 |
| 218 | | | $OCH_3$ | 6.753 | 7.111 | 6.786 | 25 | 10 | 38 | 60 | 76 |
| 219 | $C_7H_8O_3S$ | methyl benzenesulfonate | $SO_2OCH_3$ | 7.936 | 7.596 | 7.672 | 1 | 90 | x | 100 | 52 |
| 220 | | | $SO_2OCH_3$ | 7.859 | 7.511 | 7.588 | 4 | 0 | x | 100 | 51 |
| 221 | $C_7H_8O_3S$ | phenol methanesulfonate | $OSO_2CH_3$ | 7.21 | 7.33 | 7.25 | 4 | 0 | x | 100 | 65 |
| 222 | $C_7H_8S$ | thioanisole | $SCH_3$ | 7.10 | 7.07 | 6.93 | 12 | 5 | x | 100 | 79 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

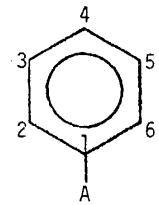



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 223 | $C_7H_9N$ | N-methylaniline | $NHCH_3$ | 6.324 | 7.064 | 6.624 | 1 | 90 | x[d] | 100 | 52 |
| 224 | | | $NHCH_3$ | 6.337 | 7.080 | 6.639 | 1 | 100 | 36 | 60 | 28 |
| 225 | | | $NHCH_3$ | 6.460 | 7.035 | 6.571 | 4 | 0[e] | x | 100 | 51 |
| 226 | | | $NHCH_3$ | 6.434 | 7.042 | 6.578 | 4 | 10 | 36 | 60 | 28 |
| 227 | $C_8H_6$ | phenylacetylene | C≡CH | 7.457 | 7.121 | 7.135 | 1 | 100 | 36 | 60 | 30 |
| 228 | | | C≡CH | 7.419 | 7.226 | 7.240 | 4 | 15 | 36 | 60 | 30 |
| 229 | $C_8H_8$ | styrene | $CH=CH_2$ | 7.230 | 7.113 | 7.059 | 1 | 100 | 36 | 60 | 95 |
| 230 | | | $CH=CH_2$ | 7.296 | 7.206 | 7.140 | 4 | 10 | 36 | 60 | 95 |
| 231 | $C_8H_8DNO$ | acetanilide-d | $CH_3COND$ | 7.644 | 7.237 | 6.999 | 8 | 11 | x | 100 | 23 |
| 232 | $C_8H_8O$ | acetophenone | $COCH_3$ | 7.888 | 7.346 | 7.448 | 1 | 90 | x | 100 | 52 |
| 233 | | | $COCH_3$ | 7.886 | 7.345 | 7.446 | 1 | 100 | 36 | 60 | 95 |
| 234 | | | $COCH_3$ | 7.874 | 7.390 | 7.467 | 4 | 0 | x | 100 | 51 |
| 235 | | | $COCH_3$ | 7.860 | 7.366 | 7.453 | 4 | 10 | 36 | 60 | 95 |
| 236 | | | $COCH_3$ | 7.86 | 7.37 | 7.45 | 5 | x[d] | x | 100 | 85 |
| 237 | $C_8H_8O_2$ | methyl benzoate | $CO_2CH_3$ | 8.051 | 7.352 | 7.455 | 1 | 90 | x | 100 | 52 |
| 238 | | | $CO_2CH_3$ | 8.037 | 7.339 | 7.440 | 1 | 100 | 36 | 60 | 95 |
| 239 | | | $CO_2CH_3$ | 8.03 | 7.40 | 7.51 | 3 | 13 | x | 100 | 3 |
| 240 | | methyl benzoate-carboxyl-$^{13}C$ | $^{13}CO_2CH_3$ | 8.03 | 7.40 | 7.52 | 3 | 13 | x | 100 | 3 |
| 241 | | methyl benzoate | $CO_2CH_3$ | 7.968 | 7.364 | 7.464 | 4 | 0 | x | 100 | 51 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

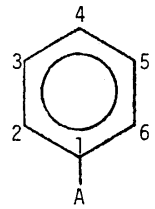



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 242 | $C_8H_8O_2$ | methyl benzoate | $CO_2CH_3$ | 7.974 | 7.342 | 7.445 | 4 | 10 | 36 | 60 | 95 |
| 243 | | | $CO_2CH_3$ | 8.016 | 7.496 | 7.618 | 8 | 1.0M | x[d] | 100 | 9 |
| 244 | $C_8H_8O_2$ | phenol acetate | $OCOCH_3$ | 7.073 | 7.230 | 7.075 | 1 | 90 | x | 100 | 52 |
| 245 | | | $OCOCH_3$ | 7.003 | 7.282 | 7.123 | 4 | 0[e] | x | 100 | 51 |
| 246 | | | $OCOCH_3$ | 7.103 | 7.374 | 7.213 | 8 | 1.0M | x | 100 | 12 |
| 247 | $C_8H_8O_2$ | phenylacetic acid | $CH_2CO_2H$ | 7.305 | 7.295 | 7.233 | 8 | 1.0M | x | 100 | 12 |
| 248 | $C_8H_9NO$ | acetanilide | $NHCOCH_3$ | 7.44 | 7.25 | 7.04 | 3 | 0 | x | 100 | 65 |
| 249 | $C_8H_{11}N$ | N,N-dimethylaniline | $N(CH_3)_2$ | 6.535 | 7.127 | 6.667 | 1 | 90 | x | 100 | 52 |
| 250 | | | $N(CH_3)_2$ | 6.541 | 7.128 | 6.667 | 1 | 100 | 36 | 60 | 28 |
| 251 | | | $N(CH_3)_2$ | 6.596 | 7.075 | 6.582 | 4 | 0 | x | 100 | 51 |
| 252 | | | $N(CH_3)_2$ | 6.590 | 7.085 | 6.598 | 4 | 10 | 36 | 60 | 28 |
| 253 | $C_8H_{11}O_3P$ | dimethyl phenylphosphonate | $PO(OCH_3)_2$ | 7.724 | 7.403 | 7.483 | 4 | 10 | 36 | 60 | 95 |
| 254 | $C_9H_{10}O$ | allyloxybenzene | $OCH_2CH{=}CH_2$ | 6.806 | 7.133 | 6.832 | 1 | 90 | x | 100 | 52 |
| 255 | $C_9H_{10}O$ | 2-phenyloxetane | CH—$CH_2$ \| \| O—$CH_2$ | 7.30 | 7.28 | 7.18 | 4 | 2-5 | x | 300 | 81 |
| 256 | | | CH—$CH_2$ \| \| O—$CH_2$ | 7.35 | 7.20 | 7.10 | 6 | 2-5 | x | 300 | 81 |
| 257 | $C_9H_{10}O$ | propiophenone | $COCH_2CH_3$ | 7.891 | 7.344 | 7.438 | 1 | 90 | x | 100 | 52 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

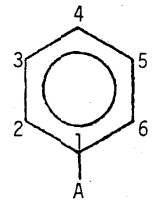



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 258 | $C_9H_{10}O$ | propiophenone | $COCH_2CH_3$ | 7.880 | 7.380 | 7.452 | 4 | 0[e] | x[d] | 100 | 51 |
| 259 | $C_9H_{14}IN$ | trimethylanilinium iodice | $N^+(CH_3)_3I^-$ | 7.979 | 7.658 | 7.604 | 22 | 15 | 36 | 60 | 28 |
| 260 | $C_9H_{15}NO_4S$ | amphetamine sulfate | $CH_2CH(CH_3)^+NH_3HSO_4^-$ | 7.32* | 7.43* | 7.36* | 30* | 0.25M | 21 | 250 | 61 |
| 261 | $C_{10}H_{12}O_2$ | isopropyl benzoate | $CO_2CH(CH_3)_2$ | 8.056 | 7.331 | 7.418 | 1 | 90 | x | 100 | 52 |
| 262 | | | $CO_2CH(CH_3)_2$ | 7.957 | 7.348 | 7.443 | 4 | 0 | x | 100 | 51 |
| 263 | $C_{10}H_{14}$ | tert-butylbenzene | $C(CH_3)_3$ | 7.267 | 7.150 | 7.019 | 1 | 100 | 36 | 60 | 95 |
| 264 | | | $C(CH_3)_3$ | 7.280 | 7.173 | 7.045 | 4 | 10 | 36 | 60 | 29 |
| 265 | $C_{11}H_{19}N$ | 2-phenylpyridine | $2\text{-}C_5H_4N^\dagger$ | 7.984 | 7.335 | 7.272 | 4 | 1-2M | 37 | 60 | 70 |
| 266 | $C_{11}H_{14}O_2$ | isobutyl benzoate | $CO_2CH_2CH(CH_3)_2$ | 7.970 | 7.364 | 7.457 | 4 | 0 | x | 100 | 51 |
| 267 | $C_{12}H_5D_5$ | biphenyl-$d_5$ | $C_6D_5$ | 7.581 | 7.416 | 7.324 | 3 | 5 | 28 | 60 | 56 |
| 268 | | | $C_6D_5$ | 7.440 | 7.265 | 7.170 | 25 | 5 | 28 | 60 | 56 |
| **269** | **$C_{12}H_9NO$** | **2-benzoylpyridine** | **$CO\text{-}(2\text{-}C_5H_4N)^\dagger$** | **8.115** | **7.372** | **7.461** | **4** | **20** | **35** | **60** | **43** |
| 270 | $C_{12}H_{10}$ | biphenyl | $C_6H_5$ | 7.59 | 7.41 | 7.32 | 3 | 5 | 28 | 60 | 56 |
| 271 | | | $C_6H_5$ | 7.479 | 7.320 | 7.224 | 4 | 5 | 36 | 60 | 95 |
| 272 | | | $C_6H_5$ | 7.468 | 7.301 | 7.207 | 4 | 10 | 36 | 60 | 95 |
| 273 | | | $C_6H_5$ | 7.436 | 7.260 | 7.169 | 25 | 5 | 28 | 60 | 56 |

*Shifts measured relative to DSS (sodium 2,2-dimethyl-2-silapentane-5-sulfonate) and converted to normal δ-scale. See Solvent Table re details of solvent No. 30.

†$2\text{-}C_5H_4N$=2-pyridyl.

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

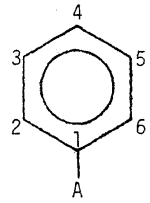



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 274 | $C_{12}H_{10}Cl_2Ge$ | dichlorodiphenylgermane | $Ge(C_6H_5)Cl_2$ | 7.555 | 7.030 | 7.073 | 6 | 5 | 33 | 100 | 74 |
| 275 | $C_{12}H_{10}Cl_2Si$ | dichlorodiphenylsilane | $Si(C_6H_5)Cl_2$ | 7.646 | 7.050 | 7.103 | 6 | 5 | 33 | 100 | 74 |
| 276 | $C_{12}H_{10}Cl_2Sn$ | dichlorodiphenylstannane | $Sn(C_6H_5)Cl_2$ | 7.385 | 7.041 | 7.069 | 6 | 5 | 33 | 100 | 74 |
| 277 | $C_{12}H_{10}F_2Si$ | difluorodiphenylsilane | $Si(C_6H_5)F_2$ | 7.57 | 7.06 | 7.15 | 6 | 5 | 33 | 100 | 74 |
| 278 | $C_{12}H_{10}Hg$ | diphenylmercury | $HgC_6H_5$ | 7.256 | 7.263 | 7.055 | 7 | 10 | 36 | 60 | 95 |
| 279 | $C_{12}H_{10}Mg$ | diphenylmagnesium | $MgC_6H_5$ | 7.70 | 7.04 | 6.96 | 10 | x[d] | x[d] | 60 | 77 |
| 280 | $C_{12}H_{10}N_2$ | cis-azobenzene | (cis) $N{=}N{-}C_6H_5$ | 6.728 | 7.141 | 7.021 | 4 | 10 | 36 | 60 | 95 |
| 281 | $C_{12}H_{10}N_2$ | trans-azobenzene | (trans) $N{=}N{-}C_6H_5$ | 7.883 | 7.406 | 7.347 | 4 | 10 | 36 | 60 | 95 |
| 282 | $C_{12}H_{10}O$ | diphenyl ether | $OC_6H_5$ | 6.925 | 7.094 | 6.895 | 1 | 100 | 36 | 60 | 28 |
| 283 | | | $OC_6H_5$ | 6.925 | 7.218 | 6.977 | 4 | 10 | 36 | 60 | 28 |
| 284 | $C_{12}H_{10}S$ | diphenyl sulfide | $SC_6H_5$ | 7.204 | 7.056 | 7.004 | 1 | 90 | x | 100 | 52 |
| 285 | | | $SC_6H_5$ | 7.255 | 7.025 | 6.979 | 1 | 100 | 36 | 60 | 95 |
| 286 | $C_{12}H_{10}S_2$ | diphenyldisulfide | $S_2C_6H_5$ | 7.500 | 7.277 | 7.200 | 3 | 5 | 38 | 60 | 72 |
| 287 | | | $S_2C_6H_5$ | 7.298 | 7.032 | 6.963 | 7 | 5 | 38 | 60 | 72 |
| 288 | | | $S_2C_6H_5$ | 7.427 | 7.187 | 7.113 | 8 | 5 | 38 | 60 | 72 |
| 289 | $C_{12}H_{10}Zn$ | diphenylzinc | $ZnC_6H_5$ | 7.57 | 7.19 | 7.16 | 10 | x | x | 60 | 77 |
| 290 | $C_{12}H_{20}Ge$ | phenyltriethylgermane | $Ge(C_2H_5)_3$ | 7.34 | 7.20 | 7.20 | 4 | 33 | x | 60 or 100 | 99 |
| 291 | $C_{12}H_{20}Pb$ | phenyltriethylplumbane | $Pb(C_2H_5)_3$ | 7.37 | 7.20 | 7.11 | 4 | 33 | | 60 or 100 | 99 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

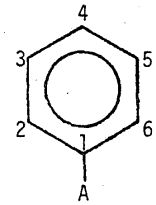
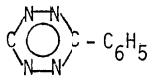



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 292 | $C_{12}H_{20}Si$ | phenyltriethylsilane | $Si(C_2H_5)_3$ | 7.48 | 7.31 | 7.22 | 4 | 33 | x[d] | 60 or 100 | 99 |
| 293 | $C_{12}H_{20}Sn$ | phenyltriethylstannane | $Sn(C_2H_5)_3$ | 7.35 | 7.19 | 7.19 | 4 | 33 | x | 60 or 100 | 99 |
| 294 | $C_{13}H_{10}Cl_2$ | dichlorodiphenylmethane | $C(C_6H_5)Cl_2$ | 7.584 | 6.986 | 6.963 | 6 | 5 | 33 | 100 | 74 |
| 295 | $C_{13}H_{10}O$ | benzophenone | $COC_6H_5$ | 7.702 | 7.363 | 7.452 | 4 | 20 | 36 | 60 | 63 |
| 296 | $C_{13}H_{10}O_2$ | phenyl benzoate | $CO_2C_6H_5$ | 8.147 | 7.425 | 7.527 | 4 | 5 | 36 | 60 | 95 |
| 297 | | | $CO_2C_6H_5$ | 8.137 | 7.407 | 7.509 | 4 | 10 | 36 | 60 | 95 |
| 298 | $C_{13}H_{10}O_2$ | phenyl benzoate | $OCOC_6H_5$ | 7.160 | 7.339 | 7.173 | 4 | 5 | 36 | 60 | 95 |
| 299 | | | $OCOC_6H_5$ | 7.154 | 7.327 | 7.162 | 4 | 10 | 36 | 60 | 95 |
| 300 | $C_{14}H_{10}$ | diphenylacetylene | $C{\equiv}C\text{-}C_6H_5$ | 7.458 | 7.251 | 7.224 | 4 | 7 | 36 | 60 | 30 |
| 301 | | | $C{\equiv}C\text{-}C_6H_5$ | 7.461 | 7.218 | 7.194 | 4 | 14 | 36 | 60 | 30 |
| 302 | $C_{14}H_{10}N_4$ | 3,6-diphenyl-s-tetrazine |  | 8.561 | 7.550 | 7.567 | 35 | 17 | 36 | 60 | 95 |
| 303 | $C_{14}H_{10}O_2$ | benzil | $COCOC_6H_5$ | 7.919 | 7.444 | 7.563 | 4 | 5 | 36 | 60 | 95 |
| 304 | | | $COCOC_6H_5$ | 7.903 | 7.423 | 7.547 | 4 | 10 | 36 | 60 | 95 |
| 305 | | | $COCOC_6H_5$ | 8.115 | 7.372 | 7.461 | 4 | 18 | 36 | 60 | 95 |
| 306 | | | $COCOC_6H_5$ | 7.971 | 7.602 | 7.747 | 8 | 10 | 36 | 60 | 95 |
| 307 | $C_{14}H_{12}$ | trans-stilbene | (trans) $CH{=}CHC_6H_5$ | 7.417 | 7.260 | 7.161 | 4 | 2 | 36 | 60 | 95 |

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

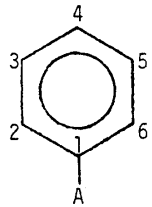
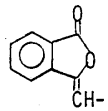



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H{}^a$ 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 308 | $C_{14}H_{12}$ | trans-stilbene | (trans) $CH{=}CHC_6H_5$ | 7.329 | 7.195 | 7.104 | 7 | x[c*] | 36 | 60 | 95 |
| 309 | $C_{15}H_{10}O_2$ | 3-phenylmethylidenephthalide | R[†] | 7.88 | 7.40 | [§] | 8 | 0.5M | 24 | 80 | 84 |
| 310 | $C_{15}H_{10}O_2S$ | 3-phenylthiomethylidenephthalide | S-R[†] | 7.30 | 7.59 | [§] | 8 | 0.5M | 24 | 80 | 84 |
| 311 | $C_{16}H_{13}N_3$ | diphenylmethyl-s-triazine | $C_3N_3(C_6H_5)(CH_3)$[¶] | 8.564 | 7.396 | 7.431 | 4 | 1-2M | 37 | 60 | 70 |
| 312 | $C_{18}H_{15}ClPb$ | chlorotriphenylplumbane | $PbCl(C_6H_5)_2$ | 7.939 | 7.538 | 7.368 | 5 | 10 | 36 | 60 | 95 |
| 313 | $C_{18}H_{15}ClSi$ | chlorotriphenylsilane | $SiCl(C_6H_5)_2$ | 7.579 | 7.332 | 7.381 | 4 | 5 | 36 | 60 | 95 |
| 314 | | | $SiCl(C_6H_5)_2$ | 7.579 | 7.309 | 7.357 | 4 | 10 | 36 | 60 | 95 |
| 315 | | | $SiCl(C_6H_5)_2$ | 7.589 | 7.314 | 7.373 | 10 | 5 | 29 | 100 | 97 |
| 316 | $C_{18}H_{15}ClSn$ | chlorotriphenylstannane | $SnCl(C_6H_5)_2$ | 7.856 | 7.448 | 7.396 | 5 | 10 | 36 | 60 | 95 |
| 317 | $C_{18}H_{15}FSi$ | fluorotriphenylsilane | $SiF(C_6H_5)_2$ | 7.588 | 7.321 | 7.389 | 10 | 5 | 29 | 100 | 97 |
| 318 | $C_{18}H_{15}GeN_3$ | azidotriphenylgermane | $Ge(C_6H_5)_2N_3$ | 7.589 | 7.411 | 7.443 | 3 | 5 | 33 | 100 | 74 |
| 319 | $C_{18}H_{15}N_3Pb$ | azidotriphenylplumbane | $Pb(C_6H_5)_2N_3$ | 7.57 | 7.44 | 7.34 | 3 | <5 | 33 | 100 | 74 |
| 320 | $C_{18}H_{15}N_3Si$ | azidotriphenylsilane | $Si(C_6H_5)_2N_3$ | 7.603 | 7.375 | 7.433 | 3 | 5 | 33 | 100 | 74 |
| 321 | $C_{18}H_{15}N_3Sn$ | azidotriphenylstannane | $Sn(C_6H_5)_2N_3$ | 7.610 | 7.432 | 7.431 | 3 | 5 | 33 | 100 | 74 |
| 322 | $C_{18}H_{15}OAs$ | triphenylarsine oxide | $AsO(C_6H_5)_2$ | 7.722 | 7.487 | 7.540 | 3 | 15 | 36 | 60 | 95 |

*Low concentration - saturated solution; †R- =  ; §shift not reported; ¶$C_3N_2(C_6H_5)(CH_3)$ = methylphenyl-s-triazenyl.

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

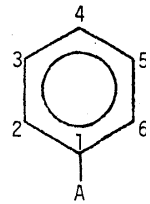



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 323 | $C_{18}H_{15}OP$ | triphenylphosphine oxide | $PO(C_6H_5)_2$ | 7.672 | 7.419 | 7.492 | 3 | 15 | 36 | 60 | 95 |
| 324 | $C_{18}H_{15}P$ | triphenylphosphine | $P(C_6H_5)_2$ | 7.236 | 6.934 | 6.926 | 6 | 12 | 32 | 100 | 86 |
| 325 | $C_{18}H_{15}P$ | triphenylphosphine | $P(C_6H_5)_2$ | 7.372 | 7.051 | 7.042 | 6 | 55 | 31 | 100 | 64 |
| 326 | $C_{18}H_{16}OSi$ | triphenylsilanol | $Si(C_6H_5)_2OH$ | 7.560 | 7.248 | 7.248 | 10 | 5 | 29 | 100 | 97 |
| 327 | $C_{18}H_{16}Si$ | triphenylsilane | $Si(C_6H_5)_2H$ | 7.512 | 7.275 | 7.309 | 10 | 5 | 29 | 100 | 97 |
| 328 | $C_{19}H_{15}N_3$ | azidotriphenylmethane | $C(C_6H_5)_2N_3$ | 7.28 | 7.28 | 7.28 | 3 | 5 | 33 | 100 | 74 |
| 329 | | | $C(C_6H_5)_2N_3$ | 7.292 | 7.037 | 6.998 | 6 | 5 | 33 | 100 | 74 |
| 330 | $C_{19}H_{18}OSi$ | triphenylmethoxysilane | $Si(C_6H_5)_2OCH_3$ | 7.573 | 7.282 | 7.325 | 10 | 5 | 29 | 100 | 97 |
| 331 | $C_{19}H_{18}Si$ | methyltriphenylsilane | $SiCH_3(C_6H_5)_2$ | 7.218 | 6.969 | 6.948 | 12 | 95 | 36 | 60 | 95 |
| 332 | $C_{20}H_{18}Ge$ | vinyltriphenylgermane | $(C_6H_5)_2Ge\text{-}CH{=}CH_2$ | 7.422 | 7.272 | 7.277 | 4 | 6 | 33 | 100 | 74 |
| 333 | $C_{20}H_{18}Pb$ | vinyltriphenylplumbane | $(C_6H_5)_2Pb\text{-}CH{=}CH_2$ | 7.510 | 7.315 | 7.227 | 4 | 6 | 33 | 100 | 74 |
| 334 | $C_{20}H_{18}Si$ | vinyltriphenylsilane | $(C_6H_5)_2Si\text{-}CH{=}CH_2$ | 7.457 | 7.267 | 7.300 | 4 | 6 | 33 | 100 | 74 |
| 335 | $C_{20}H_{18}Sn$ | vinyltriphenylstannane | $(C_6H_5)_2Sn\text{-}CH{=}CH_2$ | 7.488 | 7.282 | 7.268 | 4 | 6 | 33 | 100 | 74 |
| 336 | $C_{21}H_{18}$ | 1,1,1-triphenylpropene | $(C_6H_5)_2C\text{-}CH{=}CH_2$ | 7.037 | 7.182 | 7.122 | 4 | 6 | 33 | 100 | 74 |
| 337 | | | $(C_6H_5)_2C\text{-}CH{=}CH_2$ | 7.152 | 7.068 | 7.023 | 6 | 5 | 33 | 100 | 74 |
| 338 | $C_{24}H_{20}Ge$ | tetraphenylgermane | $Ge(C_6H_5)_3$ | 7.600 | 7.168 | 7.180 | 6 | 5 | 49 | 56.4 | 74 |
| 339 | $C_{24}H_{20}Pb$ | tetraphenylplumbane | $Pb(C_6H_5)_3$ | 7.630 | 7.219 | 7.125 | 6 | 5 | 57 | 56.4 | 74 |
| 340 | $C_{24}H_{20}Si$ | tetraphenylsilane | $Si(C_6H_5)_3$ | 7.652 | 7.172 | 7.203 | 6 | 5 | 30 | 56.4 | 74 |
| 341 | | | $Si(C_6H_5)_3$ | 7.641 | 7.173 | 7.194 | 6 | 5 | 40 | 56.4 | 74 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

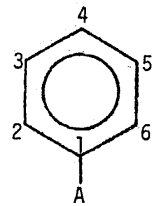



Table I

| Entry No. | Molecular Formula | Name | A | $\delta_H$[a] 2,6 (ortho) | 3,5 (meta) | 4 (para) | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 342 | $C_{24}H_{20}Sn$ | tetraphenylstannane | $Sn(C_6H_5)_3$ | 7.607 | 7.177 | 7.174 | 6 | 5 | 60 | 56.4 | 74 |
| 343 | $C_{25}H_{20}$ | tetraphenylmethane | $C(C_6H_5)_3$ | 7.324 | 7.060 | 6.995 | 6 | 5 | 60.5 | 56.4 | 74 |
| 344 | $C_{28}H_{28}Sn$ | tetrabenzyltin | $CH_2Sn(CH_2C_6H_5)_3$ | 6.68 | 7.08 | 6.93 | 4 | x[d] | x[d] | 90 | 88 |

[a] Usual δ-scale. See text, section 2, item 5.

[b] See Table V and text, section 2, item 6.

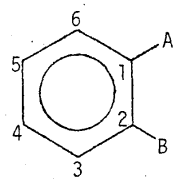
[c] Concentration is given in percent unless number is followed by "M", molarity. The designation "0" refers to the shift at "infinite dilution". See text, section 2, item 7.

[d] The designation "x" means unknown or unspecified.

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO




| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 001 | $C_6H_4BrCl$ | o-bromochlorobenzene | Cl | Br | 7.378 | 6.870 | 6.997 | 7.212 | 1 | 10 | 36 | 60 | 29 |
| 002 | | | Cl | Br | 7.53 | 7.01 | 7.14 | 7.38 | 4 | 5-10 | 40 | 60 | 33 |
| 003 | | | Cl | Br | 7.537 | 7.027 | 7.156 | 7.369 | 4 | 10 | 36 | 60 | 29 |
| 004 | | | Cl | Br | 7.475 | 6.930 | 7.060 | 7.300 | 25 | 10 | 38 | 60 | 76 |
| 005 | $C_6H_4BrF$ | o-bromofluorobenzene | F | Br | 7.350 | 6.824 | 7.078 | 6.922 | 1 | 10 | 36 | 60 | 29 |
| 006 | | | F | Br | 7.484 | 6.949 | 7.205 | 7.044 | 4 | 10 | 36 | 60 | 29 |
| 007 | | | F | Br | 7.50 | 6.97 | 7.22 | 7.06 | 4 | 10 | x[d] | 60 | 39 |
| 008 | | | F | Br | 7.44 | 6.88 | 7.13 | 6.97 | 12 | 10 | x | 60 | 39 |
| 009 | | | F | Br | 7.404 | 6.844 | 7.100 | 6.937 | 25 | 10 | 38 | 60 | 31 |
| 010 | $C_6H_4BrI$ | o-bromoiodobenzene | I | Br | 7.411 | 6.996 | 6.791 | 7.655 | 1 | 100 | 36 | 60 | 29 |
| 011 | | | I | Br | 7.55 | 7.10 | 6.88 | 7.78 | 4 | 5-10 | 40 | 60 | 33 |
| 012 | | | I | Br | 7.552 | 7.125 | 6.913 | 7.793 | 4 | 10 | 36 | 60 | 29 |
| 013 | | | I | Br | 7.483 | 7.018 | 6.806 | 7.737 | 25 | 10 | 38 | 60 | 76 |
| 014 | $C_6H_4BrNO_2$ | o-bromonitrobenzene | $NO_2$ | Cl | 7.71 | 7.40 | 7.44 | 7.78 | 4 | x[d] | x | x[d] | 7 |
| 015 | $C_6H_4Br_2$ | o-dibromobenzene | Br | Br | 7.393 | 6.929 | 6.929 | 7.393 | 1 | 100 | 36 | 60 | 29 |
| 016 | | | Br | Br | 7.55 | 7.09 | 7.09 | 7.55 | 4 | 5-10 | 40 | 60 | 33 |
| 017 | | | Br | Br | 7.544 | 7.079 | 7.079 | 7.544 | 4 | 10 | 36 | 60 | 29 |
| 018 | | | Br | Br | 7.480 | 6.977 | 6.977 | 7.480 | 25 | 10 | 38 | 60 | 76 |
| 019 | $C_6H_4ClF$ | o-chlorofluorobenzene | F | Cl | 7.34 | 7.01 | 7.16 | 7.07 | 4 | 10 | x | 60 | 39 |
| 020 | | | F | Cl | 7.258 | 6.917 | 7.066 | 6.971 | 25 | 10 | 38 | 60 | 31 |

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

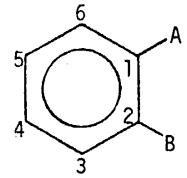


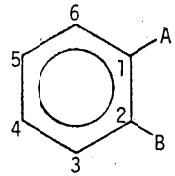

Table II

| Entry No. | Molecular Formula | Name | A | B | $\delta_H{}^a$ 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 021 | $C_6H_4ClI$ | o-chloroiodobenzene | I | Cl | 7.37 | 7.21 | 6.84 | 7.79 | 4 | 5-10 | 40 | 60 | 33 |
| 022 | | | I | Cl | 7.284 | 7.087 | 6.751 | 7.714 | 25 | 10 | 38 | 60 | 76 |
| 023 | $C_6H_4ClNO_2$ | o-chloronitrobenzene | $NO_2$ | Cl | 7.54 | 7.49 | 7.41 | 7.82 | 4 | x[d] | x[d] | x[d] | 7 |
| 024 | | | $NO_2$ | Cl | 7.520 | 7.502 | 7.406 | 7.807 | 4 | 10 | 36 | 60 | 29 |
| 025 | $C_6H_4Cl_2$ | o-dichlorobenzene | Cl | Cl | 7.202 | 6.942 | 6.942 | 7.202 | 1 | 10 | 36 | 60 | 29 |
| 026 | | | Cl | Cl | 7.37 | 7.12 | 7.12 | 7.37 | 4 | 5-10 | 40 | 60 | 33 |
| 027 | | | Cl | Cl | 7.366 | 7.110 | 7.110 | 7.366 | 4 | 10 | 36 | 60 | 29 |
| 028 | | | Cl | Cl | 7.293 | 7.011 | 7.011 | 7.293 | 25 | 10 | 38 | 60 | 76 |
| 029 | $C_6H_4FI$ | o-fluoroiodobenzene | I | F | 6.883 | 7.124 | 6.721 | 7.564 | 1 | 10 | 36 | 60 | 29 |
| 030 | | | I | F | 6.992 | 7.240 | 6.827 | 7.688 | 4 | 10 | 36 | 60 | 29 |
| 031 | | | I | F | 7.00 | 7.25 | 6.84 | 7.70 | 4 | 10 | x | 60 | 39 |
| 032 | | | I | F | 6.92 | 7.17 | 6.76 | 7.66 | 12 | 10 | x | 60 | 39 |
| 033 | | | I | F | 6.884 | 7.134 | 6.719 | 7.618 | 25 | 10 | 38 | 60 | 31 |
| 034 | $C_6H_4FNO_2$ | o-fluoronitrobenzene | $NO_2$ | F | 7.31 | 7.66 | 7.33 | 8.03 | 4 | 10 | x | 60 | 39 |
| 035 | $C_6H_4F_2$ | o-difluorobenzene | F | F | 7.07 | 7.07 | 7.07 | 7.07 | 4 | 10 | x | 60 | 39 |
| 036 | | | F | F | 7.077 | 6.997 | 6.997 | 7.077 | 8 | 75 | 36 | 100 | 17 |
| 037 | | | F | F | 6.99 | 6.99 | 6.99 | 6.99 | 12 | 10 | x | 60 | 39 |
| 038 | | | F | F | 7.008 | 6.936 | 6.936 | 7.008 | 25 | 10 | x | 100 | 46 |
| 039 | $C_6H_4INO_2$ | o-iodonitrobenzene | $NO_2$ | I | 7.99 | 7.29 | 7.36 | 7.80 | 4 | x | x | x | 7 |
| 040 | $C_6H_4I_2$ | o-diiodobenzene | I | I | 7.81 | 6.96 | 6.96 | 7.81 | 4 | 5-10 | 40 | 60 | 33 |

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO




| Entry No. | Molecular Formula | Name | A | B | $\delta_H{}^a$ 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 041 | $C_6H_4I_2$ | o-diiodobenzene | I | I | 7.809 | 6.959 | 6.959 | 7.809 | 4 | 10 | 36 | 60 | 29 |
| 042 | | | I | I | 7.806 | 6.949 | 6.949 | 7.806 | 25 | 10 | 38 | 60 | 76 |
| 043 | $C_6H_4N_2O_4$ | o-dinitrobenzene | $NO_2$ | $NO_2$ | 7.97 | 7.87 | 7.87 | 7.97 | 4 | x[d] | x[d] | x[d] | 7 |
| 044 | | | $NO_2$ | $NO_2$ | 8.158 | 8.006 | 8.006 | 8.158 | 8 | 10 | 36 | 60 | 29 |
| 045 | $C_6H_5BrO$ | o-bromophenol | OH | Br | 7.40 | 6.73 | 7.15 | 6.97 | 4 | 10 | x | 60 | 38 |
| 046 | | | OH | Br | 7.53 | 6.78 | 7.24 | 7.02 | 5 | 10 | x | 60 | 38 |
| 047 | $C_6H_5ClO$ | o-chlorophenol | OH | Cl | 7.134 | 6.673 | 6.964 | 6.974 | 1 | 100 | 36 | 60 | 29 |
| 048 | | | OH | Cl | 7.213 | 6.755 | 7.068 | 6.949 | 4 | 10 | 36 | 60 | 29 |
| 049 | | | OH | Cl | 7.25 | 6.79 | 7.11 | 6.97 | 4 | 10 | x | 60 | 38 |
| 050 | | | OH | Cl | 7.37 | 6.84 | 7.20 | 7.04 | 5 | 10 | x | 60 | 38 |
| 051 | $C_6H_5IO$ | o-iodophenol | OH | I | 7.59 | 6.61 | 7.17 | 6.94 | 4 | 10 | x | 60 | 38 |
| 052 | $C_6H_5NO_3$ | o-nitrophenol | OH | $NO_2$ | 8.048 | 6.937 | 7.529 | 7.097 | 4 | 10 | 36 | 60 | 29 |
| 053 | | | OH | $NO_2$ | 8.08 | 6.95 | 7.55 | 7.12 | 4 | 10 | x | 60 | 38 |
| 054 | | | OH | $NO_2$ | 7.92 | 7.02 | 7.58 | 7.19 | 5 | 10 | x | 60 | 38 |
| 055 | $C_6H_6BrN$ | o-bromoaniline | $NH_2$ | Br | 7.32 | 6.51 | 6.99 | 6.61 | 4 | 10 | x | 100 | 40 |
| 056 | $C_6H_6ClN$ | o-chloroaniline | $NH_2$ | Cl | 7.14 | 6.57 | 6.93 | 6.58 | 4 | 10 | x | 100 | 40 |
| 057 | | | $NH_2$ | Cl | 7.14 | 6.51 | 6.98 | 6.80 | 5 | 10 | x | 100 | 40 |
| 058 | | | $NH_2$ | Cl | 7.087 | 6.420 | 6.789 | 6.247 | 6 | 10 | x | 60 | 20 |
| 059 | | | $NH_2$ | Cl | 7.089 | 6.420 | 6.790 | 6.242 | 6 | 10 | x | 100 | 20 |
| 060 | $C_6H_6ClN$ | o-chloroaniline-$^{15}N$ | $^{15}NH_2$ | Cl | 7.087 | 6.421 | 6.790 | 6.246 | 6 | 10 | x | 100 | 20 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

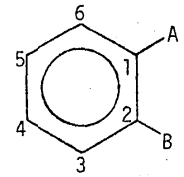
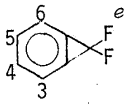



Table II

| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 061 | $C_6H_6IN$ | o-iodoaniline | $NH_2$ | I | 7.53 | 6.36 | 7.01 | 6.58 | 4 | 10 | x[d] | 100 | 40 |
| 062 | | | $NH_2$ | I | 7.51 | 6.31 | 7.04 | 6.77 | 5 | 10 | x | 100 | 40 |
| 063 | $C_6H_6N_2O_2$ | o-nitroaniline | $NH_2$ | $NO_2$ | 8.07 | 6.65 | 7.30 | 6.79 | 4 | 10 | x | 100 | 40 |
| 064 | | | $NH_2$ | $NO_2$ | 7.94 | 6.61 | 7.36 | 7.03 | 5 | 10 | x | 100 | 40 |
| 065 | $C_6H_6O_2$ | o-dihydroxybenzene | OH | OH | 6.777 | 6.842 | 6.842 | 6.777 | 3 | 1M | x | 100 | 89 |
| 066 | | | OH | OH | 6.678 | 6.824 | 6.824 | 6.678 | 8 | 10 | 36 | 60 | 29 |
| 067 | | | OH | OH | 6.96* | 6.88* | 6.88* | 6.96* | 30 | 0.2M | 22 | 250 | 82 |
| 068 | $C_6H_6S_2$ | o-benzenedithiol | SH | SH | 7.209 | 6.907 | 6.907 | 7.209 | 3 | 1M | x | 100 | 89 |
| 069 | $C_7H_4BrN$ | o-bromobenzonitrile | CN | Br | 7.67 | 7.45 | 7.43 | 7.63 | 4 | x[d] | x | x[d] | 7 |
| 070 | $C_7H_4ClN$ | o-chlorobenzonitrile | CN | Cl | 7.50 | 7.53 | 7.38 | 7.64 | 4 | x | x | x | 7 |
| 071 | $C_7H_4Cl_4$ | o-trichloromethylchlorobenzene | Cl | $CCl_3$ | 8.14 | 7.27 | 7.31 | 7.48 | 4 | 10 | x | 100 | 40 |
| 072 | $C_7H_4FN$ | o-cyanofluorobenzene | F | CN | 7.62 | 7.29 | 7.63 | 7.22 | 4 | 10 | x | 60 | 39 |
| 073 | $C_7H_4F_2$ | 7,7-difluorobenzocyclopropene |  | | 7.483 | 7.606 | 7.606 | 7.483 | 4 | 25 | x | 100 | 90 |
| 074 | $C_7H_5BrO$ | o-bromobenzaldehyde | CHO | Br | 7.582 | 7.438 | 7.406 | 7.755 | 1 | 90 | 36 | 60 | 59 |
| 075 | | | CHO | Br | 7.59 | 7.39 | 7.39 | 7.86 | 4 | 10 | x | 100 | 4 |
| 076 | $C_7H_5BrOTe$ | o-formylphenyl tellurium bromide | TeBr | CHO | 8.14 | 7.52 | 7.64 | 8.36 | 7 | 10 | x | 100 | 60 |
| 077 | $C_7H_5BrO_2$ | o-bromobenzoic acid | $CO_2H$ | Br | 7.725 | 7.438 | 7.481 | 7.801 | 5 | 10 | x | 60 or 100 | 75 |

*Shifts measured relative to DSS (sodium 2,2-dimethyl-2-silapentane-5-sulfonate) and converted to normal δ-scale.

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

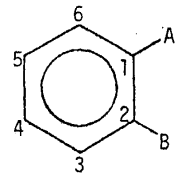
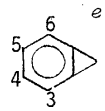



Table II

| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 078 | $C_7H_5ClO$ | o-chlorobenzaldehyde | CHO | Cl | 7.474 | 7.590 | 7.428 | 7.810 | 1 | 90 | 36 | 60 | 59 |
| 079 | | | CHO | Cl | 7.40 | 7.47 | 7.34 | 7.86 | 4 | 10 | x[d] | 100 | 4 |
| 080 | $C_7H_5ClOTe$ | o-formylphenyl tellurium chloride | TeCl | CHO | 8.18 | 7.51 | 7.68 | 8.37 | 7 | 0[c] | x | 100 | 60 |
| 081 | $C_7H_5ClO_2$ | o-chlorobenzoic acid | $CO_2H$ | Cl | 7.546 | 7.533 | 7.439 | 7.838 | 5 | 10 | x | 60 or 100 | 75 |
| 082 | $C_7H_5FO$ | o-fluorobenzaldehyde | CHO | F | 7.13 | 7.56 | 7.23 | 7.82 | 4 | 10 | x | 100 | 4 |
| 083 | | | CHO | F | 7.240 | 7.678 | 7.318 | 7.828 | 8 | 30 | 30 | 100 | 21 |
| 084 | $C_7H_5IO$ | o-iodobenzaldehyde | CHO | I | 7.89 | 7.23 | 7.42 | 7.82 | 4 | 10 | x | 100 | 4 |
| 085 | $C_7H_5IOTe$ | o-formylphenyl tellurium iodide | TeI | CHO | 8.02 | 7.54 | 7.56 | 8.28 | 7 | 0 | x | 100 | 60 |
| 086 | $C_7H_5IO_2$ | o-iodobenzoic acid | $CO_2H$ | I | 8.012 | 7.247 | 7.499 | 7.779 | 5 | 10 | x | 60 or 100 | 75 |
| 087 | $C_7H_5NO_3$ | o-nitrobenzaldehyde | CHO | $NO_2$ | 8.15 | 7.75 | 7.78 | 7.88 | 4 | 10 | x | 100 | 4 |
| 088 | $C_7H_5NO_4$ | o-nitrobenzoic acid | $CO_2H$ | $NO_2$ | 7.999 | 7.791 | 7.819 | 7.917 | 5 | 10 | x | 60 or 100 | 75 |
| 089 | $C_7H_6$ | benzocyclopropene |  | | 7.149 | 7.189 | 7.189 | 7.149 | 3 | 15 | x | 100 | 5 |
| 090 | $C_7H_6N_2$ | o-cyanoaniline | $NH_2$ | CN | 7.29 | 6.64 | 7.23 | 6.69 | 4 | 10 | x | 100 | 40 |
| 091 | | | $NH_2$ | CN | 7.28 | 6.59 | 7.21 | 6.81 | 5 | 10 | x | 100 | 40 |
| 092 | $C_7H_6O_2$ | o-hydroxybenzaldehyde | CHO | OH | 6.877 | 7.371 | 6.871 | 7.380 | 1 | 90 | 36 | 60 | 59 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

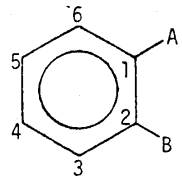



Table II

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 093 | $C_7H_6O_2$ | o-hydroxybenzaldehyde | CHO | OH | 6.90 | 7.43 | 6.92 | 7.45 | 4 | 10 | x[d] | 100 | 4 |
| 094 | $C_7H_6O_3$ | o-hydroxybenzoic acid | $CO_2H$ | OH | 7.05 | 7.56 | 6.97 | 7.97 | 3 | x[d] | x | 60 | 48 |
| 095 | | | $CO_2H$ | OH | 6.98 | 7.53 | 6.95 | 7.85 | 5 | x | x | 60 | 48 |
| 096 | | | $CO_2H$ | OH | 6.961 | 7.518 | 6.933 | 7.908 | 8 | 1.0M | x | 100 | 9 |
| 097 | $C_7H_7Br$ | o-bromotoluene | $CH_3$ | Br | 7.45 | 6.95 | 7.10 | 7.14 | 4 | 5 | x | 100 | 67 |
| 098 | | | $CH_3$ | Br | 7.44 | 6.95 | 7.09 | 7.13 | 4 | 10 | x | 100 | 40 |
| 099 | $C_7H_7BrO$ | o-bromoanisole | $OCH_3$ | Br | 7.44 | 6.73 | 7.15 | 6.77 | 4 | x | x | x[d] | 7 |
| 100 | | | $OCH_3$ | Br | 7.385 | 6.641 | 7.053 | 6.668 | 25 | 10 | 38 | 60 | 76 |
| 101 | $C_7H_7Cl$ | o-chlorctoluene | $CH_3$ | Cl | 7.26 | 7.04 | 7.06 | 7.13 | 4 | 5 | x | 100 | 67 |
| 102 | | | $CH_3$ | Cl | 7.24 | 7.02 | 7.04 | 7.11 | 4 | 10 | x | 100 | 40 |
| 103 | $C_7H_7ClO$ | o-chlorcanisole | $OCH_3$ | Cl | 7.26 | 6.80 | 7.10 | 6.81 | 4 | x | x | x | 7 |
| 104 | $C_7H_7I$ | o-iodotcluene | $CH_3$ | I | 7.73 | 6.78 | 7.14 | 7.15 | 4 | 5 | x | 100 | 67 |
| 105 | $C_7H_7IO$ | o-iodoanisole | $OCH_3$ | I | 7.69 | 6.61 | 7.20 | 6.71 | 4 | x | x | x | 7 |
| 106 | $C_7H_7NO$ | o-aminobenzaldehyde | CHO | $NH_2$ | 6.54 | 7.17 | 6.61 | 7.35 | 4 | 10 | x | 100 | 4 |
| 107 | $C_7H_7NO_2$ | o-nitrotoluene | $CH_3$ | $NO_2$ | 7.90 | 7.29 | 7.43 | 7.29 | 4 | 5 | x | 100 | 67 |
| 108 | | | $CH_3$ | $NO_2$ | 7.87 | 7.29 | 7.44 | 7.29 | 4 | 10 | x | 100 | 40 |
| 109 | $C_7H_7NO_3$ | o-nitroanisole | $OCH_3$ | $NO_2$ | 7.70 | 6.96 | 7.46 | 7.06 | 4 | x | x | x | 7 |
| 110 | | | $OCH_3$ | $NO_2$ | 7.689 | 6.955 | 7.458 | 7.066 | 25 | 10 | 38 | 60 | 76 |
| 111 | $C_7H_8O$ | o-cresol | OH | $CH_3$ | 6.99 | 6.72 | 6.94 | 6.60 | 4 | 5 | x | 100 | 67 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

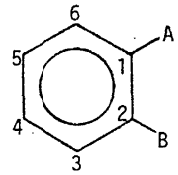
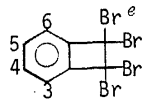
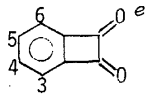
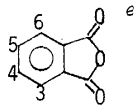
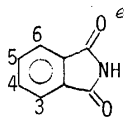



Table II

| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 112 | $C_7H_8O$ | o-cresol | OH | $CH_3$ | 6.99 | 6.73 | 6.92 | 6.59 | 4 | 10 | x[d] | 100 | 40 |
| 113 | $C_7H_8O_2$ | o-methoxyphenol | OH | $OCH_3$ | 6.73 | 6.72 | 6.78 | 6.84 | 4 | 10 | x | 60 | 38 |
| 114 | | | OH | $OCH_3$ | 6.85 | 6.85 | 6.89 | 6.89 | 5 | 10 | x | 60 | 38 |
| 115 | $C_7H_9N$ | o-toluidine | $NH_2$ | $CH_3$ | 6.89 | 6.55 | 6.88 | 6.46 | 4 | 5 | x | 100 | 67 |
| 116 | | | $NH_2$ | $CH_3$ | 6.88 | 6.55 | 6.87 | 6.43 | 4 | 10 | x | 100 | 40 |
| 117 | $C_7H_9NO$ | o-methoxylaniline | $NH_2$ | $OCH_3$ | 6.57 | 6.57 | 6.57 | 6.57 | 4 | 10 | x | 100 | 40 |
| 118 | | | $NH_2$ | $OCH_3$ | 6.60 | 6.60 | 6.60 | 6.60 | 5 | 10 | x | 100 | 40 |
| 119 | $C_8H_4Br_4$ | tetrabromobenzocyclobutene |  | | 7.503 | 7.303 | 7.303 | 7.503 | 3 | 15 | x | 100 | 5 |
| 120 | $C_8H_4N_2$ | o-phthalonitrile | CN | CN | 7.81 | 7.75 | 7.75 | 7.81 | 4 | x[d] | x | x[d] | 7 |
| 121 | $C_8H_4O_2$ | benzocyclobutadienequinone |  | | 8.080 | 7.856 | 7.856 | 8.080 | 3 | 15 | x | 100 | 5 |
| 122 | $C_8H_4O_3$ | phthalic anhydride |  | | 8.10 | 8.04 | 8.04 | 8.10 | 5 | x | x | 100 | 85 |
| 123 | $C_8H_5NO_2$ | phthalimide |  | | 7.75 | 7.75 | 7.75 | 7.75 | 5 | x | x | 100 | 85 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

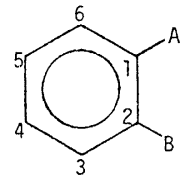
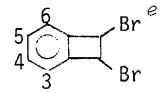
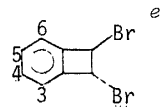
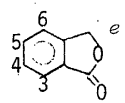



Table II

| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 124 | $C_8H_6Br_2$ | cis-dibromobenzocyclobutene |  | | 7.382 | 7.190 | 7.190 | 7.382 | 3 | 15 | x[d] | 100 | 5 |
| 125 | $C_8H_6Br_2$ | trans-dibromobenzocyclobutene |  | | 7.348 | 7.140 | 7.140 | 7.348 | 3 | 15 | x | 100 | 5 |
| 126 | $C_8H_6O_2$ | o-phthalaldehyde | CHO | CHO | 7.932 | 7.770 | 7.770 | 7.932 | 3 | 15 | x | 100 | 5 |
| 127 | | | CHO | CHO | 7.93 | 7.82 | 7.82 | 7.93 | 5 | x[d] | x | 100 | 85 |
| 128 | $C_8H_6O_2$ | phthalide |  | | 7.92 | 7.44 | 7.62 | 7.49 | 5 | x | x | 100 | 85 |
| 129 | $C_8H_6O_4$ | phthalic acid | $CO_2H$ | $CO_2H$ | 7.70 | 7.57 | 7.57 | 7.70 | 5 | x | x | 100 | 85 |
| 130 | $C_8H_7BrO$ | o-bromoacetophenone | $COCH_3$ | Br | 7.53 | 7.22 | 7.30 | 7.38 | 4 | 10 | x | 100 | 4 |
| 131 | | | $COCH_3$ | Br | 7.60 | 7.42 | 7.49 | 7.66 | 5 | 10 | x | 100 | 4 |
| 132 | $C_8H_7ClO$ | o-chloroacetophenone | $COCH_3$ | Cl | 7.34 | 7.32 | 7.25 | 7.47 | 4 | 10 | x | 100 | 4 |
| 133 | | | $COCH_3$ | Cl | 7.53 | 7.52 | 7.46 | 7.68 | 5 | 10 | x | 100 | 4 |
| 134 | $C_8H_7ClO$ | o-toluyl chloride | COCl | $CH_3$ | 7.23 | 7.44 | 7.30 | 8.17 | 4 | 5 | x | 100 | 67 |
| 135 | $C_8H_7FO$ | o-fluoroacetophenone | $COCH_3$ | F | 7.07 | 7.45 | 7.15 | 7.82 | 4 | 10 | x | 100 | 4 |
| 136 | | | $COCH_3$ | F | 7.33 | 7.67 | 7.34 | 7.83 | 5 | 10 | x | 100 | 4 |
| 137 | $C_8H_7IO$ | o-iodoacetophenone | $COCH_3$ | I | 7.86 | 7.05 | 7.34 | 7.67 | 4 | 10 | x | 100 | 4 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

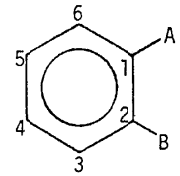
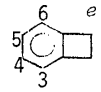



Table II

| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 138 | $C_8H_7IO$ | o-iodoacetophenone | $COCH_3$ | I | 7.97 | 7.23 | 7.51 | 7.66 | 5 | 10 | x[d] | 100 | 4 |
| 139 | $C_8H_7N$ | o-tolunitrile | CN | $CH_3$ | 7.26 | 7.41 | 7.22 | 7.52 | 4 | 5 | x | 100 | 67 |
| 140 | | | CN | $CH_3$ | 7.27 | 7.42 | 7.23 | 7.50 | 4 | 10 | x | 100 | 40 |
| 141 | $C_8H_7NO_3$ | o-nitroacetophenone | $COCH_3$ | $NO_2$ | 7.96 | 7.55 | 7.66 | 7.39 | 4 | 10 | x | 100 | 4 |
| 142 | | | $COCH_3$ | $NO_2$ | 8.09 | 7.76 | 7.86 | 7.80 | 5 | 10 | x | 100 | 4 |
| 143 | $C_8H_8$ | benzocyclobutene |  | | 6.907 | 6.764 | 6.764 | 6.907 | 3 | 15 | x | 100 | 5 |
| 144 | $C_8H_8O$ | o-tolualdehyde | CHO | $CH_3$ | 7.18 | 7.38 | 7.29 | 7.70 | 4 | 5 | x | 100 | 67 |
| 145 | | | CHO | $CH_3$ | 7.17 | 7.47 | 7.27 | 7.68 | 4 | 10 | x | 100 | 4 |
| 146 | $C_8H_8OTe$ | o-formylphenyl methyl telluride | $TeCH_3$ | CHO | 7.53 | 7.36 | 7.32 | 7.74 | 7 | 0 | x | 100 | 60 |
| 147 | $C_8H_8O_2$ | o-hydroxyacetophenone | $COCH_3$ | OH | 6.85 | 7.36 | 6.77 | 7.61 | 4 | 10 | x | 100 | 4 |
| 148 | | | $COCH_3$ | OH | 6.97 | 7.53 | 6.97 | 7.89 | 5 | 10 | x | 100 | 4 |
| 149 | $C_8H_8O_2$ | o-methoxybenzaldehyde | CHO | $OCH_3$ | 7.085 | 7.532 | 6.964 | 7.666 | 1 | 90 | 36 | 60 | 59 |
| 150 | | | CHO | $OCH_3$ | 6.81 | 7.43 | 6.93 | 7.72 | 4 | 10 | x | 100 | 4 |
| 151 | $C_8H_8O_2$ | o-toluic acid | $CO_2H$ | $CH_3$ | 7.20 | 7.37 | 7.22 | 8.06 | 4 | 5 | x | 100 | 67 |
| 152 | | | $CO_2H$ | $CH_3$ | 7.293 | 7.438 | 7.293 | 7.877 | 5 | 10 | x | 60 or 100 | 75 |
| 153 | $C_8H_8O_3$ | o-hydroxyphenylacetic acid | $CH_2CO_2H$ | OH | 6.842 | 7.072 | 6.782 | 7.164 | 8 | 1.0M | x | 100 | 12 |
| 154 | $C_8H_8O_3$ | o-methoxybenzoic acid | $CO_2H$ | $OCH_3$ | 7.07 | 7.57 | 7.12 | 8.14 | 3 | x[d] | x | 60 | 48 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

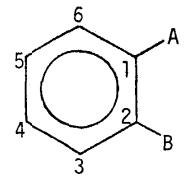



Table II

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 155 | $C_8H_8O_3$ | o-methoxybenzoic acid | $CO_2H$ | $OCH_3$ | 7.16 | 7.54 | 7.04 | 7.70 | 5 | x[d] | x[d] | 60 | 48 |
| 156 | | | $CO_2H$ | $OCH_3$ | 7.114 | 7.496 | 7.009 | 7.690 | 5 | 10 | x | 60 or 100 | 75 |
| 157 | | | $CO_2H$ | $OCH_3$ | 6.39 | 7.08 | 6.74 | 8.24 | 6 | x | x | 60 | 48 |
| 158 | $C_8H_8O_3$ | methyl o-hydroxybenzoate | $CO_2CH_3$ | OH | 7.02 | 7.48 | 6.91 | 7.86 | 3 | x | x | 60 | 48 |
| 159 | | | $CO_2CH_3$ | OH | 6.879 | 7.312 | 6.728 | 7.685 | 4 | 50 | x | 60 | 66 |
| 160 | | | $CO_2CH_3$ | OH | 7.01 | 7.54 | 6.96 | 7.81 | 5 | x | x | 60 | 48 |
| 161 | | | $CO_2CH_3$ | OH | 6.98 | 7.10 | 6.59 | 7.72 | 6 | x | x | 60 | 48 |
| 162 | | | $CO_2CH_3$ | OH | 6.957 | 7.506 | 6.916 | 7.821 | 8 | 1 | x | 100 | 9 |
| 163 | $C_8H_9Br$ | o-bromoethylbenzene | $C_2H_5$ | Br | 7.45 | 6.96 | 7.14 | 7.14 | 4 | 5 | x | 100 | 67 |
| 164 | $C_8H_9NO$ | o-aminoacetophenone | $COCH_3$ | $NH_2$ | 6.51 | 7.11 | 6.49 | 7.56 | 4 | 10 | x | 100 | 4 |
| 165 | | | $COCH_3$ | $NH_2$ | 6.77 | 7.23 | 6.54 | 7.71 | 5 | 10 | x | 100 | 4 |
| 166 | | | $COCH_3$ | $NH_2$ | 6.216 | 6.971 | 6.390 | 7.322 | 20 | 15 | x | 100 | 23 |
| 167 | $C_8H_9NO_2$ | N-methyl-o-hydroxybenzamide | $CONHCH_3$ | OH | 6.99 | 7.39 | 6.84 | 7.41 | 3 | x | x | 60 | 48 |
| 168 | | | $CONHCH_3$ | OH | 6.93 | 7.41 | 6.90 | 7.84 | 5 | x | x | 60 | 48 |
| 169 | | | $CONHCH_3$ | OH | 7.02 | 7.10 | 6.57 | 6.86 | 6 | x | x | 60 | 48 |
| 170 | $C_8H_9NO_2$ | o-nitroethylbenzene | $C_2H_5$ | $NO_2$ | 7.80 | 7.28 | 7.45 | 7.31 | 4 | 5 | x | 100 | 67 |
| 171 | $C_8H_{10}O$ | o-ethylphenol | OH | $C_2H_5$ | 7.02 | 6.76 | 6.94 | 6.58 | 4 | 5 | x | 100 | 67 |
| 172 | $C_8H_{10}O$ | o-methylanisole | $OCH_3$ | $CH_3$ | 7.00 | 6.72 | 7.02 | 6.68 | 4 | 5 | x | 100 | 67 |
| 173 | | | $OCH_3$ | $CH_3$ | 6.99 | 6.72 | 7.01 | 6.66 | 4 | 10 | x | 100 | 40 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

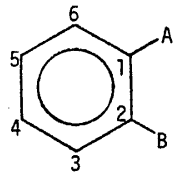
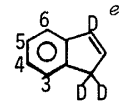
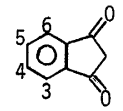
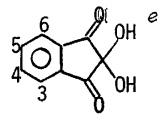
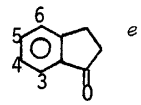
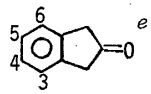



Table II

| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 174 | $C_8H_{10}O_2$ | o-dimethoxybenzene | $OCH_3$ | $OCH_3$ | 6.75 | 6.75 | 6.75 | 6.75 | 4 | x[d] | x[d] | x[d] | 7 |
| 175 | $C_8H_{11}N$ | o-ethylaniline | $NH_2$ | $C_2H_5$ | 6.91 | 6.59 | 6.88 | 6.47 | 4 | 5 | x | 100 | 67 |
| 176 | $C_8H_{11}N$ | N-methyl-o-toluidine | $NHCH_3$ | $CH_3$ | 6.88 | 6.52 | 6.99 | 6.44 | 4 | 5 | x | 100 | 67 |
| 177 | $C_9H_5D_3$ | indene-1,1,3-$d_3$ |  | | 7.085 | 6.931 | 7.017 | 7.103 | 1(?) | 100(?) | x | 100 | 16 |
| 178 | $C_9H_6O_2$ | 1,3-indandione |  | | 7.963 | 7.845 | 7.845 | 7.963 | 3 | 15 | x | 100 | 5 |
| 179 | | | " | | 7.96 | 7.84 | 7.84 | 7.96 | 5 | x | x | 100 | 85 |
| 180 | $C_9H_6O_4$ | 2,2-dihydroxy-1,3-indandione |  | | 7.99 | 7.94 | 7.94 | 7.99 | 5 | x | x | 100 | 85 |
| 181 | $C_9H_8O$ | 1-indanone |  | | 7.82 | 7.11 | 7.32 | 7.27 | 5 | x | x | 100 | 85 |
| 182 | $C_9H_8O$ | 2-indanone |  | | 7.16 | 7.16 | 7.16 | 7.16 | 5 | x | x | 100 | 85 |
| 183 | $C_9H_8O_4$ | o-acetoxybenzoic acid | $CO_2H$ | $OCOCH_3$ | 7.174 | 7.623 | 7.367 | 8.053 | 8 | 1.0M | x | 100 | 12 |

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

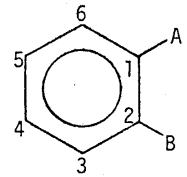
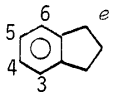
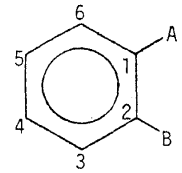



Table II

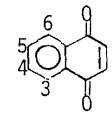
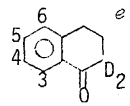
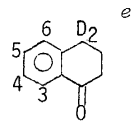
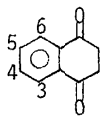
| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H{}^a$ 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 184 | $C_9H_9ClO$ | 2-(o-chlorophenyl)oxetane | | Cl | 7.27 | 7.15 | 7.24 | 7.68 | 4 | 2-5 | x[d] | 300 | 81 |
| 185 | | | " | Cl | 7.02 | 6.81 | 7.10 | 7.85 | 6 | 2-5 | x | 300 | 81 |
| 186 | $C_9H_{10}$ | indan |  | | 7.073 | 6.990 | 6.990 | 7.073 | 3 | 15 | x | 100 | 5 |
| 187 | | | " | | 7.07 | 6.99 | 6.99 | 7.07 | 5 | x | x | 100 | 85 |
| 188 | $C_9H_{10}O$ | o-methylacetophenone | $COCH_3$ | $CH_3$ | 7.15 | 7.27 | 7.16 | 7.61 | 4 | 5 | x | 100 | 67 |
| 189 | | | $COCH_3$ | $CH_3$ | 7.14 | 7.25 | 7.15 | 7.60 | 4 | 10 | x | 100 | 4 |
| 190 | | | $COCH_3$ | $CH_3$ | 7.28 | 7.42 | 7.31 | 7.79 | 5 | 10 | x | 100 | 4 |
| 191 | $C_9H_{10}O_2$ | o-cresol acetate | $OCOCH_3$ | $CH_3$ | 7.12 | 7.03 | 7.10 | 6.90 | 4 | 5 | x | 100 | 67 |
| 192 | $C_9H_{10}O_2$ | o-methoxyacetophenone | $COCH_3$ | $OCH_3$ | 6.87 | 7.33 | 6.89 | 7.63 | 4 | 10 | x | 100 | 4 |
| 193 | | | $COCH_3$ | $OCH_3$ | 7.15 | 7.53 | 7.02 | 7.60 | 5 | 10 | x | 100 | 4 |
| 194 | $C_9H_{10}O_2$ | methyl o-toluate | $CO_2CH_3$ | $CH_3$ | 7.15 | 7.29 | 7.14 | 7.85 | 4 | 5 | x | 100 | 67 |
| 195 | $C_9H_{10}O_3$ | o-methoxyphenylacetic acid | $CH_2CO_2H$ | $OCH_3$ | 6.927 | 7.218 | 6.876 | 7.199 | 8 | 1.0M | x | 100 | 12 |
| 196 | $C_9H_{10}O_3$ | methyl o-methoxybenzoate | $CO_2CH_3$ | $OCH_3$ | 6.99 | 7.47 | 6.98 | 7.80 | 3 | x | x | 60 | 48 |
| 197 | | | $CO_2CH_3$ | $OCH_3$ | 7.16 | 7.54 | 7.03 | 7.66 | 5 | x | x | 60 | 48 |
| 198 | | | $CO_2CH_3$ | $OCH_3$ | 6.54 | 7.11 | 6.74 | 7.84 | 6 | x | x | 60 | 48 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Table II




Substituent Arrangement: ORTHO

| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 199 | $C_9H_{11}NO_2$ | N-methyl-o-methoxybenzamide | $CONHCH_3$ | $OCH_3$ | 6.97 | 7.43 | 7.07 | 8.22 | 3 | x[d] | x[d] | 60 | 48 |
| 200 | | | $CONHCH_3$ | $OCH_3$ | 7.13 | 7.46 | 7.04 | 7.80 | 5 | x | x | 60 | 48 |
| 201 | | | $CONHCH_3$ | $OCH_3$ | 6.51 | 7.11 | 6.87 | 8.57 | 6 | x | x | 60 | 48 |
| 202 | $C_9H_{12}O$ | o-isopropylphenol | OH | i-$C_3H_7$ | 7.09 | 6.79 | 6.93 | 6.56 | 4 | 5 | x | 100 | 67 |
| 203 | $C_9H_{12}O$ | o-n-propylphenol | OH | n-$C_3H_7$ | 7.00 | 6.75 | 6.94 | 6.59 | 4 | 5 | x | 100 | 67 |
| 204 | $C_9H_{13}N$ | N,N-dimethyl-o-toluidine | $N(CH_3)_2$ | $CH_3$ | 7.02 | 6.81 | 7.00 | 6.91 | 4 | 5 | x | 100 | 67 |
| 205 | $C_{10}H_6O_2$ | 1,4-naphthoquinone |  | | 8.218 | 7.905 | 7.905 | 8.218 | 3 | 15 | x | 100 | 5 |
| 206 | $C_{10}H_8D_2O$ | 2,2-dideuterio-α-tetralone |  | | 7.876 | 7.148 | 7.297 | 7.098 | 4 | 15 | 32 | 100 | 83 |
| 207 | $C_{10}H_8D_2O$ | 4,4-dideuterio-α-tetralone |  | | 7.870 | 7.150 | 7.300 | 7.100 | 4 | 15 | 32 | 100 | 83 |
| 208 | $C_{10}H_8O_2$ | benzocyclohexene-1,4-dione |  | | 8.045 | 7.733 | 7.733 | 8.045 | 3 | 15 | x | 100 | 5 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

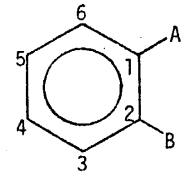
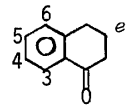
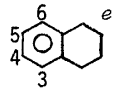
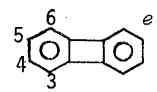


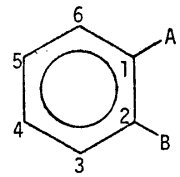

Table II

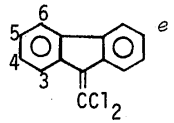
| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 209 | $C_{10}H_{10}O$ | α-tetralone |  | | 7.97 | 7.12 | 7.36 | 7.16 | 5 | x[d] | x[d] | 100 | 85 |
| 210 | $C_{10}H_{12}$ | tetralin |  | | 7.01 | 6.93 | 6.93 | 7.01 | 5 | x | x | 100 | 85 |
| 211 | $C_{10}H_{12}O_3$ | methyl o-methoxyphenylacetate | $CH_2CO_2CH_3$ | $OCH_3$ | 6.929 | 7.224 | 6.875 | 7.174 | 8 | 1.0M | x | 100 | 12 |
| 212 | $C_{10}H_{13}Br$ | o-tert-butylbromobenzene | Br | $C(CH_3)_3$ | 7.35 | 7.12 | 6.92 | 7.49 | 4 | 10 | x | 100 | 40 |
| 213 | $C_{10}H_{14}O$ | o-sec-butylphenol | OH | sec-$C_4H_9$ | 7.05 | 6.79 | 6.93 | 6.58 | 4 | 5 | x | 100 | 67 |
| 214 | $C_{10}H_{14}O$ | o-tert-butylphenol | OH | $C(CH_3)_3$ | 7.16 | 6.76 | 6.94 | 6.46 | 4 | 5 | x | 100 | 67 |
| 215 | $C_{12}H_4D_5Br$ | o-bromoperdeuteriophenylbenzene | $C_6D_5$ | Br | 7.58 | 7.08 | 7.23 | 7.23 | 4 | 10 | x | 100 | 40 |
| 216 | $C_{12}H_4D_5Cl$ | o-chloroperdeuteriophenylbenzene | $C_6D_5$ | Cl | 7.38 | 7.16 | 7.19 | 7.24 | 4 | 10 | x | 100 | 40 |
| 217 | $C_{12}H_4D_5F$ | o-fluoroperdeuteriophenylbenzene | $C_6D_5$ | F | 7.04 | 7.17 | 7.07 | 7.33 | 4 | 10 | x | 100 | 40 |
| 218 | $C_{12}H_4D_5I$ | o-iodoperdeuteriophenylbenzene | $C_6D_5$ | I | 7.87 | 6.92 | 7.27 | 7.21 | 4 | 10 | x | 100 | 40 |
| 219 | $C_{12}H_4D_5NO_2$ | o-nitroperdeuteriophenylbenzene | $C_6D_5$ | $NO_2$ | 7.71 | 7.36 | 7.48 | 7.33 | 4 | 10 | x | 100 | 40 |
| 220 | $C_{12}H_5D_5O$ | o-hydroxyperdeuteriophenylbenzene | $C_6D_5$ | OH | 6.83 | 7.11 | 6.84 | 7.10 | 4 | 10 | x | 100 | 40 |
| 221 | $C_{12}H_6D_5N$ | o-aminoperdeuteriophenylbenzene | $C_6D_5$ | $NH_2$ | 6.53 | 6.98 | 6.67 | 6.98 | 4 | 10 | x | 100 | 40 |
| 222 | $C_{12}H_8$ | biphenylene |  | | 6.664 | 6.556 | 6.556 | 6.664 | 3 | 15 | x | 100 | 5 |
| 223 | $C_{12}H_8Br_2$ | o,o'-dibromobiphenyl | o-$C_6H_4Br$ | Br | 7.304 | 6.734 | 6.899 | 7.057 | 6 | 5 | x | 60 | 32 |

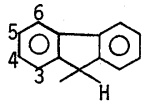
PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO



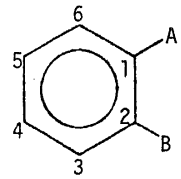

| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 224 | $C_{12}H_8Cl_2$ | o,o'-dichlorobiphenyl | o-$C_6H_4Cl$ | Cl | 7.155 | 6.815 | 6.874 | 7.138 | 6 | 5 | x[d] | 60 | 32 |
| 225 | $C_{12}H_8F_2$ | o,o'-difluorobiphenyl | o-$C_6H_4F$ | F | 6.853 | 6.890 | 6.823 | 7.214 | 6 | 5 | x | 60 | 32 |
| 226 | $C_{12}H_8I_2$ | o,o'-diiodobiphenyl | o-$C_6H_4I$ | I | 7.507 | 6.612 | 6.941 | 6.935 | 6 | 5 | x | 60 | 32 |
| 227 | $C_{12}H_8N_2O_4S$ | bis(o-nitrophenyl) sulfide | o-$NO_2C_6H_4S$ | $NO_2$ | 8.070 | 7.460 | 7.515 | 7.285 | 3 | 5-8 | 38 | 60 | 73 |
| 228 | $C_{12}H_8N_2O_4S_2$ | bis(o-nitrophenyl) disulfide | o-$NO_2C_6H_4S_2$ | $NO_2$ | 8.354 | 7.436 | 7.614 | 7.900 | 3 | 5-8 | 38 | 60 | 73 |
| 229 | $C_{12}H_{12}N_2S$ | bis(o-aminophenyl) sulfide | o-$NH_2C_6H_4S$ | $NH_2$ | 7.063 | 6.498 | 6.948 | 6.664 | 35 | 5-8 | 38 | 60 | 73 |
| 230 | $C_{12}H_{12}N_2S_2$ | bis(o-aminophenyl) disulfide | o-$NH_2C_6H_4S_2$ | $NH_2$ | 7.088 | 6.425 | 7.068 | 6.700 | 35 | 5-8 | 38 | 60 | 73 |
| 231 | $C_{13}H_4D_5N$ | o-cyanoperdeuteriophenylbenzene | $C_6D_5$ | CN | 7.64 | 7.32 | 7.51 | 7.41 | 4 | 10 | x | 100 | 40 |
| 232 | $C_{13}H_9Br$ | 9-bromofluorene | Br-R* | | 7.58 | 7.25 | 7.30 | 7.57 | 4 | 10 | x | 100 | 40 |
| 233 | $C_{13}H_9Cl$ | 9-chlorofluorene | Cl-R* | | 7.54 | 7.22 | 7.27 | 7.52 | 4 | 10 | x | 100 | 40 |
| 234 | $C_{13}H_9I$ | 9-iodofluorene | I-R* | | 7.56 | 7.20 | 7.25 | 7.54 | 4 | 10 | x | 100 | 40 |
| 235 | $C_{13}H_{10}$ | fluorene | H-R* | | 7.388 | 7.187 | 7.255 | 7.648 | 3 | 15 | x | 100 | 5 |
| 236 | | | H-R* | | 7.41 | 7.16 | 7.24 | 7.66 | 4 | 2 | x | 100 | 96 |
| 237 | | | H-R* | | 7.39 | 7.16 | 7.24 | 7.63 | 4 | 5 | x | 60 | 96 |
| 238 | | | H-R* | | 7.39 | 7.16 | 7.24 | 7.64 | 4 | 10 | x | 100 | 40 |
| 239 | $C_{14}H_8Cl_2$ | 9-dichloromethylenefluorene |  | | 8.22 | 7.20 | 7.27 | 7.54 | 4 | 10 | x | 100 | 40 |

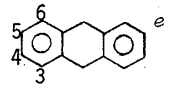
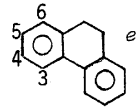
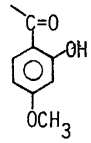
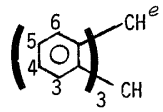
* R = 

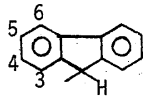
PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO



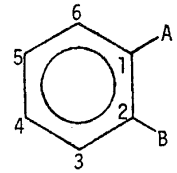

| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 240 | $C_{14}H_{12}$ | 9,10-dihydroanthracene |  | | 7.166 | 7.096 | 7.096 | 7.166 | 3 | 15 | x[d] | 100 | 5 |
| 241 | $C_{14}H_{12}$ | 9,10-dihydrophenanthrene |  | | 7.539 | 7.104 | 7.037 | 7.011 | 3 | 15 | x | 100 | 5 |
| 242 | $C_{14}H_{12}O$ | 9-methoxyfluorene | $CH_3O$-R* | | 7.51 | 7.21 | 7.28 | 7.56 | 4 | 10 | x | 100 | 40 |
| 243 | $C_{14}H_{12}O_4$ | 2,2'-dihydroxy-4-methoxybenzophenone |  | OH | 6.968 | 7.373 | 6.819 | 7.487 | 4 | 5 | x | 100 | 71 |
| 244 | $C_{14}H_{22}$ | o-di-t-butylbenzene | $C(CH_3)_3$ | $C(CH_3)_3$ | 6.972 | 7.447 | 7.447 | 6.972 | 4 | 10 | 36 | 60 | 29 |
| 245 | | | $C(CH_3)_3$ | $C(CH_3)_3$ | 6.96 | 7.46 | 7.46 | 6.96 | 4 | 10 | x | 100 | 40 |
| 246 | $C_{18}H_{14}$ | o-terphenyl | $C_6H_5$ | $C_6H_5$ | 7.27 | 7.31 | 7.31 | 7.27 | 4 | 10 | x | 100 | 40 |
| 247 | $C_{20}H_{14}$ | triptycene |  | | 7.228 | 6.855 | 6.855 | 7.228 | 7 | 2 | 29 | 60 | 6 |
| 248 | $C_{22}H_{22}O_2Te_2$ | o-phenylene-bis[p-ethoxyphenyl-telluride] | A = B = p-$C_2H_5OC_6H_4Te$ | | 7.255 | 6.902 | 6.902 | 7.255 | 3 | 1M | x | 100 | 89 |

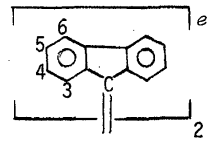
* R = 

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO




| Entry No. | Molecular Formula | Name | A[e] | B | $\delta_H$[a] 3 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 249 | $C_{26}H_{16}$ | dibiphenylene ethylene |  | | 8.38 | 7.13 | 7.23 | 7.61 | 4 | 10 | x[d] | 100 | 40 |

[a] Usual δ-scale. See text, section 2, item 5.

[b] See Table V and text, section 2, item 6.

[c] Concentration is given in percent unless number is followed by "M", molarity. The designation "0" refers to the shift at "infinite dilution". See text, section 2, item 7.

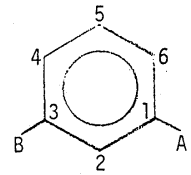
[d] The designation "x" means unknown or unspecified.

[e] Complete structure. See text, section 2, item 4.

Table III

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

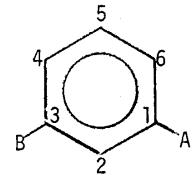



| Entry No. | Molecular Formula | Name | A | B | $\delta_H{}^a$ 2 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 001 | $C_6H_4BrCl$ | m-bromochlorobenzene | Cl | Br | 7.420 | 7.247 | 6.976 | 7.136 | 25 | 10 | 38 | 60 | 76 |
| 002 | $C_6H_4BrClMg$ | m-chlorophenylmagnesium bromide | MgBr | Cl | 7.59 | 6.98 | 7.02 | 7.49 | 10 | 1M | x[d] | 100 | 49 |
| 003 | $C_6H_4BrF$ | m-bromofluorobenzene | F | Br | 7.141 | 7.163 | 7.032 | 6.856 | 25 | 10 | 38 | 60 | 31 |
| 004 | $C_6H_4BrFMg$ | m-fluorophenylmagnesium bromide | MgBr | F | 7.41 | 6.67 | 7.06 | 7.34 | 10 | 1M | x | 100 | 49 |
| 005 | $C_6H_4BrI$ | m-bromoiodobenzene | I | Br | 7.771 | 7.312 | 6.767 | 7.481 | 25 | 10 | 38 | 60 | 76 |
| 006 | $C_6H_4BrNO_2$ | m-bromonitrobenzene | $NO_2$ | Br | 8.378 | 7.849 | 7.782 | 8.158 | 2 | 0[e] | 52 | 60 | 14 |
| 007 | | | $NO_2$ | Br | 8.367 | 7.795 | 7.420 | 8.161 | 4 | 0 | 52 | 60 | 14 |
| 008 | | | $NO_2$ | Br | 8.376 | 8.000 | 7.649 | 8.236 | 8 | 0 | 52 | 60 | 14 |
| 009 | | | $NO_2$ | Br | 8.319 | 7.694 | 7.274 | 8.079 | 9 | 0 | 52 | 60 | 14 |
| 010 | | | $NO_2$ | Br | 8.351 | 7.859 | 7.484 | 8.168 | 10 | 0 | 52 | 60 | 14 |
| 011 | | | $NO_2$ | Br | 8.409 | 7.984 | 7.619 | 8.254 | 11 | 0 | 52 | 60 | 14 |
| 012 | | | $NO_2$ | Br | 8.314 | 7.684 | 7.264 | 8.066 | 12 | 0 | 52 | 60 | 14 |
| 013 | | | $NO_2$ | Br | 8.381 | 7.953 | 7.590 | 8.230 | 13 | 0 | 52 | 60 | 14 |
| 014 | | | $NO_2$ | Br | 8.365 | 7.999 | 7.647 | 8.232 | 15 | 0 | 52 | 60 | 14 |
| 015 | | | $NO_2$ | Br | 8.366 | 7.862 | 7.474 | 8.163 | 16 | 0 | 52 | 60 | 14 |
| 016 | | | $NO_2$ | Br | 8.327 | 7.834 | 7.455 | 8.138 | 17 | 0 | 52 | 60 | 14 |
| 017 | | | $NO_2$ | Br | 8.349 | 7.960 | 7.600 | 8.198 | 18 | 0 | 52 | 60 | 14 |
| 018 | | | $NO_2$ | Br | 8.352 | 7.928 | 7.557 | 8.190 | 19 | 0 | 52 | 60 | 14 |
| 019 | $C_6H_4Br_2$ | m-dibromobenzene | Br | Br | 7.581 | 7.292 | 6.916 | 7.292 | 25 | 10 | 38 | 60 | 76 |
| 020 | $C_6H_4ClF$ | m-chlorofluorobenzene | F | Cl | 6.980 | 7.009 | 7.094 | 6.814 | 25 | 10 | 38 | 60 | 31 |

Table III

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

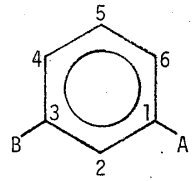



| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 021 | $C_6H_4ClI$ | m-chloroiodobenzene | I | Cl | 7.626 | 7.170 | 6.836 | 7.454 | 25 | 10 | 38 | 60 | 76 |
| 022 | $C_6H_4ClLi$ | m-chlorophenyllithium | Li | Cl | 7.90 | 6.94 | 6.97 | 7.81 | 10 | 1M | x[d] | 100 | 49 |
| 023 | $C_6H_4ClNO_2$ | m-chloronitrobenzene | $NO_2$ | Cl | 8.076 | 7.532 | 7.368 | 7.997 | 25 | 10 | 38 | 60 | 76 |
| 024 | $C_6H_4Cl_2$ | m-dichlorobenzene | Cl | Cl | 7.270 | 7.104 | 7.051 | 7.104 | 25 | 10 | 38 | 60 | 76 |
| 025 | $C_6H_4FI$ | m-fluoroiodobenzene | I | F | 7.337 | 6.884 | 6.881 | 7.362 | 25 | 10 | 38 | 60 | 31 |
| 026 | $C_6H_4F_2$ | m-difluorobenzene | F | F | 6.719 | 6.774 | 7.195 | 6.774 | 4 | 30 | x | 100 | 47 |
| 027 | | | F | F | 6.675 | 6.727 | 7.134 | 6.727 | 25 | 10 | 38 | 60 | 31 |
| 028 | $C_6H_4I_2$ | m-diiodobenzene | I | I | 8.001 | 7.537 | 6.648 | 7.537 | 25 | 10 | 38 | 60 | 76 |
| 029 | $C_6H_4Li_2$ | m-dilithiobenzene | Li | Li | 9.60 | 7.62 | 6.68 | 7.62 | 27 | 0.5M | x | 60 | 37 |
| 030 | $C_6H_4N_2O_4$ | m-dinitrobenzene | $NO_2$ | $NO_2$ | 9.030 | 8.553 | 7.802 | 8.553 | 2 | 0[e] | 52 | 60 | 14 |
| 031 | | | $NO_2$ | $NO_2$ | 9.018 | 8.542 | 7.779 | 8.542 | 4 | 0 | 52 | 60 | 14 |
| 032 | | | $NO_2$ | $NO_2$ | 8.954 | 8.658 | 8.010 | 8.658 | 8 | 0 | 52 | 60 | 14 |
| 033 | | | $NO_2$ | $NO_2$ | 8.968 | 8.578 | 7.865 | 8.578 | 10 | 0 | 52 | 60 | 14 |
| 034 | | | $NO_2$ | $NO_2$ | 8.982 | 8.636 | 7.958 | 8.636 | 11 | 0 | 52 | 60 | 14 |
| 035 | | | $NO_2$ | $NO_2$ | 9.000 | 8.676 | 8.006 | 8.676 | 13 | 0 | 52 | 60 | 14 |
| 036 | | | $NO_2$ | $NO_2$ | 8.944 | 8.662 | 8.029 | 8.662 | 15 | 0 | 52 | 60 | 14 |
| 037 | | | $NO_2$ | $NO_2$ | 8.984 | 8.554 | 7.825 | 8.554 | 16 | 0 | 52 | 60 | 14 |
| 038 | | | $NO_2$ | $NO_2$ | 8.952 | 8.530 | 7.803 | 8.530 | 17 | 0 | 52 | 60 | 14 |
| 039 | | | $NO_2$ | $NO_2$ | 8.930 | 8.601 | 7.931 | 8.501 | 18 | 0 | 52 | 60 | 14 |
| 040 | | | $NO_2$ | $NO_2$ | 8.933 | 8.583 | 7.903 | 8.583 | 19 | 0 | 52 | 60 | 14 |

Table III

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

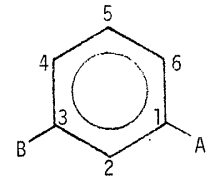



| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 041 | $C_6H_6N_2O_2$ | m-nitroaniline | $NH_2$ | $NO_2$ | 7.516 | 7.445 | 7.258 | 6.943 | 2 | 0[c] | 52 | 60 | 14 |
| 042 | | | $NH_2$ | $NO_2$ | 7.489 | 7.392 | 7.105 | 7.044 | 8 | 0 | 52 | 60 | 14 |
| 043 | | | $NH_2$ | $NO_2$ | 7.452 | 7.390 | 7.157 | 6.857 | 10 | 0 | 52 | 60 | 14 |
| 044 | | | $NH_2$ | $NO_2$ | 7.488 | 7.400 | 7.225 | 6.973 | 11 | 0 | 52 | 60 | 14 |
| 045 | | | $NH_2$ | $NO_2$ | 7.500 | 7.416 | 7.249 | 7.002 | 13 | 0 | 52 | 60 | 14 |
| 046 | | | $NH_2$ | $NO_2$ | 7.456 | 7.350 | 7.235 | 7.012 | 15 | 0 | 52 | 60 | 14 |
| 047 | | | $NH_2$ | $NO_2$ | 7.475 | 7.459 | 7.242 | 6.952 | 16 | 0 | 52 | 60 | 14 |
| 048 | | | $NH_2$ | $NO_2$ | 7.467 | 7.449 | 7.218 | 6.923 | 17 | 0 | 52 | 60 | 14 |
| 049 | | | $NH_2$ | $NO_2$ | 7.455 | 7.410 | 7.279 | 7.030 | 18 | 0 | 52 | 60 | 14 |
| 050 | $C_7H_4BrF_3Mg$ | m-trifluoromethylmagnesium bromide | MgBr | $CF_3$ | 7.98 | 7.24 | 7.28 | 7.90 | 10 | 1M | x[d] | 100 | 49 |
| 051 | $C_7H_4F_3Li$ | m-trifluoromethylphenyllithium | Li | $CF_3$ | 8.17 | 7.03 | 7.07 | 8.05 | 10 | 1M | x | 100 | 49 |
| 052 | $C_7H_5BrO$ | m-bromobenzaldehyde | CHO | Br | 7.720 | 7.478 | 7.196 | 7.596 | 1 | 90 | x | 60 | 59 |
| 053 | $C_7H_5BrO_2$ | m-bromobenzoic acid | $CO_2H$ | Br | 8.104 | 7.806 | 7.480 | 7.991 | 5 | 10 | x | 60 or 100 | 75 |
| 054 | $C_7H_5ClO_2$ | m-chlorobenzoic acid | $CO_2H$ | Cl | 7.955 | 7.667 | 7.543 | 7.949 | 5 | 10 | x | 60 or 100 | 75 |
| 055 | $C_7H_5FO$ | m-fluorobenzaldehyde | CHO | F | 7.576 | 7.389 | 7.589 | 7.736 | 8 | 30 | 30 | 100 | 21 |
| 056 | $C_7H_5IO$ | m-iodobenzaldehyde | CHO | I | 8.072 | 7.781 | 7.234 | 7.839 | 1 | 90 | x | 60 | 59 |
| 057 | $C_7H_5NO_4$ | m-nitrobenzoic acid | $CO_2H$ | $NO_2$ | 8.626 | 8.449 | 7.819 | 8.354 | 5 | 10 | x | 60 or 100 | 75 |

Table III

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

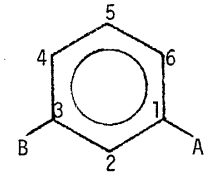



| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 058 | $C_7H_6O_3$ | m-hydroxybenzoic acid | $CO_2H$ | OH | 7.476 | 7.069 | 7.325 | 7.482 | 5 | 10 | x[d] | 60 or 100 | 75 |
| 059 | | | $CO_2H$ | OH | 7.572 | 7.123 | 7.347 | 7.576 | 8 | 1.0M | x | 100 | 9 |
| 060 | $C_7H_7Br$ | m-bromotoluene | $CH_3$ | Br | 7.26 | 7.22 | 7.03 | 7.00 | 4 | 5 | x | 100 | 67 |
| 061 | $C_7H_7BrMg$ | m-tolylmagnesium bromide | MgBr | $CH_3$ | 7.45 | 6.79 | 6.93 | 7.39 | 10 | 1M | x | 100 | 49 |
| 062 | $C_7H_7BrMgO$ | m-anisylmagnesium bromide | MgBr | $OCH_3$ | 7.22 | 6.57 | 7.02 | 7.21 | 10 | 1M | x | 100 | 49 |
| 063 | $C_7H_7Cl$ | m-chlorotoluene | $CH_3$ | Cl | 7.10 | 7.06 | 7.09 | 6.95 | 4 | 5 | x | 100 | 67 |
| 064 | $C_7H_7I$ | m-iodotoluene | $CH_3$ | I | 7.48 | 7.42 | 6.90 | 7.03 | 4 | 5 | x | 100 | 67 |
| 065 | $C_7H_7Li$ | m-tolyllithium | Li | $CH_3$ | 7.86 | 6.80 | 6.95 | 7.80 | 10 | 1M | x | 100 | 49 |
| 066 | $C_7H_7LiO$ | m-anisyllithium | Li | $OCH_3$ | 7.64 | 6.52 | 7.00 | 7.53 | 10 | 1M | x | 100 | 49 |
| 067 | $C_7H_7NO_2$ | m-nitrotoluene | $CH_3$ | $NO_2$ | 7.98 | 7.96 | 7.37 | 7.43 | 4 | 5 | x | 100 | 67 |
| 068 | $C_7H_8O$ | m-cresol | OH | $CH_3$ | 6.53 | 6.63 | 6.99 | 6.52 | 4 | 5 | x | 100 | 67 |
| 069 | $C_7H_9N$ | m-toluidine | $NH_2$ | $CH_3$ | 6.31 | 6.42 | 6.89 | 6.29 | 4 | 5 | x | 100 | 67 |
| 070 | $C_8H_7Br$ | m-bromostyrene | $CH{=}CH_2$ | Br | 7.415 | 7.248 | 7.073 | 7.183 | 7 | 5 | x | 100 | 62 |
| 071 | $C_8H_7ClO$ | m-toluyl chloride | COCl | $CH_3$ | 7.86 | 7.42 | 7.34 | 7.88 | 4 | 5 | x | 100 | 67 |
| 072 | $C_8H_7N$ | m-tolunitrile | CN | $CH_3$ | 7.41 | 7.34 | 7.31 | 7.39 | 4 | 5 | x | 100 | 67 |
| 073 | $C_8H_8O$ | m-tolualdehyde | CHO | $CH_3$ | 7.61 | 7.35 | 7.35 | 7.59 | 4 | 5 | x | 100 | 67 |
| 074 | $C_8H_8O_2$ | m-toluic acid | $CO_2H$ | $CH_3$ | 7.90 | 7.33 | 7.29 | 7.89 | 4 | 5 | x | 100 | 67 |
| 075 | | | $CO_2H$ | $CH_3$ | 7.831 | 7.417 | 7.385 | 7.810 | 5 | 10 | x | 60 or 100 | 75 |

Table III

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

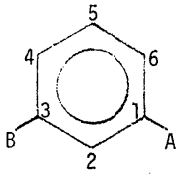



| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 076 | $C_8H_8O_3$ | m-hydroxyphenylacetic acid | $CH_2CO_2H$ | OH | 6.818 | 6.724 | 7.109 | 6.766 | 8 | 1.0M | x[d] | 100 | 12 |
| 077 | $C_8H_8O_3$ | m-methoxybenzoic acid | $CO_2H$ | $OCH_3$ | 7.531 | 7.193 | 7.425 | 7.610 | 5 | 10 | x | 60 or 100 | 75 |
| 078 | $C_8H_9Br$ | m-bromoethylbenzene | $C_2H_5$ | Br | 7.27 | 7.23 | 7.06 | 7.03 | 4 | 5 | x | 100 | 67 |
| 079 | $C_8H_9NO_2$ | m-nitroethylbenzene | $C_2H_5$ | $NO_2$ | 8.00 | 7.98 | 7.40 | 7.46 | 4 | 5 | x | 100 | 67 |
| 080 | $C_8H_{10}O$ | m-ethylphenol | OH | $C_2H_5$ | 6.56 | 6.65 | 7.01 | 6.54 | 4 | 5 | x | 100 | 67 |
| 081 | $C_8H_{10}O$ | m-methylanisole | $OCH_3$ | $CH_3$ | 6.59 | 6.63 | 7.03 | 6.57 | 4 | 5 | x | 100 | 67 |
| 082 | $C_8H_{11}N$ | m-ethylaniline | $NH_2$ | $C_2H_5$ | 6.40 | 6.48 | 6.91 | 6.38 | 4 | 5 | x | 100 | 67 |
| 083 | $C_8H_{11}N$ | N-methyl-m-toluidine | $NHCH_3$ | $CH_3$ | 6.24 | 6.39 | 6.91 | 6.23 | 4 | 5 | x | 100 | 67 |
| 084 | $C_9H_{10}O$ | m-methylacetophenone | $COCH_3$ | $CH_3$ | 7.67 | 7.26 | 7.25 | 7.65 | 4 | 5 | x | 100 | 67 |
| 085 | $C_9H_{10}O_2$ | m-cresol acetate | $OCOCH_3$ | $CH_3$ | 6.81 | 6.92 | 7.14 | 6.79 | 4 | 5 | x | 100 | 67 |
| 086 | $C_9H_{10}O_2$ | methyl m-toluate | $CO_2CH_3$ | $CH_3$ | 7.78 | 7.26 | 7.24 | 7.75 | 4 | 5 | x | 100 | 67 |
| 087 | $C_9H_{10}O_3$ | m-methoxyphenylacetic acid | $CH_2CO_2H$ | $OCH_3$ | 6.893 | 6.805 | 7.206 | 6.875 | 8 | 1.0M | x | 100 | 12 |
| 088 | $C_9H_{10}O_3$ | methyl m-methoxybenzoate | $CO_2CH_3$ | $OCH_3$ | 7.518 | 7.171 | 7.396 | 7.583 | 8 | 1.0M | x | 100 | 9 |
| 089 | $C_9H_{13}N$ | N,N-dimethyl m-toluidine | $N(CH_3)_2$ | $CH_3$ | 6.40 | 6.41 | 6.96 | 6.40 | 4 | 5 | x | 100 | 67 |
| 090 | $C_{10}H_{10}O_4$ | methyl m-acetoxybenzoate | $CO_2CH_3$ | $OCOCH_3$ | 7.737 | 7.377 | 7.527 | 7.878 | 8 | 1.0M | x | 100 | 12 |
| 091 | $C_{10}H_{12}O_3$ | methyl m-methoxyphenylacetate | $CH_2CO_2CH_3$ | $OCH_3$ | 6.862 | 6.812 | 7.208 | 6.846 | 8 | 1.0M | x | 100 | 12 |
| 092 | $C_{11}H_{12}O_4$ | methyl m-acetoxyphenylacetate | $CH_2CO_2CH_3$ | $OCOCH_3$ | 7.055 | 7.012 | 7.321 | 7.156 | 8 | 1.0M | x | 100 | 12 |
| 093 | $C_{12}H_8Br_2$ | m,m'-dibromobiphenyl | m-$C_6H_4Br$ | Br | 7.548 | 7.225 | 6.813 | 7.143 | 6 | 5 | x | 60 | 32 |

Table III

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META




| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2 | 4 | 5 | 6 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 094 | $C_{12}H_8Cl_2$ | m,m'-dichlorobiphenyl | m-$C_6H_4Cl$ | Cl | 7.398 | 7.075 | 6.894 | 7.118 | 6 | 5 | x[d] | 60 | 32 |
| 095 | $C_{12}H_8F_2$ | m,m'-difluorobiphenyl | m-$C_6H_4F$ | F | 7.097 | 6.774 | 6.970 | 7.067 | 6 | 5 | x | 60 | 32 |
| 096 | $C_{12}H_8I_2$ | m,m'-diiodobiphenyl | m-$C_6H_4I$ | I | 7.751 | 7.427 | 6.691 | 7.185 | 6 | 5 | x | 60 | 32 |
| 097 | $C_{12}H_{18}$ | m-tert-butylethylbenzene | $C_2H_5$ | $C(CH_3)_3$ | 6.76 | 6.85 | 7.04 | 6.55 | 4 | 5 | x | 100 | 67 |
| 098 | $C_{15}H_{12}N_2O_2$ | cinnamaldehyde m-nitroanil | $N{=}CHCH{=}CHC_6H_5$ | $NO_2$ | 7.98 | 7.99 | 7.46 | 7.35 | 4 | x[d] | x | 100 | 13 |
| 099 | | | $N{=}CHCH{=}CHC_6H_5$ | $NO_2$ | 7.82 | 7.72 | 6.81 | 7.10 | 6 | x | x | 100 | 13 |
| 100 | | | $N{=}CHCH{=}CHC_6H_5$ | $NO_2$ | 7.80 | 7.91 | 7.42 | 7.34 | 7 | x | x | 100 | 13 |

[a] Usual δ-scale. See text, section 2, item 5.

[b] See Table V and text, section 2, item 6.

[c] Concentration is given in percent unless number is followed by "M", molarity. The designation "0" refers to the shift at "infinite dilution". See text, section 2, item 7.

[d] The designation "x" means unknown or unspecified.

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

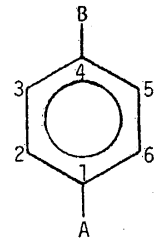



Table IV

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 001 | $C_6H_4BrCl$ | p-bromochlorobenzene | Cl | Br | 7.12 | 7.39 | 3 | x[d] | x[d] | x[d] | 2 |
| 002 | | | Cl | Br | 7.30 | 7.50 | 4 | 14 | 25 | 60 | 78 |
| 003 | | | Cl | Br | 7.070 | 7.284 | 25 | 10 | 38 | 60 | 76 |
| 004 | $C_6H_4BrClMg$ | p-chlorophenylmagnesium bromide | MgBr | Cl | 7.58 | 7.04 | 10 | 1M | x | 100 | 49 |
| 005 | | | MgBr | Cl | 7.54 | 7.09 | 10 | 0.5M | x | 60 | 37 |
| 006 | $C_6H_4BrF$ | p-bronofluorobenzene | F | Br | 6.77 | 7.25 | 1 | 100 | 25 | 60 | 78 |
| 007 | | | F | Br | 6.90 | 7.42 | 3 | x | x | x | 2 |
| 008 | | | F | Br | 6.83 | 7.33 | 7 | 29 | x | 60 | 94 |
| 009 | | | F | Br | 6.794 | 7.311 | 25 | 10 | 38 | 60 | 31 |
| 010 | $C_6H_4BrFMg$ | p-fluorophenylmagnesium bromide | MgBr | F | 7.62 | 6.88 | 10 | 1M | x | 100 | 49 |
| 011 | $C_6H_4BrI$ | p-bromoiodobenzene | I | Br | 7.50 | 7.39 | 3 | x | x | x | 2 |
| 012 | | | I | Br | 7.462 | 7.148 | 25 | 10 | 38 | 60 | 76 |
| 013 | $C_6H_4BrNO_2$ | p-bromonitrobenzene | $NO_2$ | Br | 8.04 | 7.58 | 3 | x | x | 60 or 100 | 80 |
| 014 | | | $NO_2$ | Br | 8.02 | 7.61 | 3 | x | x | x | 2 |
| 015 | | | $NO_2$ | Br | 8.19 | 7.87 | 8 | 6 | 25 | 60 | 78 |
| 016 | $C_6H_4Br_2$ | p-dibromobenzene | Br | Br | 7.67 | 7.67 | 3 | x | x | x | 2 |
| 017 | | | Br | Br | 7.50 | 7.50 | 8 | 2 | 40 | 60 | 34 |
| 018 | | | Br | Br | 7.33 | 7.33 | 12 | 2 | 40 | 60 | 34 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

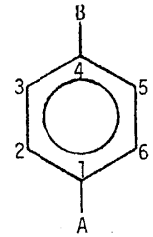



TABLE IV

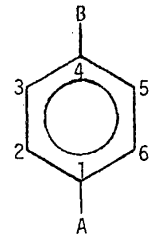
Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 019 | $C_6H_4Br_2$ | p-dibromobenzene | Br | Br | 7.222 | 7.222 | 25 | 10 | 38 | 60 | 76 |
| 020 | | | Br | Br | 7.43 | 7.43 | 26 | 2 | 40 | 60 | 34 |
| 021 | $C_6H_4Br_2Mg_2$ | p-bis(bromomagnesio)benzene | MgBr | MgBr | 7.70 | 7.70 | 27 | 0.5M | x[d] | 60 | 37 |
| 022 | $C_6H_4ClF$ | p-chlorofluorobenzene | F | Cl | 6.81 | 7.09 | 1 | 100 | 25 | 60 | 78 |
| 023 | | | F | Cl | 6.87 | 7.17 | 7 | 24 | x | 60 | 94 |
| 024 | | | F | Cl | 6.832 | 7.147 | 25 | 10 | 38 | 60 | 31 |
| 025 | $C_6H_4ClI$ | p-chloroiodobenzene | I | Cl | 7.57 | 7.03 | 3 | x[d] | x | x[d] | 2 |
| 026 | | | I | Cl | 7.478 | 6.941 | 25 | 10 | 38 | 60 | 76 |
| 027 | $C_6H_4ClLi$ | p-chlorophenyllithium | Li | Cl | 7.46(?) | 7.26(?) | 10 | 0.5 | x | 60 | 37 |
| 028 | | | Li | Cl | 7.89(?) | 7.02(?) | 10 | 1M | x | 100 | 49 |
| 029 | $C_6H_4ClNO_2$ | p-chloronitrobenzene | $NO_2$ | Cl | 8.29 | 7.71 | 8 | 8 | 25 | 60 | 78 |
| 030 | $C_6H_4Cl_2$ | p-dichlorobenzene | Cl | Cl | 7.22 | 7.22 | 3 | x | x | x | 2 |
| 031 | | | Cl | Cl | 7.40 | 7.40 | 8 | 2 | 40 | 60 | 34 |
| 032 | | | Cl | Cl | 7.18 | 7.18 | 12 | 2 | 40 | 60 | 34 |
| 033 | | | Cl | Cl | 7.070 | 7.070 | 25 | 10 | 38 | 60 | 76 |
| 034 | | | Cl | Cl | 7.36 | 7.36 | 26 | 2 | 40 | 60 | 34 |
| 035 | $C_6H_4Cl_2FP$ | p-fluorophenyldichlorophosphine | $PCl_2$ | F | 7.46 | 6.72 | 6 | 30 | 32 | 100 | 91 |
| 036 | $C_6H_4DBrMg$ | p-deuteriophenylmagnesium bromide | MgBr | D | 7.64 | 7.02 | 10 | 1.0M | 33 | 60 | 36 |
| 037 | $C_6H_4DLi$ | p-deuteriophenyllithium | Li | D | 8.02 | 7.02 | 10 | 1.0M | 33 | 60 | 36 |

TABLE IV

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA




| Entry No. | Molecular Formula | Name | A | B | $\delta_H{}^a$ 2,6 | $\delta_H{}^a$ 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 038 | $C_6H_4FI$ | p-fluoroiodobenzene | I | F | 7.33 | 6.57 | 1 | 100 | 25 | 60 | 78 |
| 039 | | | I | F | 7.492 | 6.671 | 25 | 10 | 38 | 60 | 31 |
| 040 | $C_6H_4FLi$ | p-fluorophenyllithium | Li | F | 7.98 | 6.85 | 10 | 1M | x[d] | 100 | 49 |
| 041 | $C_6H_4FNO_2$ | p-fluoronitrobenzene | $NO_2$ | F | 8.26 | 7.24 | 1 | 100 | 25 | 60 | 78 |
| 042 | | | $NO_2$ | F | 8.28 | 7.20 | 3 | x[d] | x | x[d] | 2 |
| 043 | $C_6H_4F_2$ | p-difluorobenzene | F | F | 6.847 | 6.847 | 1 | 100 | x | 60 | 50 |
| 044 | | | F | F | 7.33 | 7.33 | 3 | x | x | x | 2 |
| 045 | $C_6H_4INO_2$ | p-iodonitrobenzene | $NO_2$ | I | 7.90 | 7.90 | 3 | x | x | x | 2 |
| 046 | | | $NO_2$ | I | 8.00 | 8.08 | 8 | 2 | 25 | 60 | 78 |
| 047 | $C_6H_4I_2$ | p-diiodobenzene | I | I | 7.62 | 7.62 | 3 | x | x | x | 2 |
| 048 | | | I | I | 7.306 | 7.306 | 25 | 10 | 38 | 60 | 76 |
| 049 | $C_6H_4N_2O_4$ | p-dinitrobenzene | $NO_2$ | $NO_2$ | 8.34 | 8.34 | 3 | x | x | x | 2 |
| 050 | $C_6H_5BrO$ | p-bromophenol | OH | Br | 6.60 | 7.25 | 3 | x | x | x | 2 |
| 051 | $C_6H_5ClNO_2$ | p-chloronitrobenzene | $NO_2$ | Cl | 8.11 | 7.45 | 3 | x | x | x | 2 |
| 052 | $C_6H_5ClO$ | p-chlorophenol | OH | Cl | 6.64 | 7.12 | 3 | x | x | x | 2 |
| 053 | | | OH | Cl | 6.68 | 7.14 | 4 | 10 | x | 100 | 40 |
| 054 | | | OH | Cl | 6.87 | 7.17 | 8 | 25 | 25 | 60 | 78 |
| 055 | $C_6H_5FO$ | p-fluorophenol | OH | F | 6.72 | 6.92 | 3 | x | x | x | 2 |
| 056 | $C_6H_5NO_3$ | p-nitrophenol | OH | $NO_2$ | 6.92 | 8.10 | 3 | x | x | x | 2 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

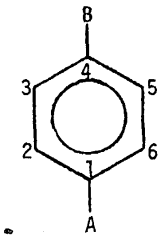


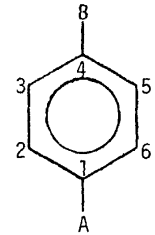

TABLE IV

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 057 | $C_6H_5NO_3$ | p-nitrophenol | OH | $NO_2$ | 6.69 | 7.83 | 8 | 11 | 25 | 60 | 78 |
| 058 | $C_6H_6BrN$ | p-bromoaniline | $NH_2$ | Br | 6.61 | 7.15 | 8 | 13 | 25 | 60 | 78 |
| 059 | $C_6H_6FN$ | p-fluoroaniline | $NH_2$ | F | 6.40 | 6.78 | 1 | 100 | 25 | 60 | 78 |
| 060 | | | $NH_2$ | F | 6.48 | 6.81 | 3 | x[d] | x[d] | x[d] | 2 |
| 061 | $C_6H_6IN$ | p-iodoaniline | $NH_2$ | I | 6.32 | 7.34 | 3 | x | x | x | 2 |
| 062 | | | $NH_2$ | I | 6.50 | 7.30 | 8 | 11 | 25 | 60 | 78 |
| 063 | $C_6H_6N_2O_2$ | p-nitroaniline | $NH_2$ | $NO_2$ | 6.61 | 8.05 | 3 | x | x | x | 2 |
| 064 | | | $NH_2$ | $NO_2$ | 6.742 | 8.019 | 8 | x | 33 | 60 | 8 |
| 065 | | | $NH_2$ | $NO_2$ | 6.76 | 8.02 | 8 | 9 | 25 | 60 | 78 |
| 066 | $C_6H_6OS$ | p-hydroxybenzenethiol | SH | OH | 7.066 | 6.644 | 3 | 1M | x | 100 | 89 |
| 067 | $C_6H_6O_2$ | p-hydroquinone | OH | OH | 7.11 | 7.11 | 12 | 2 | 40 | 60 | 34 |
| 068 | $C_7H_4BrClO$ | p-bromobenzoyl chloride | COCl | Br | 7.92 | 7.63 | 3 | x | x | x | 2 |
| 069 | $C_7H_4BrF_3Mg$ | p-trifluoromethylphenylmagnesium bromide | MgBr | $CF_3$ | 7.82 | 7.30 | 10 | 1M | x | 100 | 49 |
| 070 | $C_7H_4ClFO$ | p-fluorobenzoyl chloride | COCl | F | 8.06 | 7.14 | 3 | x | x | x | 2 |
| 071 | $C_7H_4ClFO$ | p-chlorobenzoyl fluoride | COF | Cl | 7.935 | 7.462 | 10 | x | 31 | 100 | 15 |
| 072 | $C_7H_4ClF_3$ | p-trifluoromethylchlorobenzene | Cl | $CF_3$ | 7.51 | 7.48 | 4 | 10 | x | 100 | 40 |
| 073 | $C_7H_4ClIO$ | p-iodobenzoyl chloride | COCl | I | 7.78 | 7.78 | 3 | x | x | x | 2 |
| 074 | $C_7H_4ClN$ | p-chlorobenzonitrile | CN | Cl | 7.56 | 7.43 | 3 | x | x | x | 2 |

TABLE IV

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA




| Entry No. | Molecular Formula | Name | A | B | $\delta_H{}^a$ 2,6 | $\delta_H{}^a$ 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 075 | $C_7H_4ClNO_3$ | p-nitrobenzoyl chloride | COCl | $NO_2$ | 8.32 | 8.32 | 3 | x[d] | x[d] | x[d] | 2 |
| 076 | | | COCl | $NO_2$ | 8.42 | 8.36 | 8 | 15 | 25 | 60 | 78 |
| 077 | $C_7H_4Cl_2O$ | p-chlorobenzoyl chloride | COCl | Cl | 7.94 | 7.41 | 3 | x | x | x | 2 |
| 078 | $C_7H_4Cl_4$ | p-trichloromethylchlorobenzene | Cl | $CCl_3$ | 7.36 | 7.86 | 4 | 10 | x | 100 | 40 |
| 079 | $C_7H_4FN$ | p-fluorobenzonitrile | CN | F | 7.67 | 7.17 | 3 | x | x | x | 2 |
| 080 | $C_7H_4F_3Li$ | p-trifluoromethylphenyllithium | Li | $CF_3$ | 8.05 | 7.23 | 10 | 1M | x | 100 | 49 |
| 081 | $C_7H_4IN$ | p-iodobenzonitrile | CN | I | 7.35 | 7.80 | 3 | x | x | x | 2 |
| 082 | $C_7H_4N_2O_2$ | p-nitrobenzonitrile | CN | $NO_2$ | 7.90 | 8.33 | 3 | x | x | x | 2 |
| 083 | | | CN | $NO_2$ | 8.15 | 8.45 | 8 | 5 | 25 | 60 | 78 |
| 084 | $C_7H_5BrO_2$ | p-bromobenzoic acid | $CO_2H$ | Br | 7.96 | 7.68 | 3 | x | x | x | 2 |
| 085 | | | $CO_2H$ | Br | 7.925 | 7.707 | 5 | 10 | x | 60 or 100 | 75 |
| 086 | | | $CO_2H$ | Br | 7.96 | 7.70 | 8 | 0.8 | 25 | 60 | 78 |
| 087 | $C_7H_5ClO_2$ | p-chlorobenzoic acid | $CO_2H$ | Cl | 7.96 | 7.52 | 3 | x | x | x | 2 |
| 088 | | | $CO_2H$ | Cl | 8.018 | 7.543 | 5 | 10 | x | 60 or 100 | 75 |
| 089 | $C_7H_5FO$ | p-fluorobenzaldehyde | CHO | F | 7.976 | 7.289 | 8 | 30 | 30 | 100 | 21 |
| 090 | $C_7H_5FO_2$ | p-fluorobenzoic acid | $CO_2H$ | F | 8.03 | 7.29 | 3 | x | x | x | 2 |
| 091 | | | $CO_2H$ | F | 8.089 | 7.304 | 5 | 10 | x | 60 or 100 | 75 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

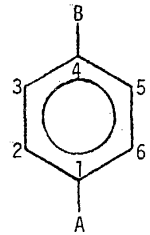



TABLE IV

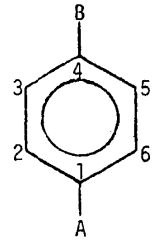
Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 092 | $C_7H_5FO_2$ | p-fluorobenzoic acid | $CO_2H$ | F | 8.09 | 7.25 | 8 | 0.9 | 25 | 60 | 78 |
| 093 | $C_7H_5IO_2$ | p-iodobenzoic acid | $CO_2H$ | I | 7.86 | 7.70 | 3 | x[d] | x[d] | x[d] | 2 |
| 094 | | | $CO_2H$ | I | 7.898 | 7.765 | 5 | 10 | x | 60 or 100 | 75 |
| 095 | $C_7H_5NO$ | p-hydroxybenzonitrile | CN | OH | 7.51 | 6.95 | 3 | x | x | x | 2 |
| 096 | $C_7H_5NO_3$ | p-nitrobenzaldehyde | CHO | $NO_2$ | 8.22 | 8.44 | 8 | 7 | 25 | 60 | 78 |
| 097 | $C_7H_6N_2$ | p-aminobenzonitrile | CN | $NH_2$ | 7.30 | 6.57 | 3 | x | x | x | 2 |
| 098 | $C_7H_6O_2$ | p-hydroxybenzaldehyde | CHO | OH | 7.82 | 7.04 | 8 | 9 | 25 | 60 | 78 |
| 099 | $C_7H_6O_3$ | p-hydroxybenzoic acid | $CO_2H$ | OH | 7.83 | 6.88 | 3 | x | x | x | 2 |
| 100 | | | $CO_2H$ | OH | 7.889 | 6.904 | 5 | 10 | x | 60 or 100 | 75 |
| 101 | | | $CO_2H$ | OH | 7.978 | 6.962 | 8 | 1.0M | x | 100 | 9 |
| 102 | $C_7H_7Br$ | p-bromotoluene | $CH_3$ | Br | 6.98 | 7.33 | 3 | x | x | x | 2 |
| 103 | | | $CH_3$ | Br | 6.96 | 7.29 | 4 | 5 | x | 100 | 67 |
| 104 | | | $CH_3$ | Br | 6.59 | 7.19 | 6 | 1-3 | x | 100 | 93 |
| 105 | | | $CH_3$ | Br | 6.86 | 7.20 | 7 | 45 | 25 | 60 | 78 |
| 106 | | | $CH_3$ | Br | 6.90 | 7.25 | 12 | 1-3 | x | 100 | 93 |
| 107 | $C_7H_7BrMg$ | p-tolylmagnesium bromide | MgBr | $CH_3$ | 7.48 | 6.86 | 10 | 0.8M | x | 60 | 37 |
| 108 | | | MgBr | $CH_3$ | 7.48 | 6.87 | 10 | 1M | x | 100 | 49 |

TABLE IV

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

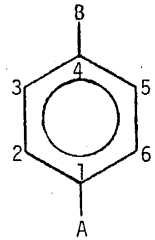



| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 109 | $C_7H_7BrMg$ | p-tolylmagnesium bromide | MgBr | $CH_3$ | 7.42 | 6.70 | 27 | 0.4M | x[d] | 60 | 37 |
| 110 | $C_7H_7BrMgO$ | p-anisylmagnesium bromide | MgBr | $OCH_3$ | 7.40(?) | 6.66(?) | 10 | 0.58M | x | 60 | 37 |
| 111 | | | MgBr | $OCH_3$ | 7.54(?) | 6.72(?) | 10 | 1M | x | 100 | 49 |
| 112 | | | MgBr | $OCH_3$ | 7.50 | 6.60 | 27 | 0.68M | x | 60 | 37 |
| 113 | $C_7H_7BrO$ | p-bromoanisole | $OCH_3$ | Br | 6.592 | 7.207 | 25 | 10 | 38 | 60 | 76 |
| 114 | $C_7H_7CaI$ | p-tolylcalcium iodide | CaI | $CH_3$ | 8.24 | 6.96 | 27 | 0.5M | x | 60 | 37 |
| 115 | $C_7H_7Cl$ | p-chlorotoluene | $CH_3$ | Cl | 7.04 | 7.18 | 3 | x | x | x | 2 |
| 116 | | | $CH_3$ | Cl | 7.01 | 7.14 | 4 | 5 | x | 100 | 67 |
| 117 | | | $CH_3$ | Cl | 6.66 | 7.04 | 6 | 1-3 | x | 100 | 93 |
| 118 | | | $CH_3$ | Cl | 6.95 | 7.08 | 12 | 1-3 | x | 100 | 93 |
| 119 | $C_7H_7ClO$ | p-chloroanisole | $OCH_3$ | Cl | 6.65 | 7.09 | 1 | 100 | 25 | 60 | 78 |
| 120 | $C_7H_7Cl_3OSn$ | p-anisyltrichlorostannane | $SnCl_3$ | $OCH_3$ | 7.57 | 7.13 | 2 | x | 21 | 60 | 87 |
| 121 | | | $SnCl_3$ | $OCH_3$ | 7.66 | 6.90 | 5 | x | 21 | 60 | 87 |
| 122 | | | $SnCl_3$ | $OCH_3$ | 7.80 | 7.13 | 8 | x | 21 | 60 | 87 |
| 123 | | | $SnCl_3$ | $OCH_3$ | 7.46 | 6.96 | 12 | x | 21 | 60 | 87 |
| 124 | | | $SnCl_3$ | $OCH_3$ | 7.78 | 7.11 | 26 | x | 21 | 60 | 87 |
| 125 | | | $SnCl_3$ | $OCH_3$ | 7.69 | 7.21 | 36 | x | 21 | 60 | 87 |
| 126 | $C_7H_7Cl_3Si$ | p-tolyltrichlorosilane | $SiCl_3$ | $CH_3$ | 7.69 | 7.32 | 2 | x | 21 | 60 | 87 |
| 127 | | | $SiCl_3$ | $CH_3$ | 7.66 | 7.29 | 3 | x | 21 | 60 | 87 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

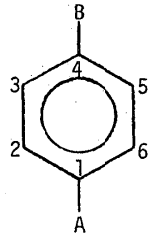



| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 128 | $C_7H_7Cl_3Si$ | p-tolyltrichlorosilane | $SiCl_3$ | $CH_3$ | 7.72 | 7.41 | 8 | x[d] | 21 | 60 | 87 |
| 129 | | | $SiCl_3$ | $CH_3$ | 7.61 | 7.17 | 12 | x | 21 | 60 | 87 |
| 130 | | | $SiCl_3$ | $CH_3$ | 7.72 | 7.38 | 26 | x | 21 | 60 | 87 |
| 131 | | | $SiCl_3$ | $CH_3$ | 7.68 | 7.32 | 27 | x | 21 | 60 | 87 |
| 132 | | | $SiCl_3$ | $CH_3$ | 7.74 | 7.40 | 36 | x | 21 | 60 | 87 |
| 133 | $C_7H_7Cl_3Sn$ | p-tolyltrichlorostannane | $SnCl_3$ | $CH_3$ | 7.52 | 7.44 | 2 | x | 21 | 60 | 87 |
| 134 | | | $SnCl_3$ | $CH_3$ | 7.50 | 7.41 | 3 | x | 21 | 60 | 87 |
| 135 | | | $SnCl_3$ | $CH_3$ | 7.61 | 7.12 | 5 | x | 21 | 60 | 87 |
| 136 | | | $SnCl_3$ | $CH_3$ | 7.74 | 7.39 | 8 | x | 21 | 60 | 87 |
| 137 | | | $SnCl_3$ | $CH_3$ | 7.42 | 7.28 | 12 | x | 21 | 60 | 87 |
| 138 | | | $SnCl_3$ | $CH_3$ | 7.72 | 7.39 | 26 | x | 21 | 60 | 87 |
| 139 | | | $SnCl_3$ | $CH_3$ | 7.62 | 7.28 | 27 | x | 21 | 60 | 87 |
| 140 | | | $SnCl_3$ | $CH_3$ | 7.49 | 7.18 | 28 | x | 21 | 60 | 87 |
| 141 | | | $SnCl_3$ | $CH_3$ | 7.63 | 7.49 | 36 | x | 21 | 60 | 87 |
| 142 | $C_7H_7F$ | p-fluorotoluene | $CH_3$ | F | 7.05 | 6.83 | 3 | x | x | x | 2 |
| 143 | | | $CH_3$ | F | 7.128 | 6.933 | 8 | 15 | x | 100 | 26 |
| 144 | $C_7H_7FO$ | p-fluoroanisole | $OCH_3$ | F | 6.77 | 6.95 | 3 | x | x | x | 2 |
| 145 | | | $OCH_3$ | F | 6.67 | 6.81 | 7 | 28 | x | 60 | 94 |
| 146 | $C_7H_7I$ | p-iodotoluene | $CH_3$ | I | 6.86 | 7.54 | 3 | x | x | x | 2 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA




| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 147 | $C_7H_7I$ | p-iodotoluene | $CH_3$ | I | 6.84 | 7.49 | 4 | 5 | x[d] | 100 | 67 |
| 148 | | | $CH_3$ | I | 6.46 | 7.36 | 6 | 1-3 | x | 100 | 93 |
| 149 | | | $CH_3$ | I | 6.78 | 7.47 | 12 | 1-3 | x | 100 | 93 |
| 150 | $C_7H_7IO$ | p-iodoanisole | $OCH_3$ | I | 6.62 | 7.53 | 3 | x[d] | x | x[d] | 2 |
| 151 | $C_7H_7Li$ | p-tolyllithium | Li | $CH_3$ | 7.91 | 6.92 | 10 | 0.5M | x | 60 | 37 |
| 152 | | | Li | $CH_3$ | 7.83 | 6.92 | 10 | 1M | x | 100 | 49 |
| 153 | $C_7H_7LiO$ | p-anisyllithium | Li | $OCH_3$ | 7.97 | 6.80 | 10 | 0.5M | x | 60 | 37 |
| 154 | | | Li | $OCH_3$ | 7.86 | 6.70 | 10 | 1M | x | 100 | 49 |
| 155 | $C_7H_7NO_2$ | p-aminobenzoic acid | $CO_2H$ | $NH_2$ | 7.67 | 6.61 | 3 | x | x | x | 2 |
| 156 | | | $CO_2H$ | $NH_2$ | 7.710 | 6.626 | 5 | 10 | x | 60 or 100 | 75 |
| 157 | $C_7H_7NO_2$ | p-nitrotoluene | $CH_3$ | $NO_2$ | 7.20 | 7.97 | 3 | x | x | x | 2 |
| 158 | | | $CH_3$ | $NO_2$ | 7.26 | 8.03 | 3 | 20 | x | 100 | 41 |
| 159 | | | $CH_3$ | $NO_2$ | 7.27 | 8.05 | 4 | 5 | x | 100 | 67 |
| 160 | | | $CH_3$ | $NO_2$ | 6.55 | 7.79 | 6 | 1-3 | x | 100 | 93 |
| 161 | | | $CH_3$ | $NO_2$ | 7.42 | 8.08 | 8 | 11 | 25 | 60 | 78 |
| 162 | | | $CH_3$ | $NO_2$ | 7.17 | 8.00 | 12 | 1-3 | x | 100 | 93 |
| 163 | $C_7H_7NO_3$ | p-nitroanisole | $OCH_3$ | $NO_2$ | 6.89 | 8.09 | 3 | x | x | x | 2 |
| 164 | | | $OCH_3$ | $NO_2$ | 6.91 | 8.12 | 4 | 5 | x | 60 | 98 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

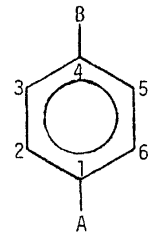



TABLE IV

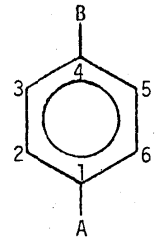
Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 165 | $C_7H_7NO_3$ | p-nitroanisole | $OCH_3$ | $NO_2$ | 6.34 | 7.89 | 6 | 5 | x[d] | 60 | 98 |
| 166 | | | $OCH_3$ | $NO_2$ | 6.88 | 8.04 | 7 | 5 | x | 60 | 98 |
| 167 | | | $OCH_3$ | $NO_2$ | 7.12 | 8.21 | 8 | 5 | x | 60 | 98 |
| 168 | | | $OCH_3$ | $NO_2$ | 6.83 | 8.10 | 12 | <5 | x | 60 | 98 |
| 169 | | | $OCH_3$ | $NO_2$ | 7.01 | 8.14 | 22 | 5 | x | 60 | 98 |
| 170 | | | $OCH_3$ | $NO_2$ | 7.02 | 8.16 | 26 | 5 | x | 60 | 98 |
| 171 | $C_7H_8O$ | p-cresol | OH | $CH_3$ | 6.61 | 6.90 | 4 | 5 | x | 100 | 67 |
| 172 | | | OH | $CH_3$ | 6.54 | 6.84 | 6 | 1-3 | x | 100 | 93 |
| 173 | | | OH | $CH_3$ | 6.61 | 6.89 | 12 | 1-3 | x | 100 | 93 |
| 174 | $C_7H_9N$ | p-toluidine | $NH_2$ | $CH_3$ | 6.40 | 6.81 | 4 | 5 | x | 100 | 67 |
| 175 | | | $NH_2$ | $CH_3$ | 6.32 | 6.88 | 6 | 1-3 | x | 100 | 93 |
| 176 | | | $NH_2$ | $CH_3$ | 6.55 | 6.85 | 8 | 11 | 25 | 60 | 78 |
| 177 | | | $NH_2$ | $CH_3$ | 6.39 | 6.78 | 12 | 1-3 | x | 100 | 93 |
| 178 | $C_7H_9NO$ | p-methoxyaniline | $NH_2$ | $OCH_3$ | 6.501 | 6.722 | 4 | x | 33 | 60 | 8 |
| 179 | | | $NH_2$ | $OCH_3$ | 6.92 | 6.68 | 8 | 5 | 25 | 60 | 78 |
| 180 | $C_8H_5NO_2$ | p-cyanobenzoic acid | $CO_2H$ | CN | 8.126 | 7.968 | 5 | 10 | x | 60 or 100 | 75 |
| 181 | $C_8H_7BrO_2$ | methyl p-bromobenzoate | $CO_2CH_3$ | Br | 7.82 | 7.52 | 3 | x | x | x | 2 |
| 182 | $C_8H_7ClO$ | p-toluyl chloride | COCl | $CH_3$ | 7.91 | 7.22 | 3 | x | x | x | 2 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA




| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 183 | $C_8H_7ClO$ | p-toluyl chloride | COCl | $CH_3$ | 7.95 | 7.24 | 4 | 5 | x[d] | 100 | 67 |
| 184 | $C_8H_7ClO_2$ | methyl-p-chlorobenzoate | $CO_2CH_3$ | Cl | 7.91 | 7.07 | 3 | x[d] | x | x[d] | 2 |
| 185 | $C_8H_7ClO_2$ | p-methoxybenzoyl chloride | COCl | $OCH_3$ | 7.94 | 6.89 | 3 | x | x | x | 2 |
| 186 | $C_8H_7FO$ | p-toluyl fluoride | COF | $CH_3$ | 7.892 | 7.337 | 10 | x | 31 | 100 | 15 |
| 187 | $C_8H_7FO_2$ | methyl p-fluorobenzoate | $CO_2CH_3$ | F | 7.99 | 7.07 | 3 | x | x | x | 2 |
| 188 | $C_8H_7IO_2$ | methyl p-iodobenzoate | $CO_2CH_3$ | I | 7.70 | 7.70 | 3 | x | x | x | 2 |
| 189 | $C_8H_7LiN$ | p-dimethylaminophenyllithium | Li | $N(CH_3)_2$ | 7.91 | 6.69 | 10 | 0.5M | x | 60 | 37 |
| 190 | $C_8H_7N$ | p-tolunitrile | CN | $CH_3$ | 7.46 | 7.22 | 3 | x | x | x | 2 |
| 191 | | | CN | $CH_3$ | 7.46 | 7.22 | 4 | 5 | x | 100 | 67 |
| 192 | | | CN | $CH_3$ | 6.97 | 6.53 | 6 | 1-3 | x | 100 | 93 |
| 193 | | | CN | $CH_3$ | 7.36 | 7.14 | 12 | 1-3 | x | 100 | 93 |
| 194 | $C_8H_7NO$ | p-methoxybenzonitrile | CN | $OCH_3$ | 7.56 | 6.97 | 3 | x | x | x | 2 |
| 195 | $C_8H_7NO_2$ | p-nitrostyrene | $CH{=}CH_2$ | $NO_2$ | 7.463 | 8.062 | 7 | 5 | 30 | 100 | 24 |
| 196 | $C_8H_7NO_3$ | methyl p-nitrobenzoate | $CO_2CH_3$ | $NO_2$ | 8.21 | 8.21 | 3 | x | x | x | 2 |
| 197 | $C_8H_8BrNO$ | p-bromoacetanilide | $NHCOCH_3$ | Br | 7.77 | 7.39 | 3 | x | x | x | 2 |
| 198 | $C_8H_8ClNO$ | p-chloroacetanilide | $NHCOCH_3$ | Cl | 7.80 | 7.23 | 3 | x | x | x | 2 |
| 199 | $C_8H_8FNO$ | p-fluoroacetanilide | $NHCOCH_3$ | F | 7.60 | 6.93 | 3 | x | x | x | 2 |
| 200 | $C_8H_8INO$ | p-iodoacetanilide | $NHCOCH_3$ | I | 7.58 | 7.58 | 3 | x | x | x | 2 |
| 201 | $C_8H_8O$ | p-tolualdehyde | CHO | $CH_3$ | 7.69 | 7.25 | 4 | 5 | x | 100 | 67 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

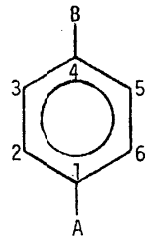



TABLE IV

Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 202 | $C_8H_8O_2$ | p-hydroxyphenylacetic acid | $CH_2CO_2H$ | OH | 7.125 | 6.785 | 8 | 1.0M | x[d] | 100 | 12 |
| 203 | $C_8H_8O_2$ | p-methoxybenzaldehyde | CHO | $OCH_3$ | 7.79 | 6.95 | 1 | 100 | 25 | 60 | 78 |
| 204 | $C_8H_8O_2$ | p-toluic acid | $CO_2H$ | $CH_3$ | 7.88 | 7.30 | 3 | x[d] | x | x[d] | 2 |
| 205 | | | $CO_2H$ | $CH_3$ | 7.98 | 7.20 | 4 | 5 | x | 100 | 67 |
| 206 | $C_8H_8O_3$ | p-methoxybenzoic acid | $CO_2H$ | $OCH_3$ | 7.92 | 7.03 | 3 | x | x | x | 2 |
| 207 | | | $CO_2H$ | $OCH_3$ | 7.964 | 7.026 | 5 | 10 | x | 60 or 100 | 75 |
| 208 | $C_8H_8O_3$ | methyl p-hydroxybenzoate | $CO_2CH_3$ | OH | 7.88 | 6.87 | 3 | x | x | x | 2 |
| 209 | $C_8H_9Br$ | p-methylbenzyl bromide | $CH_2Br$ | $CH_3$ | 7.12 | 7.00 | 7 | 11 | x | 60 | 92 |
| 210 | | | $CH_2Br$ | $CH_3$ | 7.077 | 7.240 | 8 | 20 | x | 100 | 25 |
| 211 | $C_8H_9NO$ | p-aminoacetophenone | $COCH_3$ | $NH_2$ | 7.77 | 6.71 | 8 | 13 | 25 | 60 | 78 |
| 212 | $C_8H_9NO_2$ | p-ethylnitrobenzene | $NO_2$ | $C_2H_5$ | 8.04 | 7.27 | 3 | 20 | x | 100 | 41 |
| 213 | | | $NO_2$ | $C_2H_5$ | 8.00 | 7.27 | 3 | x | x | x | 2 |
| 214 | $C_8H_9NO_2$ | methyl p-aminobenzoate | $CO_2CH_3$ | $NH_2$ | 7.79 | 6.61 | 3 | x | x | x | 2 |
| 215 | $C_8H_{10}$ | p-xylene | $CH_3$ | $CH_3$ | 6.98 | 6.98 | 4 | 1 | x | 60 | 55 |
| 216 | | | $CH_3$ | $CH_3$ | 7.03 | 7.03 | 8 | 2 | 40 | 60 | 34 |
| 217 | | | $CH_3$ | $CH_3$ | 6.94 | 6.94 | 12 | 2 | 40 | 60 | 34 |
| 218 | | | $CH_3$ | $CH_3$ | 7.06 | 7.06 | 26 | 2 | 40 | 60 | 34 |
| 219 | | | $CH_3$ | $CH_3$ | 6.92 | 6.92 | 32 | 0.02M | 10 | 60 | 1 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

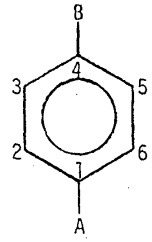



TABLE IV

Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 220 | $C_8H_{10}BrN$ | p-N,N-dimethylaminobromobenzene | Br | $N(CH_3)_2$ | 7.21 | 6.48 | 3 | x[d] | x[d] | x[d] | 2 |
| 221 | $C_8H_{10}ClN$ | p-N,N-dimethylaminochlorobenzene | Cl | $N(CH_3)_2$ | 7.12 | 6.55 | 3 | x | x | x | 2 |
| 222 | $C_8H_{10}FN$ | p-N,N-dimethylaminofluorobenzene | F | $N(CH_3)_2$ | 6.86 | 6.55 | 3 | x | x | x | 2 |
| 223 | $C_8H_{10}IN$ | p-N,N-dimethylaminoiodobenzene | I | $N(CH_3)_2$ | 7.37 | 6.37 | 3 | x | x | x | 2 |
| 224 | $C_8H_{10}N_2O$ | N,N-dimethyl-p-nitrosoaniline* | $N(CH_3)_2$ | NO | *s 7.01<br>*a 6.71 | s 8.93<br>a 6.62 | 8 | 2 | -56 | 60 | 68 |
| 225 | | | $N(CH_3)_2$ | NO | s 6.82<br>a 6.53 | s 8.91<br>a 6.78 | 3 | 2 | -56(?) | 60 | 69 |
| 226 | $C_8H_{10}N_2O_2$ | p-N,N-dimethylaminonitrobenzene | $NO_2$ | $N(CH_3)_2$ | 8.07 | 6.56 | 3 | x | x | x | 2 |
| 227 | | | $NO_2$ | $N(CH_3)_2$ | 8.088 | 6.780 | 8 | x | 33 | 60 | 8 |
| 228 | | | $NO_2$ | $N(CH_3)_2$ | 8.05 | 6.79 | 8 | 1.3 | 25 | 60 | 78 |
| 229 | $C_8H_{10}O$ | p-methylanisole | $OCH_3$ | $CH_3$ | 6.66 | 6.94 | 4 | 5 | x | 100 | 67 |
| 230 | | | $OCH_3$ | $CH_3$ | 6.68 | 6.94 | 6 | 1-3 | x | 100 | 93 |
| 231 | | | $OCH_3$ | $CH_3$ | 6.66 | 6.93 | 12 | 1-3 | x | 100 | 93 |
| 232 | $C_8H_{11}N$ | N-methyl-p-toluidine | $NHCH_3$ | $CH_3$ | 6.35 | 6.84 | 4 | 5 | x | 100 | 67 |
| 233 | $C_9H_9ClO$ | 2-(p-chlorophenyl)oxetane | CH—$CH_2$<br>\| \|<br>O—$CH_2$ | Cl | 7.28 | 7.28 | 4 | 2-5 | x | 300 | 81 |

* Slow rotational exchange limit shifts are given: s = proton syr to O of N=O; a = proton anti to O of N=O.

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

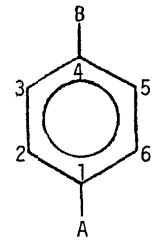
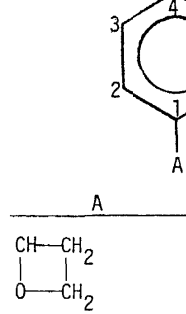



TABLE IV

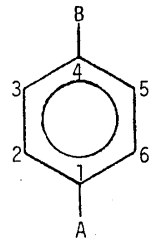
Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 234 | $C_9H_9ClO$ | 2-(p-chlorophenyl)oxetane |  | Cl | 7.03 | 7.14 | 6 | 2-5 | x[d] | 300 | 81 |
| 235 | $C_9H_9ClO$ | p-ethylbenzoyl chloride | COCl | $C_2H_5$ | 7.95 | 7.28 | 3 | x[d] | x | x[d] | 2 |
| 236 | $C_9H_9N$ | p-ethylbenzonitrile | CN | $C_2H_5$ | 7.52 | 7.27 | 3 | x | x | x | 2 |
| 237 | $C_9H_{10}N_2$ | p-N,N-dimethylaminobenzonitrile | CN | $N(CH_3)_2$ | 7.33 | 6.57 | 3 | x | x | x | 2 |
| 238 | $C_9H_{10}O$ | p-methoxystyrene | $CH{=}CH_2$ | $OCH_3$ | 7.160 | 6.683 | 7 | 5 | 30 | 100 | 24 |
| 239 | $C_9H_{10}O$ | p-methylacetophenone | $COCH_3$ | $CH_3$ | 7.75 | 7.16 | 4 | 5 | x | 100 | 67 |
| 240 | $C_9H_{10}O_2$ | p-cresol acetate | $OCOCH_3$ | $CH_3$ | 6.88 | 7.06 | 4 | 5 | x | 100 | 67 |
| 241 | $C_9H_{10}O_2$ | p-ethylbenzoic acid | $CO_2H$ | $C_2H_5$ | 7.85 | 7.28 | 3 | x | x | x | 2 |
| 242 | $C_9H_{10}O_2$ | methyl p-toluate | $CO_2CH_3$ | $CH_3$ | 7.87 | 7.19 | 3 | x | x | x | 2 |
| 243 | | | $CO_2CH_3$ | $CH_3$ | 7.85 | 7.14 | 4 | 5 | x | 100 | 67 |
| 244 | | | $CO_2CH_3$ | $CH_3$ | 8.05 | 6.89 | 6 | 1-3 | x | 100 | 93 |
| 245 | | | $CO_2CH_3$ | $CH_3$ | 7.87 | 7.08 | 12 | 1-3 | x | 100 | 93 |
| 246 | $C_9H_{10}O_3$ | p-methoxyphenylacetic acid | $CH_2CO_2H$ | $OCH_3$ | 7.208 | 6.853 | 8 | 1.0M | x | 100 | 12 |
| 247 | $C_9H_{10}O_3$ | methyl p-methoxybenzoate | $CO_2CH_3$ | $OCH_3$ | 7.90 | 6.85 | 3 | x | x | x | 2 |
| 248 | | | $CO_2CH_3$ | $OCH_3$ | 7.952 | 6.999 | 8 | 1.0M | x | 100 | 9 |
| 249 | $C_9H_{11}NO$ | N,N-dimethyl-p-aminobenzaldehyde | CHO | $N(CH_3)_2$ | 7.68 | 6.72 | 8 | 11 | 25 | 60 | 78 |
| 250 | $C_9H_{11}NO_2$ | p-N,N-dimethylaminobenzoic acid | $CO_2H$ | $N(CH_3)_2$ | 7.72 | 6.64 | 3 | x | x | x | 2 |
| 251 | $C_9H_{11}NO_2$ | p-isopropylnitrobenzene | $NO_2$ | $CH(CH_3)_2$ | 8.13 | 7.38 | 3 | 20 | x | 100 | 41 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA




| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 252 | $C_9H_{11}NO_2$ | p-isopropylnitrobenzene | $NO_2$ | $CH(CH_3)_2$ | 8.06 | 7.35 | 3 | x[d] | x[d] | x[d] | 2 |
| 253 | $C_9H_{13}N$ | N,N-dimethyl-p-toluidine | $N(CH_3)_2$ | $CH_3$ | 6.52 | 6.89 | 4 | 5 | x | 100 | 67 |
| 254 | | | $N(CH_3)_2$ | $CH_3$ | 6.61 | 7.03 | 6 | 1-3 | x | 100 | 93 |
| 255 | | | $N(CH_3)_2$ | $CH_3$ | 6.56 | 6.91 | 12 | 1-3 | x | 100 | 93 |
| 256 | $C_{10}H_8$ | 4-ethynylstyrene | $CH{=}CH_2$ | $C{\equiv}CH$ | 6.985 | 7.341 | 6 | 5 | 30 | 100 | 24 |
| 257 | $C_{10}H_{10}O_4$ | methyl p-acetoxybenzoate | $CO_2CH_3$ | $OCOCH_3$ | 8.035 | 7.245 | 8 | 1.0 | x | 100 | 12 |
| 258 | $C_{10}H_{11}ClO$ | p-isopropylbenzoyl chloride | COCl | $CH(CH_3)_2$ | 7.96 | 7.31 | 3 | x | x | x | 2 |
| 259 | $C_{10}H_{11}N$ | p-isopropylbenzonitrile | CN | $CH(CH_3)_2$ | 7.49 | 7.26 | 3 | x | x | x | 2 |
| 260 | $C_{10}H_{12}O_2$ | p-isopropylbenzoic acid | $CO_2H$ | $CH(CH_3)_2$ | 7.88 | 7.33 | 3 | x | x | x | 2 |
| 261 | $C_{10}H_{12}O_2$ | methyl p-ethylbenzoate | $CO_2CH_3$ | $C_2H_5$ | 7.89 | 7.20 | 3 | x | x | x | 2 |
| 262 | $C_{10}H_{12}O_3$ | methyl p-methoxyphenylacetate | $CH_2CO_2CH_3$ | $OCH_3$ | 7.180 | 6.852 | 8 | 1.0M | x | 100 | 12 |
| 263 | $C_{10}H_{13}Br$ | p-tert-butylbromobenzene | Br | $C(CH_3)_3$ | 7.30 | 7.16 | 4 | 10 | x | 100 | 40 |
| 264 | $C_{10}H_{13}Cl$ | p-tert-butylchlorobenzene | Cl | $C(CH_3)_3$ | 7.19 | 7.19 | 3 | x | x | x | 2 |
| 265 | $C_{10}H_{13}Cl_2NS_2Sn$ | p-tolyldichlorotin N,N-dimethyldithiocarbamate | $SnCl_2SCSN(CH_3)_2$ | $CH_3$ | 7.80 | 7.36 | 2 | x | 21 | 60 | 87 |
| 266 | | | $SnCl_2SCSN(CH_3)_2$ | $CH_3$ | 7.82 | 7.16 | 5 | x | 21 | 60 | 87 |
| 267 | | | $SnCl_2SCSN(CH_3)_2$ | $CH_3$ | 7.78 | 7.39 | 8 | x | 21 | 60 | 87 |
| 268 | | | $SnCl_2SCSN(CH_3)_2$ | $CH_3$ | 7.76 | 7.37 | 26 | x | 21 | 60 | 87 |
| 269 | | | $SnCl_2SCSN(CH_3)_2$ | $CH_3$ | 7.57 | 7.17 | 27 | x | 21 | 60 | 87 |
| 270 | | | $SnCl_2SCSN(CH_3)_2$ | $CH_3$ | 7.82 | 7.44 | 36 | x | 21 | 60 | 87 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

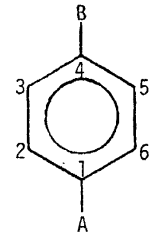



TABLE IV

Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 271 | $C_{10}H_{13}Cl_3Sn$ | p-tert-butylphenyltrichlorostannane | $SnCl_3$ | $C(CH_3)_3$ | 7.61 | 7.61 | 2 | x[d] | 21 | 60 | 87 |
| 272 | | | $SnCl_3$ | $C(CH_3)_3$ | 7.62 | 7.34 | 5 | x | 21 | 60 | 87 |
| 273 | | | $SnCl_3$ | $C(CH_3)_3$ | 7.79 | 7.63 | 8 | x | 21 | 60 | 87 |
| 274 | | | $SnCl_3$ | $C(CH_3)_3$ | 7.52 | 7.52 | 12 | x | 21 | 60 | 87 |
| 275 | | | $SnCl_3$ | $C(CH_3)_3$ | 7.78 | 7.63 | 26 | x | 21 | 60 | 87 |
| 276 | | | $SnCl_3$ | $C(CH_3)_3$ | 7.70 | 7.70 | 36 | x | 21 | 60 | 87 |
| 277 | $C_{10}H_{13}N$ | p-N,N-dimethylaminostyrene | $CH{=}CH_2$ | $N(CH_3)_2$ | 7.301 | 6.512 | 6 | 5 | 30 | 100 | 24 |
| 278 | $C_{10}H_{13}NO_2$ | p-tert-butylnitrobenzene | $NO_2$ | $C(CH_3)_3$ | 8.19 | 7.61 | 3 | 20 | x[d] | 100 | 41 |
| 279 | | | $NO_2$ | $C(CH_3)_3$ | 8.07 | 7.50 | 3 | x | x | x[d] | 2 |
| 280 | $C_{10}H_{14}N_2O$ | N,N-diethyl-p-nitrosoaniline* | $N(C_2H_5)_2$ | NO | *s 7.07<br>*a 6.77 | s 8.89<br>a 6.66 | 8 | 2 | -56 | 60 | 68 |
| 281 | | | $N(C_2H_5)_2$ | NO | s 6.83<br>a 6.54 | s 8.86<br>a 6.84 | 3 | 2 | -56(?) | 60 | 69 |
| 282 | | | $N(C_2H_5)$ | NO | s 6.01<br>a 5.67 | s 8.96<br>a 6.74 | 20 | 2 | -56(?) | 60 | 69 |
| 283 | $C_{11}H_{12}O_4$ | methyl p-acetoxyphenylacetate | $CH_2CO_2CH_3$ | $OCOCH_3$ | 7.298 | 7.051 | 8 | 1.0M | x | 100 | 12 |
| 284 | $C_{11}H_{13}ClO$ | p-tert-butylbenzoyl chloride | COCl | $C(CH_3)_3$ | 7.99 | 7.49 | 3 | x | x | x | 2 |
| 285 | $C_{11}H_{13}N$ | p-tert-butylbenzonitrile | CN | $C(CH_3)_3$ | 7.49 | 7.49 | 3 | x | x | x | 2 |

*Slow rotational exchange limit shifts are given: s = proton syn to O of N=O; a = proton anti to O of N=O.

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN DISUBSTITUTED BENZENES

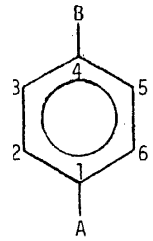



TABLE IV

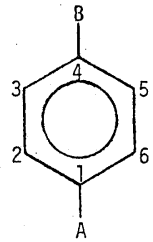
Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H{}^a$ 2,6 | $\delta_H{}^a$ 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 286 | $C_{11}H_{14}O_2$ | p-tert-butylbenzoic acid | $CO_2H$ | $C(CH_3)_3$ | 7.90 | 7.49 | 3 | x[d] | x[d] | x[d] | 2 |
| 287 | $C_{11}H_{14}O_2$ | methyl p-isopropylbenzoate | $CO_2CH_3$ | $CH(CH_3)_2$ | 7.89 | 7.21 | 3 | x | x | x | 2 |
| 288 | $C_{11}H_{16}$ | p-ethyl-n-propylbenzene | n-$C_3H_7$ | $C_2H_5$ | 6.90 | 6.64 | 4 | 5 | x | 100 | 67 |
| 289 | $C_{12}H_4D_5Cl$ | p-chloroperdeuteriophenylbenzene | $C_6D_5$ | Cl | 7.39 | 7.30 | 4 | 10 | x | 100 | 40 |
| 290 | $C_{12}H_4D_5NO_2$ | p-nitroperdeuterophenylbenzene | $C_6D_5$ | $NO_2$ | 7.66 | 8.22 | 4 | 10 | x | 100 | 40 |
| 291 | $C_{12}H_8Br_2$ | p,p'-dibromobiphenyl | p-$C_6H_4Br$ | Br | 7.057 | 7.304 | 6 | 1 | x | 60 | 32 |
| 292 | $C_{12}H_8Cl_2$ | p,p'-dichlorobiphenyl | p-$C_6H_4Cl$ | Cl | 7.138 | 7.154 | 6 | 1 | x | 60 | 32 |
| 293 | $C_{12}H_8F_2$ | p,p'-difluorobiphenyl | p-$C_6H_4F$ | F | 7.214 | 6.853 | 6 | 5 | x | 60 | 32 |
| 294 | | | p-$C_6H_4F$ | F | 7.33 | 6.95 | 7 | 21 | x | 60 | 94 |
| 295 | $C_{12}H_8I_2$ | p,p'-diiodobiphenyl | p-$C_6H_4I$ | I | 6.935 | 7.507 | 6 | 1 | x | 60 | 32 |
| 296 | $C_{12}H_8N_2O_4S$ | bis(p-nitrophenyl) sulfide | p-$NO_2C_6H_4S$ | $NO_2$ | 7.589 | 8.207 | 35 | 5-8 | 38 | 60 | 73 |
| 297 | $C_{12}H_8N_2O_4S_2$ | bis(p-nitrophenyl) disulfide | p-$NO_2C_6H_4S_2$ | $NO_2$ | 7.758 | 8.216 | 35 | 5-8 | 38 | 60 | 73 |
| 298 | $C_{12}H_{12}N_2S$ | bis(p-aminophenyl) sulfide | p-$NH_2C_6H_4S$ | $NH_2$ | 6.966 | 6.480 | 35 | 5-8 | 38 | 60 | 73 |
| 299 | $C_{12}H_{12}N_2S_2$ | bis(p-aminophenyl) disulfide | p-$NH_2C_6H_4S_2$ | $NH_2$ | 7.153 | 6.517 | 35 | 5-8 | 38 | 60 | 73 |
| 300 | $C_{12}H_{16}O_2$ | methyl p-tert-butylbenzoate | $CO_2CH_3$ | $C(CH_3)_3$ | 7.89 | 7.39 | 3 | x | x | x | 2 |
| 301 | $C_{12}H_{18}$ | p-sec-butylethylbenzene | $C_2H_5$ | sec-$C_4H_9$ | 6.66 | 6.93 | 4 | 5 | x | 100 | 67 |
| 302 | $C_{12}H_{18}$ | p-tert-butylethylbenzene | $C_2H_5$ | tert-$C_4H_9$ | 6.66 | 7.13 | 4 | 5 | x | 100 | 67 |
| 303 | $C_{13}H_{11}NO_2S$ | p-tolylthio-p-nitrobenzene | $NO_2$ | p-$CH_3C_6H_4S$ | 8.02 | 7.83 | 3 | x | x | 60 or 100 | 80 |

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA




| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 304 | $C_{14}H_{14}Cl_2Sn$ | di(p-tolyl)dichlorostannane | $SnCl_2$-p-$CH_3C_6H_4$ | $CH_3$ | 7.54 | 7.33 | 2 | x[d] | 21 | 60 | 87 |
| 305 | | | $SnCl_2$-p-$CH_3C_6H_4$ | $CH_3$ | 7.77 | 7.14 | 5 | x | 21 | 60 | 87 |
| 306 | | | $SnCl_2$-p-$CH_3C_6H_4$ | $CH_3$ | 7.71 | 7.34 | 8 | x | 21 | 60 | 87 |
| 307 | | | $SnCl_2$-p-$CH_3C_6H_4$ | $CH_3$ | 7.46 | 7.18 | 12 | x | 21 | 60 | 87 |
| 308 | | | $SnCl_2$-p-$CH_3C_6H_4$ | $CH_3$ | 7.70 | 7.36 | 26 | x | 21 | 60 | 87 |
| 309 | | | $SnCl_2$-p-$CH_3C_6H_4$ | $CH_3$ | 7.65 | 7.41 | 36 | x | 21 | 60 | 87 |
| 310 | $C_{14}H_{14}N_2O_3$ | p,p'-azoxyanisole (ring adjacent to NO) | p-$CH_3O$-$C_6H_4$-N-NO | $OCH_3$ | 8.13 | 6.79 | 7 | 5 | 70 | 60 | 78 |
| 311 | $C_{14}H_{14}N_2O_3$ | p,p'-azoxyanisole (ring remote from NO) | p-$CH_3O$-$C_6H_4$-NO-N | $OCH_3$ | 8.15 | 6.90 | 7 | 5 | 70 | 60 | 78 |
| 312 | $C_{14}H_{22}$ | p-di-t-butylbenzene | $C(CH_3)_3$ | $C(CH_3)_3$ | 7.18 | 7.18 | 4 | 1 | x[d] | 100 | 55 |
| 313 | $C_{15}H_{11}BrO$ | 3-(p-bromphenyl)methylidenephthalide | R* | Br | 7.80 | 7.59 | 8 | .05M | 24 | 80 | 84 |
| 314 | $C_{15}H_{11}BrOS$ | 3-(p-bromophenyl)thiomethylidene-phthalide | S-R* | Br | 7.49 | 7.73 | 8 | .05M | 24 | 80 | 84 |
| 315 | $C_{15}H_{11}ClO$ | 3-(p-chlorophenyl)methylidenephthalide | R* | Cl | 7.86 | 7.46 | 8 | .05M | 24 | 80 | 84 |
| 316 | $C_{15}H_{11}ClOS$ | 3-(p-chlorophenyl)thiomethylidene-phthalide | S-R* | Cl | 7.43 | 7.61 | 8 | .05M | 24 | 80 | 84 |
| 317 | $C_{15}H_{11}IO$ | 3-(p-iodophenyl)methylidenephthalide | R* | I | 7.84 | 7.63 | 8 | .05M | 24 | 80 | 84 |
| 318 | $C_{15}H_{11}IOS$ | 3-(p-iodophenyl)thiomethylidene-phthalide | S-R* | I | 7.37 | 7.79 | 8 | .05M | 24 | 80 | 84 |

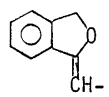
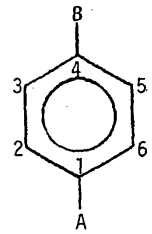
* R = 

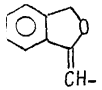
TABLE IV

PROTON CHEMICAL SHIFTS, $\delta_H{}^a$, IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA




| Entry No. | Molecular Formula | Name | A | B | $\delta_H{}^a$ 2,6 | $\delta_H{}^a$ 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 319 | $C_{15}H_{11}NO_3$ | 3-(p-nitrophenyl)methylidenephthalide | R* | $NO_2$ | 8.32 | 8.08 | 8 | .05M | 24 | 80 | 84 |
| 320 | $C_{15}H_{11}NO_3S$ | 3-(p-nitrophenyl)thiomethylidene-phthalide | S-R* | $NO_2$ | 7.80 | 8.27 | 8 | .05M | 24 | 80 | 84 |
| 321 | $C_{15}H_{12}BrN$ | cinnamaldehyde p-bromoanil | Br | $N{=}CHCH{=}CHC_6H_5$ | 6.93 | 7.38 | 4 | x[d] | x[d] | 100 | 13 |
| 322 | | | Br | $N{=}CHCH{=}CHC_6H_5$ | 6.81 | 7.27 | 6 | x | x | 100 | 13 |
| 323 | | | Br | $N{=}CHCH{=}CHC_6H_5$ | 6.90 | 7.33 | 7 | x | x | 100 | 13 |
| 324 | $C_{15}H_{12}FN$ | cinnamaldehyde p-fluoroanil | F | $N{=}CHCH{=}CHC_6H_5$ | 6.96 | 6.87 | 6 | x | x | 100 | 13 |
| 325 | $C_{15}H_{12}O_2S$ | 3-(p-hydroxyphenyl)thiomethylidene-phthalide | S-R* | OH | 7.50 | 7.68 | 8 | .05M | 24 | 80 | 84 |
| 326 | $C_{15}H_{13}NO$ | 3-(p-aminophenyl)methylidenephthalide | R* | $NH_2$ | 7.61 | 6.72 | 8 | .05M | 24 | 80 | 84 |
| 327 | $C_{16}H_{14}O$ | 3-(p-tolyl)methylidenephthalide | R* | $CH_3$ | 7.75 | 7.25 | 8 | .05M | 24 | 80 | 84 |
| 328 | $C_{16}H_{14}OS$ | 3-(p-tolyl)thiomethylidenephthalide | S-R* | $CH_3$ | 7.23 | 7.45 | 8 | .05M | 24 | 80 | 84 |
| 329 | $C_{16}H_{14}O_2$ | 3-(p-anisyl)methylidenephthalide | R* | $OCH_3$ | 7.83 | 7.02 | 8 | .05M | 24 | 80 | 84 |
| 330 | $C_{17}H_{15}NO$ | cinnamaldehyde p-acetylanil | $COCH_3$ | $N{=}CHCH{=}CHC_6H_5$ | 7.96 | 7.18 | 3 | x | x | 100 | 13 |
| 331 | | | $COCH_3$ | $N{=}CHCH{=}CHC_6H_5$ | 7.84 | 7.04 | 6 | x | x | 100 | 13 |
| 332 | $C_{17}H_{17}NO$ | cinnamaldehyde p-ethoxyanil | $OC_2H_5$ | $N{=}CHCH{=}CHC_6H_5$ | 6.75 | 7.02 | 4 | x | x | 100 | 13 |
| 333 | | | $OC_2H_5$ | $N{=}CHCH{=}CHC_6H_5$ | 6.83 | 7.22 | 6 | x | x | 100 | 13 |
| 334 | | | $OC_2H_5$ | $N{=}CHCH{=}CHC_6H_5$ | 6.40 | 6.66 | 7 | x | x | 100 | 13 |

* R = 

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

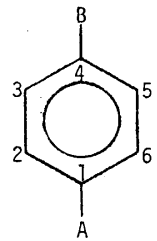



TABLE IV

Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 335 | $C_{18}H_{12}Br_3OP$ | tris-p-bromophenylphosphine oxide | $PO(p\text{-}BrC_6H_4)_2$ | Br | 7.50 | 7.64 | 2 | 0.5M | x[d] | 60 | 44 |
| 336 | $C_{18}H_{12}Br_3P$ | tris-p-bromophenylphosphine | $P(p\text{-}BrC_6H_4)_2$ | Br | 7.14 | 7.47 | x | 0.5M | x | 60 | 44 |
| 337 | $C_{18}H_{12}Br_3PS$ | tris-p-bromophenylphosphine sulfide | $PS(p\text{-}BrC_6H_4)_2$ | Br | 7.54 | 7.62 | 2 | 0.5M | x | 60 | 44 |
| 338 | $C_{18}H_{12}Cl_3OP$ | tris-p-chlorophenylphosphine oxide | $PO(p\text{-}ClC_6H_4)_2$ | Cl | 7.59 | 7.47 | 3 | 0.5M | x | 60 | 44 |
| 339 | $C_{18}H_{12}Cl_3P$ | tris-p-chlorophenylphosphine | $P(p\text{-}ClC_6H_4)_2$ | Cl | 7.19 | 7.30 | 3 | 0.5M | x | 60 | 44 |
| 340 | $C_{18}H_{12}Cl_3PS$ | tris-p-chlorophenylphosphine sulfide | $PS(p\text{-}ClC_6H_4)_2$ | Cl | 7.63 | 7.44 | 2 | 0.5M | x | 60 | 44 |
| 341 | $C_{18}H_{12}D_3OP$ | tris-p-deuteriophenylphosphine oxide | $PO(p\text{-}DC_6H_4)_2$ | D | 7.65 | 7.44 | 2 | 0.5M | x | 60 | 44 |
| 342 | $C_{18}H_{12}D_3P$ | tris-p-deuteriophenylphosphine | $P(p\text{-}DC_6H_4)_2$ | D | 7.29 | 7.28 | 2 | 0.5M | x | 60 | 44 |
| 343 | $C_{18}H_{12}D_3PS$ | tris-p-deuteriophenylphosphine sulfide | $PS(p\text{-}DC_6H_4)_2$ | D | 7.70 | 7.44 | 2 | 0.5M | x | 60 | 44 |
| 344 | $C_{18}H_{12}F_3OP$ | tris(p-fluorophenyl)phosphine oxide | $PO(p\text{-}FC_6H_4)_2$ | F | 7.70 | 7.35 | 5 | 50 | x | 60 | 35 |
| 345 | $C_{18}H_{12}F_3P$ | tris-p-fluorophenylphosphine | $P(p\text{-}FC_6H_4)_2$ | F | 7.05 | 6.74 | 6 | 20 | 32 | 100 | 91 |
| 346 | $C_{18}H_{14}$ | p-terphenyl | $C_6H_5$ | $C_6H_5$ | 7.667 | 7.567 | 3 | 5 | 28 | 60 | 56 |
| 347 | $C_{19}H_{15}Cl_3IP$ | methyl(tris-p-chlorophenyl)phosphonium iodide | $\overset{+}{P}(p\text{-}ClC_6H_4)_2CH_3I^-$ | Cl | 7.87 | 7.58 | 3 | 0.5M | x | 60 | 44 |
| 348 | $C_{19}H_{15}D_3IP$ | methyl(tris-p-deuteriophenyl)phosphonium iodide | $\overset{+}{P}(p\text{-}DC_6H_4)_2CH_3I^-$ | D | 7.83 | 7.71 | 2 | 0.5M | x | 60 | 44 |
| 349 | $C_{20}H_{17}OTe_2$ | o-phenylene-bis[p-ethoxyphenyltelluride] | R* | $OC_2H_5$ | 7.741 | 6.779 | 3 | 1M | x | 100 | 89 |
| 350 | $C_{20}H_{18}F_3O_3P$ | dimethyl p-fluorophenylphosphonate | $PO(OCH_3)_2(p\text{-}FC_6H_4)_2$ | F | 7.80 | 7.27 | 1 | 100 | x | 60 | 35 |
| 351 | | | $PO(OCH_3)_2(p\text{-}FC_6H_4)_2$ | F | 7.83 | 7.33 | 4 | 50 | x | 60 | 35 |

*R- = p-$C_2H_5OC_6H_4Te$-o-$C_6H_4$-Te-

PROTON CHEMICAL SHIFTS, $\delta_H$[a], IN DISUBSTITUTED BENZENES

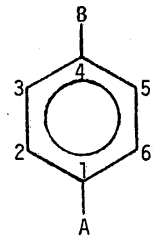



TABLE IV

Substituent Arrangement: PARA

| Entry No. | Molecular Formula | Name | A | B | $\delta_H$[a] 2,6 | $\delta_H$[a] 3,5 | Solvent Code[b] | Concn.[c] (%) | Temp. (°C) | Spect. Freq. (MHz) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 352 | $C_{21}H_{21}OP$ | tris-p-tolylphosphine oxide | $PO(p\text{-}CH_3C_6H_4)_2$ | $CH_3$ | 7.50 | 7.22 | 2 | 0.5M | x[d] | 60 | 44 |
| 353 | $C_{21}H_{21}O_3P$ | tris-p-anisylphosphine | $P(p\text{-}CH_3OC_6H_4)_2$ | $OCH_3$ | 7.26 | 6.87 | 3 | 0.5M | x | 60 | 44 |
| 354 | $C_{21}H_{21}O_3PS$ | tris-p-anisylphosphine sulfide | $PS(p\text{-}CH_3OC_6H_4)_2$ | $OCH_3$ | 7.62 | 6.92 | 3 | 0.5M | x | 60 | 44 |
| 355 | $C_{21}H_{21}O_4P$ | tris-p-anisylphosphine oxide | $PO(p\text{-}CH_3OC_6H_4)_2$ | $OCH_3$ | 7.53 | 6.94 | 2 | 0.5M | x | 60 | 44 |
| 356 | $C_{21}H_{21}P$ | tris-p-tolylphosphine | $P(p\text{-}CH_3C_6H_4)_2$ | $CH_3$ | 7.19 | 7.09 | 3 | 1.0M | x | 60 | 44 |
| 357 | $C_{21}H_{21}PS$ | tris-p-tolylphosphine sulfide | $PS(p\text{-}CH_3C_6H_4)_2$ | $CH_3$ | 7.56 | 7.18 | 2 | 1.0M | x | 60 | 44 |
| 358 | $C_{22}H_{24}IO_3P$ | methyl(tris-p-anisyl)phosphonium iodide | $\overset{+}{P}(p\text{-}CH_3OC_6H_4)_2CH_3I^-$ | $OCH_3$ | 7.63 | 7.20 | 3 | 0.5M | x | 60 | 44 |
| 359 | $C_{22}H_{24}IP$ | methyl(tris-p-tolyl)phosphonium iodide | $\overset{+}{P}(p\text{-}CH_3C_6H_4)_2CH_3I^-$ | $CH_3$ | 7.62 | 7.53 | 2 | 0.5M | x | 60 | 44 |
| 360 | $C_{24}H_{30}N_3OP$ | tris-p-dimethylaminophenylphosphine oxide | $PO(p\text{-}(CH_3)_2NC_6H_4)_2$ | $N(CH_3)_2$ | 7.40 | 6.68 | 2 | 0.2M | x | 60 | 44 |

[a] Usual δ-scale. See text, section 2, item 5.

[b] See Table V and text, section 2, item 6.

[c] Concentration is given in percent unless number is followed by "M", molarity. The designation '0" refers to the shift at "infinite dilution". See text, section 2, item 7.

[d] The designation "x" means unknown or unspecified.

Table V: Solvents and Solvent Code Numbers

| Solvent Code | Solvent |
|---|---|
| 1 | (none; neat liquid + TMS*) |
| 2 | methylene chloride |
| 3 | chloroform-d |
| 4 | carbon tetrachloride |
| 5 | dimethylsulfoxide(-$d_6$) |
| 6 | benzene(-$d_6$) |
| 7 | carbon disulfide |
| 8 | acetone(-$d_6$) |
| 9 | n hexane |
| 10 | diethyl ether |
| 11 | ethyl acetate |
| 12 | cyclohexane |
| 13 | methyl acetate |
| 14 | paraldehyde |
| 15 | cyclohexanone |
| 16 | ethyl bromide |
| 17 | bromocyclopentane |
| 18 | propylene carbonate |
| 19 | acetic anhydride |
| 20 | toluene-$d_8$ |
| 21 | 1,1,1-trichloro-1,1,1-trifluoroethane |
| 22 | methanol |
| 23 | carbon tetrabromide |
| 24 | squalane |
| 25 | *tetramethylsilane (TMS) |
| 26 | acetonitrile |
| 27 | tetrahydrofuran |
| 28 | dimethylformamide |
| 29 | methylpropionamide |
| 30 | water ($H_2O$ or $D_2O$) |
| 31 | acetic acid |
| 32 | 1,2-dichloroethane |
| 33 | dioxane |
| 34 | trifluoroacetic acid |
| 35 | 2-methoxyethyl ether (diglyme) |
| 36 | nitromethane |
| 37 | ethanol |
| 38 | triethylamine |
| 39 | deuterium oxide containing an unspecified low concentration of NaOD |
| 40 | deuterium oxide containing an unspecified high concentration of NaOD |

| Solvent | Solvent Code |
|---|---|
| (none: neat liquid + TMS*) | 1 |
| acetic acid | 31 |
| acetic anhydride | 19 |
| acetone(-$d_6$) | 8 |
| acetonitrile | 26 |
| benzene(-$d_6$) | 6 |
| bromocyclopentane | 17 |
| carbon disulfide | 7 |
| carbon tetrabromide | 23 |
| carbon tetrachloride | 4 |
| chloroform-d | 3 |
| cyclohexane | 12 |
| cyclohexanone | 15 |
| deuterium oxide containing an unspecified low concentration of NaOD | 39 |
| deuterium oxide containing an unspecified high concentration of NaOD | 40 |
| 1,2-dichloroethane | 32 |
| diethyl ether | 10 |
| dimethylformamide | 28 |
| dimethylsulfoxide(-$d_6$) | 5 |
| dioxane | 33 |
| ethanol | 37 |
| ethyl acetate | 11 |
| ethyl bromide | 16 |
| n-hexane | 9 |
| methanol | 22 |
| 2-methoxyethyl ether (diglyn | 35 |
| methyl acetate | 13 |
| methylene chloride | 2 |
| methylpropionamide | [illegible] |
| nitromethane | 36 |
| paraldehyde | 14 |
| propylene carbonate | 18 |
| squalane | 24 |
| tetrahydrofuran | 27 |
| *tetramethylsilane (TMS) | 25 |
| 1,1,1-trichloro-1,1,1-trifluoroethane | 21 |
| triethylamine | 38 |
| toluene-$d_8$ | 20 |
| water ($H_2O$ or $D_2O$) | 30 |

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