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

B. L. Shapiro and L. E. Mohrmann

Department of Chemistry, Texas A&M University, College Station, TX 77843

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.

Contents

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

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, δ_H: All shifts are reported on the conventional δ-scale, i.e., δ_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 careful 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 δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

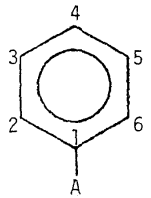


Table I

Entry No.	Molecular Formula	Name	A	δ_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			MgBr	7.656	7.067	7.000	10	10	36	60	95
019			MgBr	7.640	6.952	6.870	27	10	36	60	95

PROTON CHEMICAL SHIFTS, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

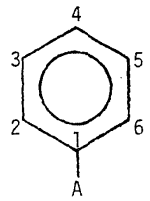


Table I

Entry No.	Molecular Formula	Name	A	δ_H[a] 2,6 (ortho)	3,5 (meta)	4 (para)	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
020	C_6H_5Cl	chlorobenzene	Cl	7.139	7.005	6.970	1	30	x[d]	100	52
021			Cl	7.141	6.999	6.966	1	100	36	60	27
022			Cl	7.340	7.300	7.248	2	0[e]	52	60	10
023			Cl	7.264	7.196	7.141	4	10	36	60	27
024			Cl	7.288	7.238	7.173	4	0	52	60	10
025			Cl	7.281	7.233	7.167	4	0	x	100	51
026			Cl	7.378	7.370	7.308	8	0	52	60	10
027			Cl	7.245	7.153	7.098	9	0	52	60	10
028			Cl	7.307	7.257	7.197	10	0	52	60	10
029			Cl	7.350	7.323	7.260	11	0	52	60	10
030			Cl	7.235	7.150	7.093	12	0	52	60	10
031			Cl	7.365	7.343	7.280	13	0	52	60	10
032			Cl	7.338	7.333	7.277	14	0	52	60	10
033			Cl	7.353	7.348	7.285	15	0	52	60	10
034			Cl	7.223	7.128	7.078	25	10	38	60	53
035	$C_6H_5ClO_2S$	benzenesulfonyl chloride	SO_2Cl	7.939	7.487	7.605	1+6	80	x	100	52
036			SO_2Cl	8.020	7.603	7.701	4	0	x	100	51
037	$C_6H_5Cl_3Ge$	phenyltrichlorogermane	$GeCl_3$	7.67	7.52	7.46	4	33	x	60 or 100	99

PROTON CHEMICAL SHIFTS, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

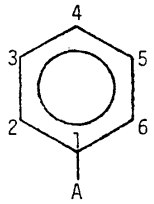


Table I

Entry No.	Molecular Formula	Name	A	δ_H[a] 2,6 (ortho)	3,5 (meta)	4 (para)	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
038	$C_6H_5Cl_3Si$	phenyltrichlorosilane	$SiCl_3$	7.73	7.44	7.37	4	33	x[d]	60 or 100	99
039	$C_6H_5Cl_3Sn$	phenyltrichlorostannane	$SnCl_3$	7.55	7.53	7.50	4	33	x	60 or 100	99
040	C_6H_5F	fluorobenzene	F	6.863	7.072	6.896	1	100	36	60	27
041			F	7.050	7.337	7.128	2	0[e]	52	60	10
042			F	6.973	7.241	7.034	4	10	36	60	27
043			F	6.970	7.246	7.037	4	10	38	60	58
044			F	6.988	7.270	7.050	4	0	52	60	10
045			F	7.100	7.393	7.177	8	0	52	60	10
046			F	7.080	7.371	7.155	8	10	38	60	58
047			F	6.927	7.202	7.000	9	0	52	60	10
048			F	7.010	7.290	7.035	10	0	52	60	10
049			F	7.067	7.353	7.143	11	0	52	60	10
050			F	6.918	7.193	6.990	12	0	52	60	10
051			F	7.080	7.370	7.155	13	0	52	60	10
052			F	7.060	7.353	7.140	14	0	52	60	10
053			F	7.073	7.370	7.150	15	0	52	60	10
054			F	6.889	7.100	6.922	21	85	36	60	27

PROTON CHEMICAL SHIFTS, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

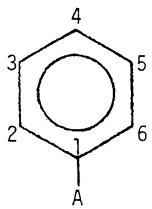


Table I

Entry No.	Molecular Formula	Name	A	δ_H[a] 2,6 (ortho)	δ_H[a] 3,5 (meta)	δ_H[a] 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[e]	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
071			I	7.625	6.960	7.185	9	0	52	60	11
072			I	7.678	7.062	7.283	10	0	52	60	11

PROTON CHEMICAL SHIFTS, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

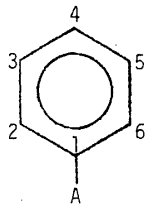


Table I

Entry No.	Molecular Formula	Name	A	δ_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

PROTON CHEMICAL SHIFTS, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

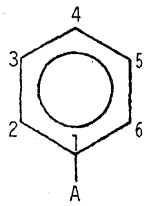


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

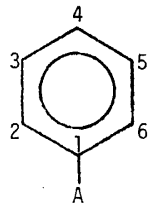


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

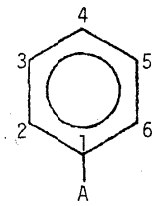


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

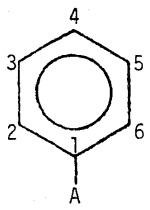


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

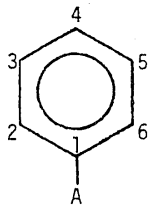


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

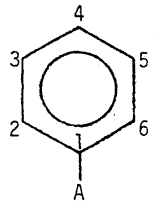


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

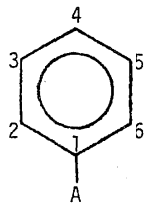


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

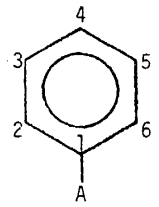


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

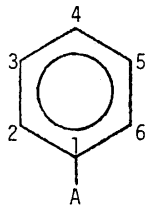


Table I

Entry No.	Molecular Formula	Name	A	δ_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		7.30	7.28	7.18	4	2-5	x	300	81
256				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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

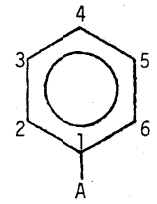


Table I

Entry No.	Molecular Formula	Name	A	δ_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	$CH_2CH(CH_3)^{\dagger}NH_3HSO_4^-$	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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

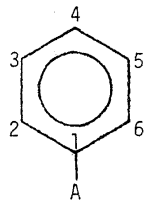


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

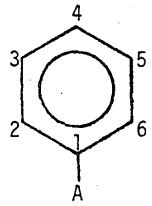
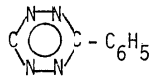


Table I

Entry No.	Molecular Formula	Name	A	δ_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	$C(C_6H_5)Cl_2$	7.384	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	$C\equiv C-C_6H_5$	7.458	7.251	7.224	4	7	36	60	30
301			$C\equiv C-C_6H_5$	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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

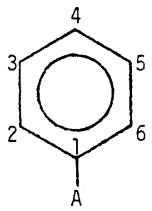
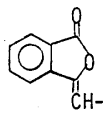


Table I

Entry No.	Molecular Formula	Name	A	δ_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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

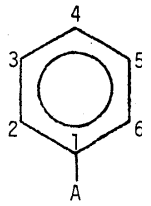


Table I

Entry No.	Molecular Formula	Name	A	δ_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	$(C_6H_5)_2Ge\text{-}CH\text{=}CH_2$	7.422	7.272	7.277	4	6	33	100	74
333	$C_{20}H_{18}Pb$	vinyltriphenylplumbane	$(C_6H_5)_2Pb\text{-}CH\text{=}CH_2$	7.510	7.315	7.227	4	6	33	100	74
334	$C_{20}H_{18}Si$	vinyltriphenylsilane	$(C_6H_5)_2Si\text{-}CH\text{=}CH_2$	7.457	7.267	7.300	4	6	33	100	74
335	$C_{20}H_{18}Sn$	vinyltriphenylstannane	$(C_6H_5)_2Sn\text{-}CH\text{=}CH_2$	7.488	7.282	7.268	4	6	33	100	74
336	$C_{21}H_{18}$	1,1,1-triphenylpropene	$(C_6H_5)_2C\text{-}CH\text{=}CH_2$	7.037	7.182	7.122	4	6	33	100	74
337			$(C_6H_5)_2C\text{-}CH\text{=}CH_2$	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, δ_H[a], IN MONOSUBSTITUTED BENZENES (AND IN BENZENE ITSELF)

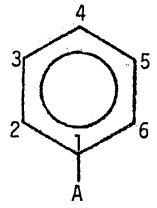


Table I

Entry No.	Molecular Formula	Name	A	δ_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.

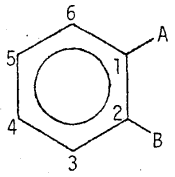
[c] Concentration is given in percent unless number is followed by "M", molarity. The designation "0" refers to the shift at "infinite dilution". See text, section 2, item 7.

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

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

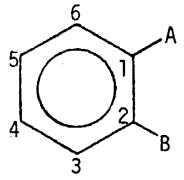


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
001	C_6H_4BrCl	o-bromochlorobenzene	Cl	Br	7.378	6.870	6.997	7.212	1	10	36	60	29
002			Cl	Br	7.53	7.01	7.14	7.38	4	5-10	40	60	33
003			Cl	Br	7.537	7.027	7.156	7.369	4	10	36	60	29
004			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-dibronobenzene	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

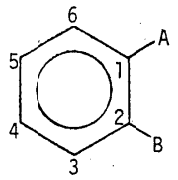


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
021	C_6H_4ClI	o-chloroiodobenzene	I	Cl	7.37	7.21	6.84	7.79	4	5-10	40	60	33
022			I	Cl	7.284	7.087	6.751	7.714	25	10	38	60	76
023	$C_6H_4ClNO_2$	o-chloronitrobenzene	NO_2	Cl	7.54	7.49	7.41	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

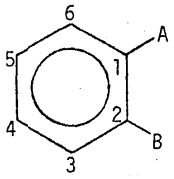


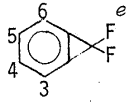
Entry No.	Molecular Formula	Name	A	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
041	$C_6H_4I_2$	o-diiodobenzene	I	I	7.809	6.959	6.959	7.809	4	10	36	60	29
042			I	I	7.806	6.949	6.949	7.806	25	10	38	60	76
043	$C_6H_4N_2O_4$	o-dinitrobenzene	NO_2	NO_2	7.97	7.87	7.87	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO



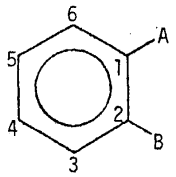
Entry No.	Molecular Formula	Name	A [e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
061	C_6H_6IN	o-iodoaniline	NH_2	I	7.53	6.36	7.01	6.58	4	10	x[d]	100	40
062			NH_2	I	7.51	6.31	7.04	6.77	5	10	x	100	40
063	$C_6H_6N_2O_2$	o-nitroaniline	NH_2	NO_2	8.07	6.65	7.30	6.79	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

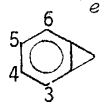
*Shifts measured relative to DSS (sodium 2,2-dimethyl-2-silapentane-5-sulfonate) and converted to normal δ-scale.

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

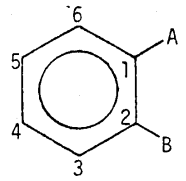


Entry No.	Molecular Formula	Name	A [e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
078	C_7H_5ClO	o-chlorobenzaldehyde	CHO	Cl	7.474	7.590	7.428	7.810	1	90	36	60	59
079			CHO	Cl	7.40	7.47	7.34	7.86	4	10	x[d]	100	4
080	C_7H_5ClOTe	o-formylphenyl tellurium chloride	TeCl	CHO	8.18	7.51	7.68	8.37	7	0[e]	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

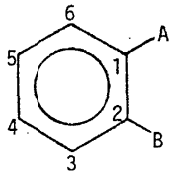


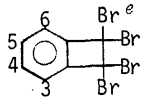
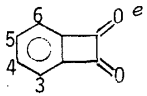
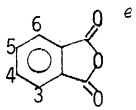
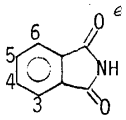
Entry No.	Molecular Formula	Name	A	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
093	$C_7H_6O_2$	o-hydroxybenzaldehyde	CHO	OH	6.90	7.43	6.92	7.45	4	10	x[d]	100	4
094	$C_7H_6O_3$	o-hydroxybenzoic acid	CO_2H	OH	7.05	7.56	6.97	7.97	3	x[d]	x	60	48
095			CO_2H	OH	6.98	7.53	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-nitrotcluene	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

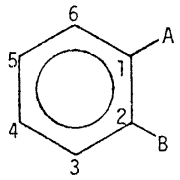


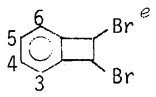
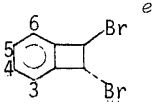
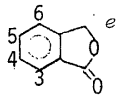
Entry No.	Molecular Formula	Name	A[e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
112	C_7H_8O	o-cresol	OH	CH_3	6.99	6.73	6.92	6.59	4	10	x[d]	100	40
113	$C_7H_8O_2$	o-methoxyphenol	OH	OCH_3	6.73	6.72	6.78	6.84	4	10	x	60	38
114			OH	OCH_3	6.85	6.85	6.89	6.89	5	10	x	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

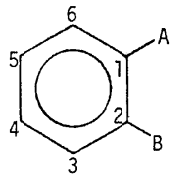


Entry No.	Molecular Formula	Name	A[e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
124	$C_8H_6Br_2$	cis-dibromobenzocyclobutene			7.382	7.190	7.190	7.382	3	15	x[d]	100	5
125	$C_8H_6Br_2$	trans-dibromobenzocyclobutene			7.348	7.140	7.140	7.348	3	15	x	100	5
126	$C_8H_6O_2$	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

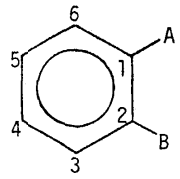


Entry No.	Molecular Formula	Name	A[e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
138	C_8H_7IO	o-iodoacetophenone	$COCH_3$	I	7.97	7.23	7.51	7.66	5	10	x[d]	100	4
139	C_8H_7N	o-tolunitrile	CN	CH_3	7.26	7.41	7.22	7.52	4	5	x	100	67
140			CN	CH_3	7.27	7.42	7.23	7.50	4	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

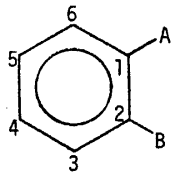


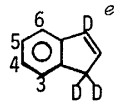
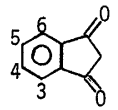
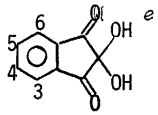
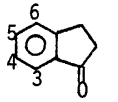
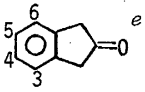
Entry No.	Molecular Formula	Name	A	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
155	$C_8H_8O_3$	o-methoxybenzoic acid	CO_2H	OCH_3	7.16	7.54	7.04	7.70	5	x[d]	x[d]	60	48
156			CO_2H	OCH_3	7.114	7.496	7.009	7.690	5	10	x	60 or 100	75
157			CO_2H	OCH_3	6.39	7.08	6.74	8.24	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

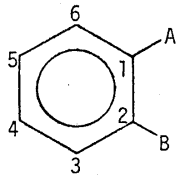


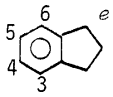
Entry No.	Molecular Formula	Name	A [e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
174	$C_8H_{10}O_2$	o-dimethoxybenzene	OCH_3	OCH_3	6.75	6.75	6.75	6.75	4	x[d]	x[d]	x[d]	7
175	$C_8H_{11}N$	o-ethylaniline	NH_2	C_2H_5	6.91	6.59	6.88	6.47	4	5	x	100	67
176	$C_8H_{11}N$	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

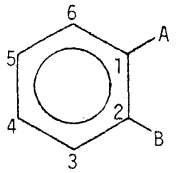


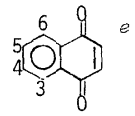
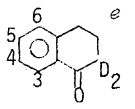
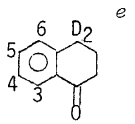
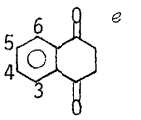
Entry No.	Molecular Formula	Name	A [e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
184	C_9H_9ClO	2-(o-chlorophenyl)oxetane		Cl	7.27	7.15	7.24	7.68	4	2-5	x[d]	300	81
185			"	Cl	7.02	6.81	7.10	7.85	6	2-5	x	300	81
186	C_9H_{10}	indan			7.073	6.990	6.990	7.073	3	15	x	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, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO

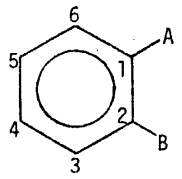


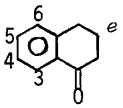
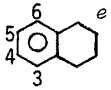
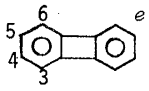
Entry No.	Molecular Formula	Name	A [e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
199	$C_9H_{11}NO_2$	N-methyl-o-methoxybenzamide	$CONHCH_3$	OCH_3	6.97	7.43	7.07	8.22	3	x[d]	x[d]	60	48
200			$CONHCH_3$	OCH_3	7.13	7.46	7.04	7.80	5	x	x	60	48
201			$CONHCH_3$	OCH_3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

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO



Entry No.	Molecular Formula	Name	A [e]	B	δ_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, δ_H[a], IN DISUBSTITUTED BENZENES

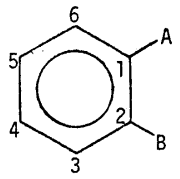
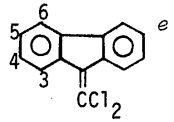
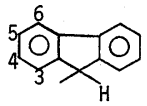


Table II

Substituent Arrangement: ORTHO

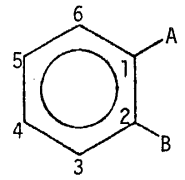
Entry No.	Molecular Formula	Name	A [e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
224	$C_{12}H_8Cl_2$	o,o'-dichlorobiphenyl	o-C_6H_4Cl	Cl	7.155	6.815	6.874	7.138	6	5	x[d]	60	32
225	$C_{12}H_8F_2$	o,o'-difluorobiphenyl	o-C_6H_4F	F	6.853	6.890	6.823	7.214	6	5	x	60	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-dichloromethylenefluorere	 [e]		8.22	7.20	7.27	7.54	4	10	x	100	40

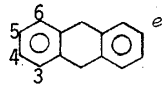
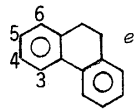
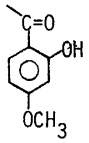
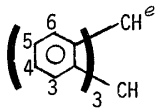
* R = 

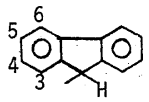
PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO



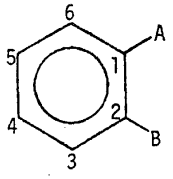
Entry No.	Molecular Formula	Name	A [e]	B	δ_H[a] 3	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
240	$C_{14}H_{12}$	9,10-dihydroanthracene			7.166	7.096	7.096	7.166	3	15	x[d]	100	5
241	$C_{14}H_{12}$	9,10-dihydrophenanthrene			7.539	7.104	7.037	7.011	3	15	x	100	5
242	$C_{14}H_{12}O$	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

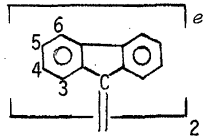
* R = 

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

Table II

Substituent Arrangement: ORTHO



Entry No.	Molecular Formula	Name	A [e] B	δ_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.

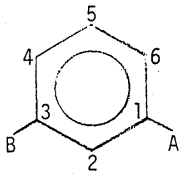
[d] The designation "x" means unknown or unspecified.

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

Table III

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

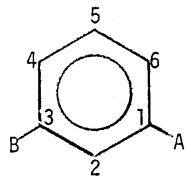


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
001	C_6H_4BrCl	m-bromochlorobenzene	Cl	Br	7.420	7.247	6.976	7.136	25	10	38	60	76
002	$C_6H_4BrClMg$	m-chlorophenylmagnesium bromide	MgBr	Cl	7.59	6.98	7.02	7.49	10	1M	x[d]	100	49
003	C_6H_4BrF	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, δ_H[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

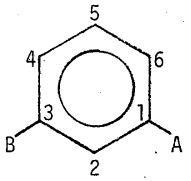


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
021	C_6H_4ClI	m-chloroiodobenzene	I	Cl	7.626	7.170	6.836	7.454	25	10	38	60	76
022	C_6H_4ClLi	m-chlorophenyllithium	Li	Cl	7.90	6.94	6.97	7.81	10	1M	x[d]	100	49
023	$C_6H_4ClNO_2$	m-chloronitrobenzene	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, δ_H[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

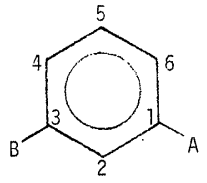


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
041	$C_6H_6N_2O_2$	m-nitroaniline	NH_2	NO_2	7.516	7.445	7.258	6.943	2	0[e]	52	60	14
042			NH_2	NO_2	7.489	7.392	7.105	7.044	8	0	52	60	14
043			NH_2	NO_2	7.452	7.390	7.157	6.857	10	0	52	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, δ_H[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

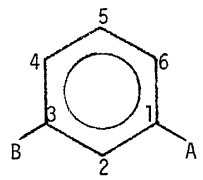


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2	4	5	6	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
058	$C_7H_6O_3$	m-hydroxybenzoic acid	CO_2H	OH	7.476	7.069	7.325	7.482	5	10	x[d]	60 or 100	75
059			CO_2H	OH	7.572	7.123	7.347	7.576	8	1.0M	x	100	9
060	C_7H_7Br	m-bromotoluene	CH_3	Br	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, δ_H[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

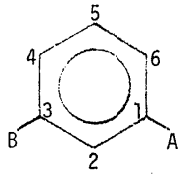


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2	4	5	6	Solvent Code[b]	Concn[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
076	$C_8H_8O_3$	m-hydroxyphenylacetic acid	CH_2CO_2H	OH	6.818	6.724	7.109	6.766	8	1.0M	x[d]	100	12
077	$C_8H_8O_3$	m-methoxybenzoic acid	CO_2H	OCH_3	7.531	7.193	7.425	7.610	5	10	x	60 or 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'-dibromobipheryl	m-C_6H_4Br	Br	7.548	7.225	6.813	7.143	6	5	x	60	32

Table III

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

Substituent Arrangement: META



Entry No.	Molecular Formula	Name	A	B	δ_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.

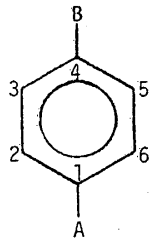
[c] Concentration is given in percent unless number is followed by "M", molarity. The designation "0" refers to the shift at "infinite dilution". See text, section 2, item 7.

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

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

Table IV

Substituent Arrangement: PARA

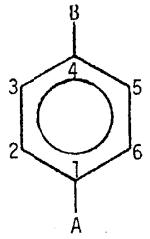


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
001	C_6H_4BrCl	p-bromochlorobenzene	Cl	Br	7.12	7.39	3	x[d]	x[d]	x[d]	2
002			Cl	Br	7.30	7.50	4	14	25	60	78
003			Cl	Br	7.070	7.284	25	10	38	60	76
004	$C_6H_4BrClMg$	p-chlorophenylmagnesium 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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

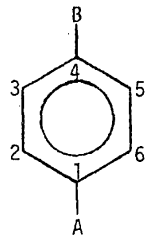


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
019	$C_6H_4Br_2$	p-dibromobenzene	Br	Br	7.222	7.222	25	10	38	60	76
020			Br	Br	7.43	7.43	26	2	40	60	34
021	$C_6H_4Br_2Mg_2$	p-bis(bromomagnesio)benzene	MgBr	MgBr	7.70	7.70	27	0.5M	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

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

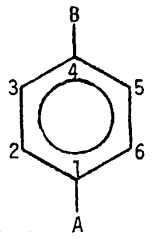


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
038	C_6H_4FI	p-fluoroiodobenzene	I	F	7.33	6.57	1	100	25	60	78
039			I	F	7.492	6.671	25	10	38	60	31
040	C_6H_4FLi	p-fluorophenyllithium	Li	F	7.98	6.85	10	1M	x[d]	100	49
041	$C_6H_4FNO_2$	p-fluoronitrobenzene	NC_2	F	8.26	7.24	1	100	25	60	78
042			NC_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	NC_2	I	7.90	7.90	3	x	x	x	2
046			NC_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	NC_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	NC_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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

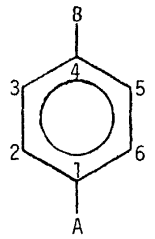


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
057	$C_6H_5NO_3$	p-nitrophenol	OH	NO_2	6.69	7.83	8	11	25	60	78
058	C_6H_6BrN	p-bromoaniline	NH_2	Br	6.61	7.15	8	13	25	60	78
059	C_6H_6FN	p-fluoroaniline	NH_2	F	6.40	6.78	1	100	25	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

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

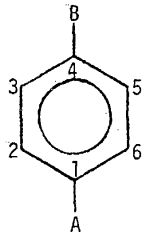
Substituent Arrangement: PARA



Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV



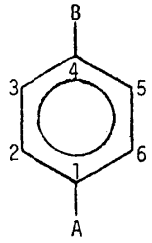
Substituent Arrangement: PARA

Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_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

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

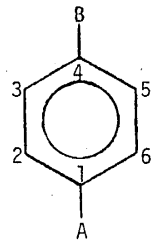


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
109	C_7H_7BrMg	p-tolylmagnesium bromide	MgBr	CH_3	7.42	6.70	27	0.4M	x[d]	60	37
110	C_7H_7BrMgO	p-anisylmagnesium bromide	MgBr	OCH_3	7.40(?)	6.66(?)	10	0.58M	x	60	37
111			MgBr	OCH_3	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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

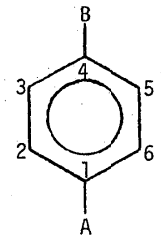


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq.[f] (MHz)	Ref.
128	$C_7H_7Cl_3Si$	p-tolyltrichlorosilane	$SiCl_3$	CH_3	7.72	7.41	8	x[d]	21	60	87
129			$SiCl_3$	CH_3	7.61	7.17	12	x	21	60	87
130			$SiCl_3$	CH_3	7.72	7.38	26	x	21	60	87
131			$SiCl_3$	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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

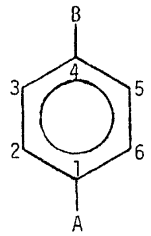


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
147	C_7H_7I	p-iodotoluene	CH_3	I	6.84	7.49	4	5	x[d]	100	67
148			CH_3	I	6.46	7.36	6	1-3	x	100	93
149			CH_3	I	6.78	7.47	12	1-3	x	100	93
150	C_7H_7IO	p-iodoanisole	OCH_3	I	6.62	7.53	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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

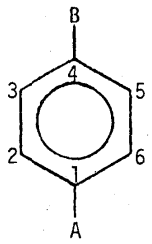


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
165	$C_7H_7NO_3$	p-nitroanisole	OCH_3	NO_2	6.34	7.89	6	5	x[d]	60	98
166			OCH_3	NO_2	6.88	8.04	7	5	x	60	98
167			OCH_3	NO_2	7.12	8.21	8	5	x	60	98
168			OCH_3	NO_2	6.83	8.10	12	<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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

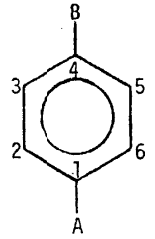


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
183	C_8H_7ClO	p-toluyl chloride	COCl	CH_3	7.95	7.24	4	5	x[d]	100	67
184	$C_8H_7ClO_2$	methyl-p-chlorobenzoate	CO_2CH_3	Cl	7.91	7.07	3	x[d]	x	x[d]	2
185	$C_8H_7ClO_2$	p-methoxybenzoyl 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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

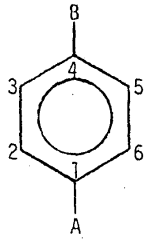


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
202	$C_8H_8O_2$	p-hydroxyphenylacetic acid	CH_2CO_2H	OH	7.125	6.785	8	1.0M	x[d]	100	12
203	$C_8H_8O_2$	p-methoxybenzaldehyde	CHO	OCH_3	7.79	6.95	1	100	25	60	78
204	$C_8H_8O_2$	p-toluic 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	$C_8H_9NC_2$	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	$C_8H_9NC_2$	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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA



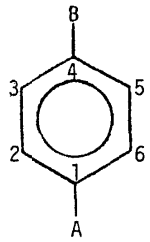
Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
220	$C_8H_{10}BrN$	p-N,N-dimethylaminobromobenzene	Br	$N(CH_3)_2$	7.21	6.48	3	x[d]	x[d]	x[d]	2
221	$C_8H_{10}ClN$	p-N,N-dimethylaminochlorobenzene	Cl	$N(CH_3)_2$	7.12	6.55	3	x	x	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 *a 6.71	s 8.93 a 6.62	8	2	-56	60	68
225			$N(CH_3)_2$	NO	s 6.82 a 6.53	s 8.91 a 6.78	3	2	-56(?)	60	69
226	$C_8H_{10}N_2O_2$	p-N,N-dimethylaminonitrobenzene	NC_2	$N(CH_3)_2$	8.07	6.56	3	x	x	x	2
227			NC_2	$N(CH_3)_2$	8.088	6.780	8	x	33	60	8
228			NC_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		Cl	7.28	7.28	4	2-5	x	300	81

* 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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

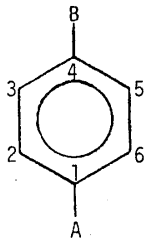


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
234	C_9H_9ClO	2-(p-chlorophenyl)oxetane		Cl	7.03	7.14	6	2-5	x[d]	300	81
235	C_9H_9ClO	p-ethylbenzoyl chloride	$COCl$	C_2H_5	7.95	7.28	3	x[d]	x	x[d]	2
236	C_9H_9N	p-ethylbenzonitrile	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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

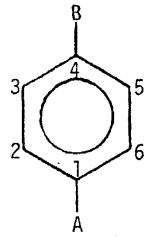
Substituent Arrangement: PARA



Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[e] (%)	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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV



Substituent Arrangement: PARA

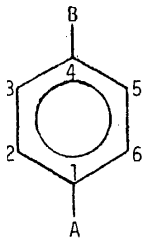
Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
271	$C_{10}H_{13}Cl_3Sn$	p-tert-butylphenyltrichlorostannane	$SnCl_3$	$C(CH_3)_3$	7.61	7.61	2	x[d]	21	60	87
272			$SnCl_3$	$C(CH_3)_3$	7.62	7.34	5	x	21	60	87
273			$SnCl_3$	$C(CH_3)_3$	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 *a 6.77	s 8.89 a 6.66	8	2	-56	60	68
281			$N(C_2H_5)_2$	NO	s 6.83 a 6.54	s 8.86 a 6.84	3	2	-56(?)	60	69
282			$N(C_2H_5)$	NO	s 6.01 a 5.67	s 8.96 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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA

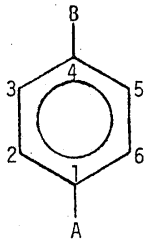


Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
286	$C_{11}H_{14}O_2$	p-tert-butylbenzoic acid	CO_2H	$C(CH_3)_3$	7.90	7.49	3	x[d]	x[d]	x[d]	2
287	$C_{11}H_{14}O_2$	methyl p-isopropylbenzoate	CO_2CH_3	$CH(CH_3)_2$	7.89	7.21	3	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

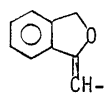
PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA



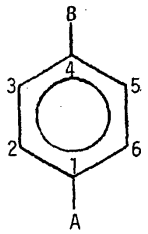
Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
304	$C_{14}H_{14}Cl_2Sn$	di(p-tolyl)dichlorostannane	$SnCl_2$-p-$CH_3C_6H_4$	CH_3	7.54	7.33	2	x[d]	21	60	87
305			$SnCl_2$-p-$CH_3C_6H_4$	CH_3	7.77	7.14	5	x	21	60	87
306			$SnCl_2$-p-$CH_3C_6H_4$	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 = 

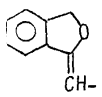
PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA



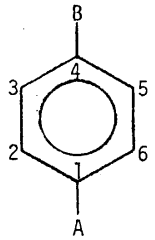
Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
319	$C_{15}H_{11}NO_3$	3-(p-nitrophenyl)methylidenephthalide	R*	NO_2	8.32	8.08	8	.05M	24	80	84
320	$C_{15}H_{11}NO_3S$	3-(p-nitrophenyl)thiomethylidene-phthalide	S-R*	NO_2	7.80	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, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA



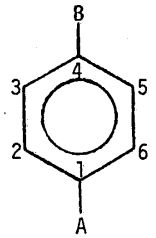
Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_H[a] 3,5	Solvent Code[b]	Concn.[c] (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
335	$C_{18}H_{12}Br_3OP$	tris-p-bromophenylphosphine oxide	$PO(p\text{-}BrC_6H_4)_2$	Br	7.50	7.64	2	0.5M	x[d]	60	44
336	$C_{18}H_{12}Br_3P$	tris-p-bromophenylphosphine	$P(p\text{-}BrC_6H_4)_2$	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- = $p\text{-}C_2H_5OC_6H_4Te\text{-}o\text{-}C_6H_4\text{-}Te$-

PROTON CHEMICAL SHIFTS, δ_H[a], IN DISUBSTITUTED BENZENES

TABLE IV

Substituent Arrangement: PARA



Entry No.	Molecular Formula	Name	A	B	δ_H[a] 2,6	δ_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

4. Author Index

5. References

[1] G. M. Janini, J. W. King, and D. E. Martire, J. Am. Chem. Soc., **96**, 5368 (1974).
[2] D. W. Beistel, H. E. Chen, and P. J. Fryatt, J. Am. Chem. Soc., **95**, 5455 (1973).
[3] A. M. Ihrig and J. L. Marshall, J. Am. Chem. Soc., **94**, 3268 (1972).
[4] W. B. Smith, D. L. Deavenport, and A. M. Ihrig, J. Am. Chem. Soc., **94**, 1959 (1972).
[5] M. A. Cooper and S. L. Manatt, J. Am. Chem. Soc., **92**, 1605 (1970).
[6] K. G. Kidd, G. Kotowycz, and T. Schaefer, Can. J. Chem. **45**, 2155 (1967).
[7] W. B. Smith and J. L. Roark, J. Am. Chem. Soc., **89**, 5018 (1967).
[8] G. Fraenkel and J. P. Kim, J. Am. Chem. Soc., **88**, 4203 (1966).

[9] K. N. Scott, J. Mag Res., **2**, 361 (1970).
[10] L. G. Robinson and G. B. Savitsky, J. Mag. Res., **3**, 269 (1970).
[11] G. M. Ford, L. G. Robinson, and G. B. Savitsky, J. Mag. Res., **4**, 109 (1971).
[12] K. N. Scott, J. Mag. Res., **6**, 55 (1972).
[13] M. Anteunis, A. De Bruyn, and J. S. Sandhu, J. Mag. Res., **8**, 7 (1972).
[14] W. A. Tallon and G. B. Savitsky, J. Mag. Res., **9**, 422 (1973).
[15] H. Bildsøe and K. Schaumburg, J. Mag. Res., **14**, 223 (1974).
[16] Y. N. Luzikov, N. M. Sergeyev, and Y. A. Ustynyuk, J. Mag. Res., **18**, 406 (1975).
[17] L. Ernst, D. N. Lincoln, and V. Wray, J. Mag. Res., **21**, 115 (1976).
[18] L. Ernst, E. Lustig, and V. Wray, J. Mag. Res., **22**, 459 (1976).
[19] R. J. Kostelnik, M. P. Williamson, D. E. Wisnosky, and S. M. Castellano, Can J. Chem., **47**, 3313 (1969).
[20] R. Wasylishen and T. Schaefer, Can. J. Chem., **49**, 3627 (1971).
[21] R. Wasylishen and T. Schaefer, Can. J. Chem., **49**, 3216 (1971).
[22] J. B. Rowbotham, A. F. Janzen, J. Peeling, and T. Schaefer, Can. J. Chem., **52**, 481 (1974).
[23] R. Wasylishen, J. B. Rowbotham, L. Ernst, and T. Schaefer, Can. J. Chem., **50**, 2575 (1972).
[24] W. F. Reynolds, I. R. Peat, and G. K. Hamer, Can. J. Chem., **52**, 3415 (1974).
[25] K. Chum, J. B. Rowbotham, and T. Schaefer, Can. J. Chem., **52**, 3489 (1974).
[26] R. Wasylishen and T. Schaefer, Can. J. Chem., **49**, 94 (1971).
[27] S. Castellano, R. Kostelnik, and C. Sun., Tetrahedron Lett., 4635 (1967).
[28] S. Castellano, C. Sun, and R. Kostelnik, Tetrahedron Lett., 5205 (1967).
[29] S. Castellano and R. Kostelnik, Tetrahedron Lett., 5211 (1967).
[30] S. Castellano and J. Lorenc, J. Phys. Chem., **69**, 3552 (1965).
[31] J. E. Loemker, J. M. Read, Jr., and J. H. Goldstein, J. Phys. Chem., **72**, 991 (1968).
[32] A. R. Tarpley, Jr. and J. H. Goldstein, J. Phys. Chem., **75**, 421 (1971).
[33] W. B. Smith and G. M. Cole, J. Phys. Chem., **69**, 4413 (1965).
[34] W. B. Smith and S. Chiranjeevi, J. Phys. Chem., **70**, 3505 (1966).
[35] C. E. Griffin, J. J. Burke, F. E. Dickson, M. Gordon, H. H. Hsieh, R. Obrycki, and M. P. Williamson, J. Phys. Chem., **71**, 4558 (1967).
[36] G. Fraenkel, D. G. Adams, and R. R. Dean, J. Phys. Chem., **72**, 944 (1968).
[37] G. Fraenkel, S. Dayagi, and S. Kobayashi, J. Phys. Chem., **72**, 953 (1968).
[38] J. L. Roark and W. B. Smith, J. Phys. Chem., **73**, 1043 (1969).
[39] J. L. Roark and W. B. Smith, J. Phys. Chem., **73**, 1046 (1969).
[40] W. B. Smith, A. M. Ihrig, and J. L. Roark, J. Phys. Chem., **74**, 812 (1970).
[41] D. W. Beistel and H. E. Chen, J. Chem. Phys., **59**, 4642 (1973).
[42] M. P. Williamson, R. J. Kostelnik, and S. M. Castellano, J. Chem. Phys., **49**, 2218 (1968).
[43] S. Castellano and A. A. Bothner-By, J. Chem. Phys., **41**, 3863 (1964).
[44] R. Benassi, M. L. Schenetti, F. Taddei, P. Vivarelli, and P. Dembech, J. Chem. Soc., Perkin II, 1338 (1974).
[45] T. Birchall and I. Drummond, J. Chem. Soc. A, 1401 (1970).
[46] J. E. Loemker, J. H. Goldstein, and J. M. Read, Jr., Chem. Comm., 744 (1968).
[47] D. B. Macdonald, Chem. Comm., 686 (1967).
[48] M. Kondo, Bull. Chem. Soc. Japan, **45**, 2790 (1972).
[49] J. A. Ladd and J. Parker, J. Chem. Soc., Dalton, 930 (1972).
[50] J. E. Loemker, J. M. Read, Jr., and J. H. Goldstein, J. Mol. Spectry., **29**, 284 (1969).
[51] K. Hayamizu and O. Yamamoto, J. Mol. Spectry., **28**, 89 (1968).
[52] K. Hayamizu and O. Yamamoto, J. Mol. Spectry., **25**, 422 (1968).
[53] J. M. Read, Jr. and J. H. Goldstein, J. Mol. Spectry., **23**, 179 (1967).
[54] J. P. Jacobsen and K. Schaumburg, Mol. Phys., **28**, 1505 (1974).
[55] W. A. Gibbons and V. M. S. Gil, Mol. Phys., **9**, 163 (1965).
[56] R. E. Mayo and J. H. Goldstein, Mol. Phys., **10**, 301 (1966).
[57] J. E. Loemker, J. M. Read, Jr., and J. H. Goldstein, Mol. Phys., **13**, 433 (1967).
[58] J. E. Loemker and J. H. Goldstein, Spectry. Lett., **1**, 153 (1968).
[59] D. G. de Kowalewski and S. Castellano, Mol. Phys., **16**, 567 (1969).
[60] M. Baiwir, G. Llabres, J. Denoel and J.-L. Piette, Mol. Phys., **25**, 1 (1973).
[61] F. Lambert, M. Ellenberger, and Y. Cohen, Spectry. Lett., **8**, 509 (1975).
[62] M. Barfield, C. J. Macdonald, I. R. Peat, and W. F. Reynolds, J. Am. Chem Soc., **93**, 4195 (1971).
[63] S. Castellano and J. Lorenc, Chim. Ind (Milan), **47**, 643 (1965).
[64] S. Sørensen and H. J. Jakobsen, Acta Chem. Scand., **A28**, 249 (1974).
[65] J. Beeby, S. Sternhell, T. Hoffmann-Ostenhof, E. Pretsch, and W. Simon, Anal. Chem., **45**, 1571 (1973).
[66] R. Freeman, N. S. Bhacca, and C. A. Reilly, J. Chem. Phys., **38**, 293 (1963).
[67] O. Yamamoto, K. Hayamizu, K. Sekine, and S. Funahira, Anal. Chem., **44**, 1794 (1972).
[68] P. D. Buckley, A. R. Furness, K. W. Jolley, and D. N. Pinder, Aust. J. Chem., **27**, 21 (1974).
[69] A. R. Furness, P. D. Buckley, and K. W. Jolley, Aust. J. Chem., **28**, 2303 (1975).
[70] H. Günther and S. Castellano, Ber. Bunsenges. Phys. Chem., **70**, 913 (1966).
[71] T. Schaefer and K. Chum, Can. J. Chem., **54**, 2231 (1976).
[72] G. C. Pappalardo and S. Gruttadauria, Z. Physik. Chem., **94**, 179 (1975).
[73] G. C. Pappalardo, Spectrochim. Acta, **29A**, 2055 (1973).
[74] P. N. Preston, L. H. Sutcliffe, and B. Taylor, Spectrochim. Acta, **28A**, 197 (1972).
[75] R. H. Cox, Spectrochim. Acta, **25A**, 1189 (1969).
[76] R. W. Creely, J. M. Read, Jr., R. S. Butler, and J. H. Goldstein, Spectrochim. Acta, **24A**, 685 (1968).
[77] J. A. Ladd, Spectrochim. Acta, **22**, 1157 (1966).
[78] B. Dischler, Z. Naturforsch., **20a**, 888 (1965).
[79] C. Glidewell, D. W. H. Rankin, and G. M. Sheldrick, Trans. Faraday Soc., **65**, 2801 (1969).
[80] P. Beltrame, P. Carniti, A. Lai, and P. Viglino, Org. Mag. Res., **7**, 465 (1975).
[81] K. Pihlaja, J. Jokisaari, P. Olavi, I. Virtanen, H. Ruotsalainen, and M. Anteunis, Org. Mag. Res., **7**, 286 (1975).
[82] F. Lambert, M. Ellenberger, L. Merlin, and Y. Cohen, Org. Mag. Res., **7**, 266 (1975).
[83] K. Gatto, J. D. Reinheimer, K. Shafer, and J. T. Gerig, Org. Mag. Res., **6**, 577 (1974).
[84] M. Vida, V. Kellö, T. Liptaj, A. Perjéssy, P. Hrnciar, and M. Lácová, Org. Mag. Res., **6**, 400 (1974).
[85] H. Sterk and H. Holzer, Org. Mag. Res., **6**, 133 (1974).
[86] L. Radics, E. Baitz-Gács, and A. Neszmélyi, Org. Mag. Res., **6**, 60 (1974).

[87] G. Matsubayashi, H. Koezuka, and T. Tanaka, Org. Mag. Res., **5**, 529 (1973).
[88] L. Zetta and G. Gatti, Org. Mag. Res., **4**, 585 (1972).
[89] K. Müllen, Org. Mag. Res., **3**, 331 (1971).
[90] H. Günther and J. B. Pawliczek, Org. Mag. Res., **3**, 267 (1971).
[91] T. J. Batterham and R. Bramley, Org. Mag. Res., **3**, 83 (1971).
[92] K. D. Bartle, D. W. Jones, and R. S. Matthews, Tetrahedron, **25**, 2701 (1969).
[93] Y. Nomura and Y. Takeuchi, Tetrahedron, **25**, 3825 (1969).
[94] B. Gestblom and S. Rodmar, Acta Chem. Scand., **18**, 1767 (1964).
[95] S. Castellano, Private communication of unpublished results.
[96] K. D. Bartle and D. W. Jones, J. Mol. Structure, **1**, 131 (1967).
[97] R. H. Cox and W. K. Austin, Jr., J. Organometal. Chem., **26**, 331 (1971).
[98] H. M. Hutton and T. Schaefer, Can. J. Chem., **43**, 3116 (1965).
[99] G. M. Whitesides, J. G. Selgestad, S. P. Thomas, D. W. Andrews, B. A. Morrison, E. J. Panek, and J. S. Filippo, Jr., J. Organometal. Chem., **22**, 365 (1970).