

NMR spectral data: A compilation of aromatic proton chemical shifts in mono- and di-substituted benzenes

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

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

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

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1. Introduction and Scope

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

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

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

(3) In a substantial number of cases, the reporting of the

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

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

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

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:

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

- 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.

- 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).

- 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

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

- 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.

- 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.

- 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.

- 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 than ± 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-d₆. 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 Frequency: 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)

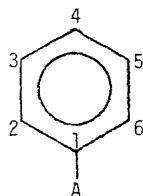


Table I

Entry No.	Molecular Formula	Name	A	δ_H^a			Solvant Code ^b	Concr. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
001	C ₆ H ₅ Br	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 ₆ H ₅ BrMg	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^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

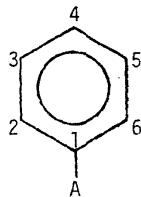


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Cope ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
020	C ₆ H ₅ Cl	chlorobenzene	C1	7.139	7.005	6.970	1	30	x ^d	100	52
021			C1	7.141	6.999	6.966	1	100	36	60	27
022			C1	7.340	7.300	7.248	2	0 ^e	52	60	10
023			C1	7.264	7.196	7.141	4	10	36	60	27
024			C1	7.288	7.238	7.173	4	0	52	60	10
025			C1	7.281	7.233	7.167	4	0	x	100	51
026			C1	7.378	7.370	7.308	8	0	52	60	10
027			C1	7.245	7.153	7.098	9	0	52	60	10
028			C1	7.307	7.257	7.197	10	0	52	60	10
029			C1	7.350	7.323	7.260	11	0	52	60	10
030			C1	7.235	7.150	7.093	12	0	52	60	10
031			C1	7.365	7.343	7.280	13	0	52	60	10
032			C1	7.338	7.333	7.277	14	0	52	60	10
033			C1	7.353	7.348	7.285	15	0	52	60	10
034			C1	7.223	7.128	7.078	25	10	38	60	53
035	C ₆ H ₅ C ₁₀ S ₂	benzenesulfonyl chloride	SO ₂ C1	7.939	7.487	7.605	1+6	80	x	100	52
036			SO ₂ C1	8.020	7.603	7.701	4	0	x	100	51
037	C ₆ H ₅ C ₁ Ge	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)

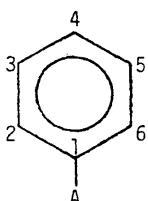


Table I

Entry No.	Molecular Formula	Name	A	δ_H^a			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
038	C ₆ H ₅ Cl ₃ Si	phenyltrichlorosilane	SiCl ₃	7.73	7.44	7.37	4	33	x ^d	60 or 100	99
039	C ₆ H ₅ Cl ₃ Sn	phenyltrichlorostannane	SnCl ₃	7.55	7.53	7.50	4	33	x	60 or 100	99
040	C ₆ H ₅ F	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^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

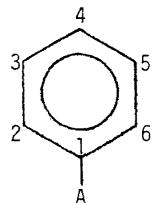


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code ^b	Concn ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
055	C ₆ H ₅ F	fluorobenzene	F	7.047	7.339	7.130	22	10	38	60	58
056			F	6.947	7.208	7.014	25	0 ^d	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 ₆ H ₅ I	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^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

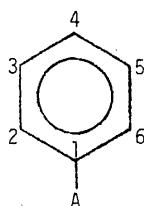


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
073	C ₆ H ₅ I	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 ₆ H ₅ Li	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 ₆ H ₅ NO	nitrosobenzene	NO	7.813	7.548	7.610	4	10	36	60	28
083	C ₆ H ₅ NO 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)

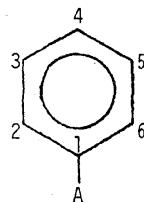


Table I

Entry No.	Molecular Formula	Name	A	δ_H^a			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
092	C ₆ H ₅ NO ₂	nitrobenzene	NO ₂	8.207	7.545	7.678	10	0 ^d	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 ₆ H ₅ N ₃	azidobenzene	N ₃	6.925	7.234	7.027	4	10	36	60	95
100	C ₆ H ₅ NaO	sodium phenolate	ONa	6.435	6.819	6.101	28	10	36	60	95
101	C ₆ H ₅ NaO ₂ S	sodium benzenesulfinate	SO ₂ Na	7.557	7.330	7.269	5	10	36	60	95
102	C ₆ H ₅ NaO ₃ S	sodium benzenesulfonate	SO ₃ Na	7.675	7.343	7.330	5	10	36	60	95
103	C ₆ H 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^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

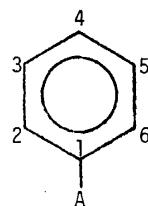


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvant Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
111	C ₆ H 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^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

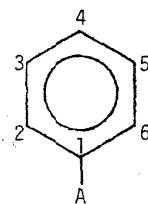


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
130	C ₆ H 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 ₆ H ₅ O	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^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

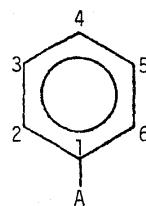


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
149	C ₆ H ₅ O	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 ₆ H ₅ S	thiophenol	SH	7.10	7.02	6.95	12	5	x ^d	100	79
152	C ₆ H ₇ BO ₂	phenylboronic acid	B(OH) ₂	7.712	7.306	7.359	22	10	36	60	95
153	C ₆ H ₇ N	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)

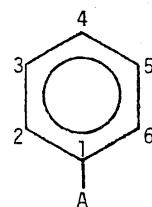


Table I

Entry No.	Molecular Formula	Name	A	δ_H^a			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
167	C ₆ H ₇ N	aniline	NH ₂	6.600	6.983	6.512	15	0 ^e	52	60	10
168	C ₆ H ₈ Ge	phenylgermane	GeH ₃	7.44	7.24	7.28	4	0	x ^d	100	45
169	C ₆ H ₈ GeO	phenoxygermane	OGeH ₃	6.67	6.99	6.72	12	5	x	100	79
170	C ₆ H ₈ GeS	thiophenoxygermane	SGeH ₃	7.10	7.02	6.95	12	5	x	100	79
171	C ₆ H ₈ N ₂	phenylhydrazine	NHNH ₂	6.700	7.171	6.765	3	10	36	60	95
172	C ₆ H ₈ OSi	phenoxy silane	OSiH ₃	6.76	7.08	6.82	12	5	x	100	79
173	C ₆ H ₈ SSi	thiophenoxy silane	SSiH ₃	7.12	7.04	6.96	12	5	x	100	79
174	C ₆ H ₈ Si	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 ₇ H ₅ BrO	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 ₇ H ₅ ClO	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 ₇ H ₅ Cl 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^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

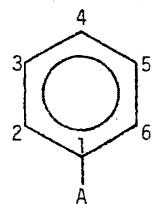


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
186	C ₇ H ₅ Cl 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 ₇ H ₅ FO	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 ₇ H ₅ F 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 ₇ H ₅ N	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 ₇ H ₅ NO	phenyl isocyanate	NCO	6.985	7.216	7.090	4	10	36	60	95
199	C ₇ H ₆ F ₂	benzal fluoride	CHF ₂	7.204	7.037	7.068	6	15	30	100	22
200	C ₇ H ₆ O	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)

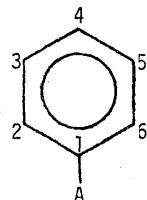


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Entry No.	Molecular Formula	Name	A	δ_H^a			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
204	C ₇ H ₆ O	benzaldehyde	CHO	7.788	7.438	7.526	4	25.4	x ^d	100	51
205			CHO	7.81	7.45	7.54	5	x ^d	x	100	85
206	C ₇ H ₆ O ₂	benzoic acid	CO ₂ H	8.11	7.44	7.53	4	0 ^e	x	100	65
207			CO ₂ H	8.081	7.510	7.624	8	1.0M	x	100	9
208			CO ₂ H	8.059	7.498	7.612	8	10	36	60	95
209	C ₇ H ₇ NO	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 ₇ H ₈	toluene	CH ₃	6.973	7.085	7.004	1(=20)	100	36	60	95
212	C ₇ H ₈ O	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 ₇ H ₈ O ₃ S	methyl benzenesulfonate	SO ₂ OCH ₃	7.936	7.596	7.672	1	90	x	100	52
220			SO ₂ OCH ₃	7.859	7.511	7.588	4	0	x	100	51
221	C ₇ H ₈ O ₃ S	phenol methanesulfonate	OSO ₂ CH ₃	7.21	7.33	7.25	4	0	x	100	65
222	C ₇ H ₈ S	thioanisole	SCH ₃	7.10	7.07	6.93	12	5	x	100	79

PROTON CHEMICAL SHIFTS, δ_H^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

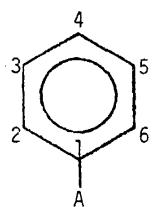


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
223	C ₇ H ₉ N	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 ₈ H 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 ₈ H 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 ₈ H ₈ DNO	acetanilide-d	CH ₃ COND	7.644	7.237	6.999	8	11	x	100	23
232	C ₈ H ₈ O	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 ₈ H ₈ O ₂	methyl benzoate	CO ₂ CH ₃	8.051	7.352	7.455	1	90	x	100	52
238			CO ₂ CH ₃	8.037	7.339	7.440	1	100	36	60	95
239			CO ₂ CH ₃	8.03	7.40	7.51	3	13	x	100	3
240		methyl benzoate- <u>carboxyl</u> - ¹³ C	¹³ CO ₂ CH ₃	8.03	7.40	7.52	3	13	x	100	3
241		methyl benzoate	CO ₂ CH 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)

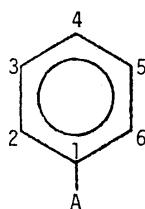


Table I

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				2,6 (ortho)	3,5 (meta)	4 (para)					
242	C ₈ H ₈ O ₂	methyl benzoate	CO ₂ CH ₃	7.974	7.342	7.445	4	10	36	60	95
243			CO ₂ CH ₃	8.016	7.496	7.618	8	1.0M	x ^d	100	9
244	C ₈ H ₈ O 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 ₈ H ₈ O ₂	phenylacetic acid	CH ₂ CO ₂ H	7.305	7.295	7.233	8	1.0M	x	100	12
248	C ₈ H ₉ NO	acetanilide	NHCOCH ₃	7.44	7.25	7.04	3	0	x	100	65
249	C ₈ H 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 ₈ H ₁₁ O ₃ P	dimethyl phenylphosphonate	PO(OCH ₃) ₂	7.724	7.403	7.483	4	10	36	60	95
254	C ₉ H ₁₀ O	allyloxybenzene	OCH ₂ CH=CH ₂	6.806	7.133	6.832	1	90	x	100	52
255	C ₉ H 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 ₉ H ₁₀ O	propiophenone	COCH ₂ CH ₃	7.891	7.344	7.438	1	90	x	100	52

PROTON CHEMICAL SHIFTS, δ_H^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

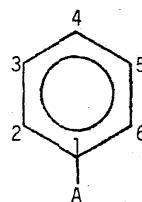


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Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
258	C ₉ H ₁₀ O	propiophenone	COCH ₂ CH ₃	7.880	7.380	7.452	4	0 ^e	x ^d	100	51
259	C ₉ H ₁₄ IN	trimethylanilinium iodide	N ⁺ (CH ₃) ₃ I ⁻	7.979	7.658	7.604	22	15	36	60	28
260	C ₉ H ₁₅ NO ₄ S	amphetamine sulfate	CH ₂ CH(CH ₃) ⁺ NH ₃ HSO ₄ ⁻	7.32*	7.43*	7.36*	30*	0.25M	21	250	61
261	C ₁₀ H ₁₂ O ₂	isopropyl benzoate	CO ₂ CH(CH ₃) ₂	8.056	7.331	7.418	1	90	x	100	52
262			CO ₂ CH(CH ₃) ₂	7.957	7.348	7.443	4	0	x	100	51
263	C ₁₀ H ₁₄	<u>tert</u> -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-C ₅ H ₄ N ⁺	7.984	7.335	7.272	4	1-2M	37	60	70
266	C ₁₁ H ₁₄ O ₂	isobutyl benzoate	CO ₂ CH ₂ CH(CH ₃) ₂	7.970	7.364	7.457	4	0	x	100	51
267	C ₁₂ H ₅ D ₅	biphenyl-d ₅	C ₆ D ₅	7.581	7.416	7.324	3	5	28	60	56
268			C ₆ D ₅	7.440	7.265	7.170	25	5	28	60	56
269	C ₁₂ H ₉ NO	2-benzoylpyridine	CO-(2-C ₅ H ₄ N) ⁺	8.115	7.372	7.461	4	20	35	60	43
270	C ₁₂ H ₁₀	biphenyl	C ₆ H ₅	7.59	7.41	7.32	3	5	28	60	56
271			C ₆ H ₅	7.479	7.320	7.224	4	5	36	60	95
272			C ₆ H ₅	7.468	7.301	7.207	4	10	36	60	95
273			C ₆ H 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.

^t2-C₅H₄N=2-pyridyl.

PROTON CHEMICAL SHIFTS, δ_H^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

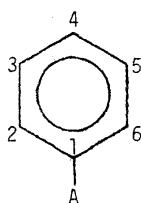


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
274	C ₁₂ H ₁₀ Cl ₂ Ge	dichlorodiphenylgermane	Ge(C ₆ H ₅)Cl ₂	7.555	7.030	7.073	6	5	33	100	74
275	C ₁₂ H ₁₀ Cl ₂ Si	dichlorodiphenylsilane	Si(C ₆ H ₅)Cl ₂	7.646	7.050	7.103	6	5	33	100	74
276	C ₁₂ H ₁₀ Cl ₂ Sn	dichlorodiphenylstannane	Sn(C ₆ H ₅)Cl ₂	7.385	7.041	7.069	6	5	33	100	74
277	C ₁₂ H ₁₀ F ₂ Si	difluorodiphenylsilane	Si(C ₆ H ₅)F ₂	7.57	7.06	7.15	6	5	33	100	74
278	C ₁₂ H ₁₀ Hg	diphenylmercury	HgC ₆ H ₅	7.256	7.263	7.055	7	10	36	60	95
279	C ₁₂ H ₁₀ Mg	diphenylmagnesium	MgC ₆ H 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 ₆ H 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 ₆ H ₅	7.883	7.406	7.347	4	10	36	60	95
282	C ₁₂ H ₁₀ O	diphenyl ether	OC ₆ H ₅	6.925	7.094	6.895	1	100	36	60	28
283			OC ₆ H ₅	6.925	7.218	6.977	4	10	36	60	28
284	C ₁₂ H ₁₀ S	diphenyl sulfide	SC ₆ H ₅	7.204	7.056	7.004	1	90	x	100	52
285			SC ₆ H ₅	7.255	7.025	6.979	1	100	36	60	95
286	C ₁₂ H ₁₀ S ₂	diphenyldisulfide	S ₂ C ₆ H ₅	7.500	7.277	7.200	3	5	38	60	72
287			S ₂ C ₆ H ₅	7.298	7.032	6.963	7	5	38	60	72
288			S ₂ C ₆ H ₅	7.427	7.187	7.113	8	5	38	60	72
289	C ₁₂ H ₁₀ Zn	diphenylzinc	ZnC ₆ H ₅	7.57	7.19	7.16	10	x	x	60	77
290	C ₁₂ H ₂₀ Ge	phenyltriethylgermane	Ge(C ₂ H ₅) ₃	7.34	7.20	7.20	4	33	x	60 or 100	99
291	C ₁₂ H ₂₀ Pb	phenyltriethylplumbane	Pb(C ₂ H ₅) ₃	7.37	7.20	7.11	4	33		60 or 100	99

PROTON CHEMICAL SHIFTS, δ_H^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

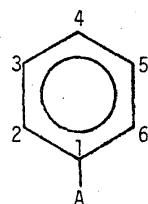
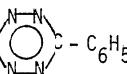


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
292	C ₁₂ H ₂₀ Si	phenyltriethylsilane	Si(C ₂ H 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 ₂ H 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 ₆ H ₅)Cl ₂	7.584	6.986	6.963	6	5	33	100	74
295	C ₁₃ H ₁₀ O	benzophenone	COOC ₆ H ₅	7.702	7.363	7.452	4	20	36	60	63
296	C ₁₃ H ₁₀ O ₂	phenyl <u>benzoate</u>	CO ₂ C ₆ H ₅	8.147	7.425	7.527	4	5	36	60	95
297			CO ₂ C ₆ H ₅	8.137	7.407	7.509	4	10	36	60	95
298	C ₁₃ H ₁₀ O ₂	<u>phenyl</u> benzoate	OCOC ₆ H ₅	7.160	7.339	7.173	4	5	36	60	95
299			OCOC ₆ H ₅	7.154	7.327	7.162	4	10	36	60	95
300	C ₁₄ H ₁₀	diphenylacetylene	C≡C-C ₆ H ₅	7.458	7.251	7.224	4	7	36	60	30
301			C≡C-C ₆ H 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	COOCOC ₆ H ₅	7.919	7.444	7.563	4	5	36	60	95
304			COOCOC ₆ H ₅	7.903	7.423	7.547	4	10	36	60	95
305			COOCOC ₆ H ₅	8.115	7.372	7.461	4	18	36	60	95
306			COOCOC ₆ H ₅	7.971	7.602	7.747	8	10	36	60	95
307	C ₁₄ H ₁₂	<u>trans</u> -stilbene	(trans) CH=CHC ₆ H ₅	7.417	7.260	7.161	4	2	36	60	95

PROTON CHEMICAL SHIFTS, δ_H^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

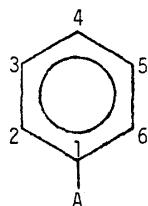


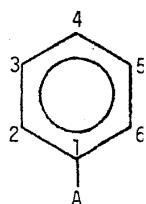
Table I

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

* Low concentration - saturated solution; ^{e†}R- = ; [§] shift not reported; ^{f†}C₃N₂(C₆H₅)(CH₃) = 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			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
323	C ₁₈ H ₁₅ OP	triphenylphosphine oxide	PO(C ₆ H ₅) ₂	7.672	7.419	7.492	3	15	36	60	95
324	C ₁₈ H ₁₅ P	triphenylphosphine	P(C ₆ H ₅) ₂	7.236	6.934	6.926	6	12	32	100	86
325	C ₁₈ H ₁₅ P	triphenylphosphine	P(C ₆ H ₅) ₂	7.372	7.051	7.042	6	55	31	100	64
326	C ₁₈ H ₁₆ OSi	triphenylsilanol	Si(C ₆ H ₅) ₂ OH	7.560	7.248	7.248	10	5	29	100	97
327	C ₁₈ H ₁₆ Si	triphenylsilane	Si(C ₆ H ₅) ₂ H	7.512	7.275	7.309	10	5	29	100	97
328	C ₁₉ H ₁₅ N ₃	azidotriphenylmethane	C(C ₆ H ₅) ₂ N ₃	7.28	7.28	7.28	3	5	33	100	74
329			C(C ₆ H ₅) ₂ N ₃	7.292	7.037	6.998	6	5	33	100	74
330	C ₁₉ H ₁₈ OSi	triphenylmethoxysilane	Si(C ₆ H ₅) ₂ OCH ₃	7.573	7.282	7.325	10	5	29	100	97
331	C ₁₉ H ₁₈ Si	methyltriphenylsilane	SiCH ₃ (C ₆ H ₅) ₂	7.218	6.969	6.948	12	95	36	60	95
332	C ₂₀ H ₁₈ Ge	vinyltriphenylgermane	(C ₆ H ₅) ₂ Ge-CH=CH ₂	7.422	7.272	7.277	4	6	33	100	74
333	C ₂₀ H ₁₈ Pb	vinyltriphenylplumbane	(C ₆ H ₅) ₂ Pb-CH=CH ₂	7.510	7.315	7.227	4	6	33	100	74
334	C ₂₀ H ₁₈ Si	vinyltriphenylsilane	(C ₆ H ₅) ₂ Si-CH=CH ₂	7.457	7.267	7.300	4	6	33	100	74
335	C ₂₀ H ₁₈ Sn	vinyltriphenylstannane	(C ₆ H ₅) ₂ Sn-CH=CH ₂	7.488	7.282	7.268	4	6	33	100	74
336	C ₂₁ H ₁₈	1,1,1-triphenylpropene	(C ₆ H ₅) ₂ C-CH=CH ₂	7.037	7.182	7.122	4	6	33	100	74
337			(C ₆ H ₅) ₂ C-CH=CH ₂	7.152	7.068	7.023	6	5	33	100	74
338	C ₂₄ H ₂₀ Ge	tetraphenylgermane	Ge(C ₆ H ₅) ₃	7.600	7.168	7.180	6	5	49	56.4	74
339	C ₂₄ H ₂₀ Pb	tetraphenylplumbane	Pb(C ₆ H ₅) ₃	7.630	7.219	7.125	6	5	57	56.4	74
340	C ₂₄ H ₂₀ Si	tetraphenylsilane	Si(C ₆ H ₅) ₃	7.652	7.172	7.203	6	5	30	56.4	74
341			Si(C ₆ H ₅) ₃	7.641	7.173	7.194	6	5	40	56.4	74

PROTON CHEMICAL SHIFTS, δ_H^α , IN MONOSUBSTITUTED
BENZENES (AND IN BENZENE ITSELF)

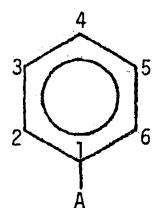


Table I

Entry No.	Molecular Formula	Name	A	δ_H^α			Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				2,6 (ortho)	3,5 (meta)	4 (para)					
342	C ₂₄ H ₂₀ Sn	tetraphenylstannane	Sn(C ₆ H ₅) ₃	7.607	7.177	7.174	6	5	60	56.4	74
343	C ₂₅ H ₂₀	tetraphenylmethane	C(C ₆ H ₅) ₃	7.324	7.060	6.995	6	5	60.5	56.4	74
344	C ₂₈ H ₂₈ Sn	tetrabenzyltin	CH ₂ Sn(CH ₂ C ₆ H 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.

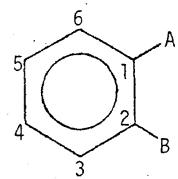
PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENESSubstituent Arrangement: OR^HO

Table II

Entry No.	Molecular Formula	Name	δ_H^α				Solvent Code ^d	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.		
			A	B	3	4	5	6					
001	C ₆ H ₄ BrCl	<u>o</u> -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 ₆ H ₄ BrF	<u>o</u> -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 ₆ H ₄ BrI	<u>o</u> -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 ₆ H ₄ BrNO ₂	<u>o</u> -bromonitrobenzene	NO ₂	Cl	7.71	7.40	7.44	7.78	4	x ^d	x	x ^d	7
015	C ₆ H ₄ Br ₂	<u>o</u> -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 ₆ H ₄ ClF	<u>o</u> -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^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

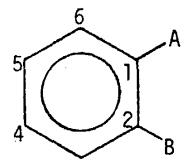


Table II

Entry No.	Molecular Formula	Name	A	B	δ_H^α				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					3	4	5	6					
021	C ₆ H ₄ ClI	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 ₆ H ₄ ClNO 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 ₆ H ₄ Cl 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 ₆ H ₄ FI	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 ₆ H ₄ FNO ₂	o-fluoronitrobenzene	NO ₂	F	7.31	7.66	7.33	8.03	4	10	x	60	39
035	C ₆ H ₄ F 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 ₆ H ₄ INO ₂	o-iodonitrobenzene	NO ₂	I	7.99	7.29	7.36	7.80	4	x	x	x	7
040	C ₆ H ₄ I ₂	o-diiodobenzene	I	I	7.81	6.96	6.96	7.81	4	5-10	40	60	33

PROTON CHEMICAL SHIFTS, δ_H^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

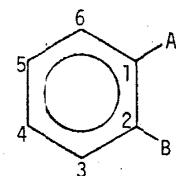
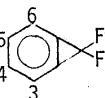


Table II

Entry No.	Molecular Formula	Name	A	B	δ_H^{α}				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					3	4	5	6					
041	C ₆ H ₄ I ₂	<u>o</u> -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 ₆ H ₄ N ₂ O ₄	<u>o</u> -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 ₆ H ₅ BrO	<u>o</u> -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 ₆ H ₅ ClO	<u>o</u> -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 ₆ H ₅ I ₀	<u>o</u> -iodophenol	OH	I	7.59	6.61	7.17	6.94	4	10	x	60	38
052	C ₆ H ₅ NO ₃	<u>o</u> -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 ₆ H ₆ BrN	<u>o</u> -bromoaniline	NH ₂	Br	7.32	6.51	6.99	6.61	4	10	x	100	40
056	C ₆ H ₆ C1N	<u>o</u> -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 ₆ H ₆ C1N	<u>o</u> -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^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

Entry No.	Molecular Formula	Name	A	e	B	δ_H^{α}				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
						3	4	5	6					
061	C ₆ H ₆ N	<u>o</u> -iodoaniline	NH ₂	I		7.53	6.36	7.01	5.58	4	10	x ^d	100	40
062			NH ₂	I		7.51	6.31	7.04	5.77	5	10	x	100	40
063	C ₆ H ₆ N ₂ O ₂	<u>o</u> -nitroaniline	NH ₂	NO ₂		8.07	6.65	7.30	5.79	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 ₆ H ₆ O ₂	<u>o</u> -dihydroxybenzene	OH	OH		6.777	6.842	6.842	5.777	3	1M	x	100	89
066			OH	OH		6.678	6.824	6.824	5.678	8	10	36	60	29
067			OH	OH		6.96*	6.88*	6.88*	5.96*	30	0.2M	22	250	82
068	C ₆ H ₆ S ₂	<u>o</u> -benzenedithiol	SH	SH		7.209	6.907	6.907	7.209	3	1M	x	100	89
069	C ₇ H ₄ BrN	<u>o</u> -bromobenzonitrile	CN	Br		7.67	7.45	7.43	7.63	4	x ^d	x	x ^d	7
070	C ₇ H ₄ CIN	<u>o</u> -chlorobenzonitrile	CN	Cl		7.50	7.53	7.38	7.64	4	x	x	x	7
071	C ₇ H ₄ Cl ₄	<u>o</u> -trichloromethylchlorobenzene	Cl	CCl ₃		8.14	7.27	7.31	7.48	4	10	x	100	40
072	C ₇ H ₄ FN	<u>o</u> -cyanofluorobenzene	F	CN		7.62	7.29	7.63	7.22	4	10	x	60	39
073	C ₇ H ₄ F ₂	7,7-difluorobenzocyclopropene		e		7.483	7.606	7.606	7.483	4	25	x	100	90
074	C ₇ H ₅ BrO	<u>o</u> -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 ₇ H ₅ BrOTe	<u>o</u> -formylphenyl tellurium bromide	TeBr	CHO	8.14	7.52	7.64	8.36	7	10	x	100	60	
077	C ₇ H ₅ BrO ₂	<u>o</u> -bromobenzoic acid	CO ₂ H	Br	7.725	7.438	7.481	7.801	5	10	x	60 or 100	75	

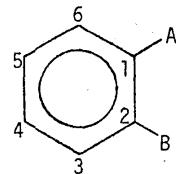
*Shifts measured relative to DSS (sodium 2,2-dimethyl-2-silapentane-5-sulfonate) and converted to normal δ -scale.

Table II

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

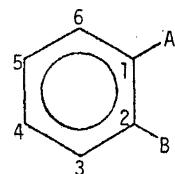


Table II

Entry No.	Molecular Formula	Name	A	ϵ	B	δ_H^α				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
						3	4	5	6					
078	C ₇ H ₅ ClO	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 ₇ H ₅ ClOTe	o-formylphenyl tellurium chloride	TeCl		CHO	8.18	7.51	7.68	8.37	7	0 ^e	x	100	60
081	C ₇ H ₅ ClO ₂	o-chlorobenzoic acid	CO ₂ H		Cl	7.546	7.533	7.439	7.838	5	10	x	60 or 100	75
082	C ₇ H ₅ F0	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 ₇ H ₅ I0	o-iodobenzaldehyde	CHO		I	7.89	7.23	7.42	7.82	4	10	x	100	4
085	C ₇ H ₅ I0Te	o-formylphenyl tellurium iodide	TeI		CHO	8.02	7.54	7.56	8.28	7	0	x	100	60
086	C ₇ H ₅ I0 ₂	o-iodobenzoic acid	CO ₂ H		I	8.012	7.247	7.499	7.779	5	10	x	60 or 100	75
087	C ₇ H ₅ N0 ₃	o-nitrobenzaldehyde	CHO		NO ₂	8.15	7.75	7.78	7.88	4	10	x	100	4
088	C ₇ H ₅ N0 ₄	o-nitrobenzoic acid	CO ₂ H		NO ₂	7.999	7.791	7.819	7.917	5	10	x	60 or 100	75
089	C ₇ H ₆	benzocyclopropene		e		7.149	7.189	7.189	7.149	3	15	x	100	5
090	C ₇ H ₆ N 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 ₇ H ₆ O 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

Substituent Arrangement: ORTHO

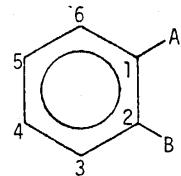


Table II

Entry No.	Molecular Formula	Name	δ_H^a						Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
			A	B	3	4	5	6					
093	C ₇ H ₆ O ₂	<u>o</u> -hydroxybenzaldehyde	CHO	OH	6.90	7.43	6.92	7.45	4	10	x ^d	100	4
094	C ₇ H ₆ O ₃	<u>o</u> -hydroxybenzoic acid	CO ₂ H	OH	7.05	7.56	6.97	7.97	3	x ^d	x	60	48
095			CO ₂ H	OH	6.98	7.53	6.95	7.85	5	x	x	60	48
096			CO ₂ H	OH	6.961	7.518	6.933	7.908	8	1.0M	x	100	9
097	C ₇ H ₇ Br	<u>o</u> -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 ₇ H ₇ BrO	<u>o</u> -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 ₇ H ₇ Cl	<u>o</u> -chlorotoluene	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 ₇ H ₇ ClO	<u>o</u> -chloranisole	OCH ₃	Cl	7.26	6.80	7.10	6.81	4	x	x	x	7
104	C ₇ H ₇ I	<u>o</u> -iodotoluene	CH ₃	I	7.73	6.78	7.14	7.15	4	5	x	100	67
105	C ₇ H ₇ I ₂ O	<u>o</u> -iodoanisole	OCH ₃	I	7.69	6.61	7.20	6.71	4	x	x	x	7
106	C ₇ H ₇ NO	<u>o</u> -aminobenzaldehyde	CHO	NH ₂	6.54	7.17	6.61	7.35	4	10	x	100	4
107	C ₇ H ₇ NO ₂	<u>o</u> -nitrotoluene	CH ₃	NO ₂	7.90	7.29	7.43	7.29	4	5	x	100	67
108			CH ₃	NO ₂	7.87	7.29	7.44	7.29	4	10	x	100	40
109	C ₇ H ₇ NO ₃	<u>o</u> -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 ₇ H ₈ O	<u>o</u> -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

Substituent Arrangement: ORTHO

Entry No.	Molecular Formula	Name
112	C ₇ H ₈ O	<u>o</u> -cresol
113	C ₇ H ₈ O ₂	<u>o</u> -methoxyphenol
114		
115	C ₇ H ₉ N	<u>o</u> -toluidine
116		
117	C ₇ H ₉ NO	<u>o</u> -methoxyaniline
118		
119	C ₈ H ₄ Br ₄	tetrabromobenzocyclobutene
120	C ₈ H ₄ N ₂	<u>o</u> -phthalonitrile
121	C ₈ H ₄ O ₂	benzocyclobutadienequinone
122	C ₈ H ₄ O ₃	phthalic anhydride
123	C ₈ H ₅ NO ₂	phthalimide

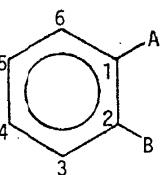


Table II

				δ_H^a	Solvent Code ^b				Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.	
					A	B	3	4	5	6			
112	C ₇ H ₈ O	<u>o</u> -cresol	OH	CH ₃	6.99	6.73	6.92	6.59	4	10	x ^d	100	40
113	C ₇ H ₈ O ₂	<u>o</u> -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 ₇ H ₉ N	<u>o</u> -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 ₇ H ₉ NO	<u>o</u> -methoxyaniline	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 ₈ H ₄ Br ₄	tetrabromobenzocyclobutene			7.503	7.303	7.303	7.503	3	15	x	100	5
120	C ₈ H ₄ N ₂	<u>o</u> -phthalonitrile	CN	CN	7.81	7.75	7.75	7.81	4	x ^d	x	x ^d	7
121	C ₈ H ₄ O ₂	benzocyclobutadienequinone			8.080	7.856	7.856	8.080	3	15	x	100	5
122	C ₈ H ₄ O ₃	phthalic anhydride			8.10	8.04	8.04	8.10	5	x	x	100	85
123	C ₈ H ₅ NO ₂	phthalimide			7.75	7.75	7.75	7.75	5	x	x	100	85

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

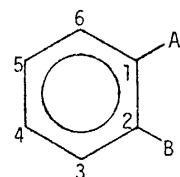


Table II

Entry No.	Molecular Formula	Name	A ^e	B ^e	δ_H^α				Solvent Code ^d	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					3	4	5	6					
124	C ₈ H ₆ Br ₂	<u>cis</u> -dibromobenzocyclobutene			7.382	7.190	7.190	7.382	3	15	x ^d	100	5
125	C ₈ H ₆ Br ₂	<u>trans</u> -dibromobenzocyclobutene			7.348	7.140	7.140	7.348	3	15	x	100	5
126	C ₈ H ₆ O ₂	<u>o</u> -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 ₈ H ₆ O ₂	phthalide			7.92	7.44	7.62	7.49	5	x	x	100	85
129	C ₈ H ₆ O ₄	phthalic acid	CO ₂ H	CO ₂ H	7.70	7.57	7.57	7.70	5	x	x	100	85
130	C ₈ H ₇ BrO	<u>o</u> -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 ₈ H ₇ ClO	<u>o</u> -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 ₈ H ₇ ClO	<u>o</u> -tolyl chloride	COCl	CH ₃	7.23	7.44	7.30	8.17	4	5	x	100	67
135	C ₈ H ₇ FO	<u>o</u> -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 ₈ H ₇ I0	<u>o</u> -iodoacetophenone	COCH ₃	I	7.86	7.05	7.34	7.67	4	10	x	100	4

PROTON CHEMICAL SHIFTS, δ_H^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

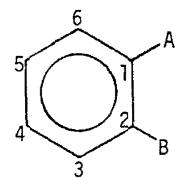


Table II

Entry No.	Molecular Formula	Name	A	^e	B	δ_H^{α}				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
						3	4	5	6					
138	C ₈ H ₇ I0	<u>o</u> -iodoacetophenone	COCH ₃		I	7.97	7.23	7.51	7.66	5	10	x ^d	100	4
139	C ₈ H ₇ N	<u>o</u> -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 ₈ H ₇ NO ₃	<u>o</u> -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 ₈ H ₈	benzocyclobutene		e		6.907	6.764	6.764	6.907	3	15	x	100	5
144	C ₈ H ₈ O	<u>o</u> -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 ₈ H ₈ OTe	<u>o</u> -formylphenyl methyl telluride	TeCH ₃		CHO	7.53	7.36	7.32	7.74	7	0	x	100	60
147	C ₈ H ₈ O ₂	<u>o</u> -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 ₈ H ₈ O ₂	<u>o</u> -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 ₈ H ₈ O ₂	<u>o</u> -toluic acid	CO ₂ H		CH ₃	7.20	7.37	7.22	8.06	4	5	x	100	67
152			CO ₂ H		CH ₃	7.293	7.438	7.293	7.877	5	10	x	60 or 100	75
153	C ₈ H ₈ O ₃	<u>o</u> -hydroxyphenylacetic acid	CH ₂ CO ₂ H		OH	6.842	7.072	6.782	7.164	8	1.0M	x	100	12
154	C ₈ H ₈ O ₃	<u>o</u> -methoxybenzoic acid	CO ₂ H		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

Substituent Arrangement: ORTHO

Entry No.	Molecular Formula	Name	δ_H^a						Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
			A	B	3	4	5	6					
155	C ₈ H ₈ O ₃	<u>o</u> -methoxybenzoic acid	CO ₂ H	OCH ₃	7.15	7.54	7.04	7.70	5	x ^d	x ^d	60	48
156			CO ₂ H	OCH ₃	7.114	7.496	7.009	7.690	5	10	x	60 or 100	75
157			CO ₂ H	OCH ₃	6.39	7.08	6.74	8.24	6	x	x	60	48
158	C ₈ H ₈ O ₃	methyl <u>o</u> -hydroxybenzoate	CO ₂ CH ₃	OH	7.02	7.48	6.91	7.86	3	x	x	60	48
159			CO ₂ CH ₃	OH	6.879	7.312	6.728	7.685	4	50	x	60	66
160			CO ₂ CH ₃	OH	7.01	7.54	6.96	7.81	5	x	x	60	48
161			CO ₂ CH ₃	OH	6.98	7.10	6.59	7.72	6	x	x	60	48
162			CO ₂ CH ₃	OH	6.957	7.506	6.916	7.821	8	1	x	100	9
163	C ₈ H ₉ Br	<u>o</u> -bromoethylbenzene	C ₂ H ₅	Br	7.45	6.96	7.14	7.14	4	5	x	100	67
164	C ₈ H ₉ NO	<u>o</u> -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 ₈ H ₉ NO ₂	N-methyl- <u>o</u> -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 ₈ H ₉ NO ₂	<u>o</u> -nitroethylbenzene	C ₂ H ₅	NO ₂	7.80	7.28	7.45	7.31	4	5	x	100	67
171	C ₈ H ₉ O	<u>o</u> -ethylphenol	OH	C ₂ H ₅	7.02	6.76	6.94	6.58	4	5	x	100	67
172	C ₈ H ₉ O	<u>o</u> -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

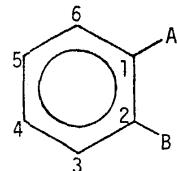


Table II

PROTON CHEMICAL SHIFTS, δ_H^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

Entry No.	Molecular Formula	Name
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174 $C_8H_{10}O_2$ o-dinethoxybenzene175 $C_8H_{11}N$ o-ethylaniline176 $C_8H_{11}N$ N-methyl-o-toluidine177 $C_9H_5D_3$ indene-1,1,3-d₃178 $C_9H_6O_2$ 1,3-indandione

179

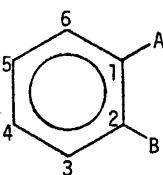
180 $C_9H_6O_4$ 2,2-dihydroxy-1,3-indandione181 C_9H_8O 1-indanone182 C_9H_8O 2-indanone183 $C_9H_8O_4$ o-acetoxybenzoic acid

Table II

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

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

Entry No.	Molecular Formula	Name
184	C_9H_9ClO	2-(<i>o</i> -chlorophenyl)oxetane
185		
186	C_9H_{10}	indan
187		
188	$C_9H_{10}O$	<i>o</i> -methylacetophenone
189		
190		
191	$C_9H_{10}O_2$	<i>o</i> -cresol acetate
192	$C_9H_{10}O_2$	<i>o</i> -methoxyacetophenone
193		
194	$C_9H_{10}O_2$	methyl <i>o</i> -toluate
195	$C_9H_{10}O_3$	<i>o</i> -methoxyphenylacetic acid
196	$C_9H_{10}O_3$	methyl <i>o</i> -methoxybenzoate
197		
198		

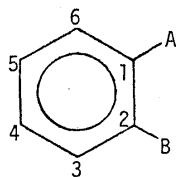


Table II

	A	e	B	δ_H^α				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.	
				3	4	5	6						
184		C1		7.27	7.15	7.24	7.68	4	2-5	x ^d	300	81	
185		"	C1	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	$C_9H_{10}O$	<i>o</i> -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	$C_9H_{10}O_2$	<i>o</i> -cresol acetate	OCOCH ₃	CH ₃	7.12	7.03	7.10	6.90	4	5	x	100	67
192	$C_9H_{10}O_2$	<i>o</i> -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 <i>o</i> -toluate	CO ₂ CH ₃	CH ₃	7.15	7.29	7.14	7.85	4	5	x	100	67
195	$C_9H_{10}O_3$	<i>o</i> -methoxyphenylacetic acid	CH ₂ CO ₂ H	OCH ₃	6.927	7.218	6.876	7.199	8	1.0M	x	100	12
196	$C_9H_{10}O_3$	methyl <i>o</i> -methoxybenzoate	CO ₂ CH ₃	OCH ₃	6.99	7.47	6.98	7.80	3	x	x	60	48
197			CO ₂ CH ₃	OCH ₃	7.16	7.54	7.03	7.66	5	x	x	60	48
198			CO ₂ CH ₃	OCH ₃	6.54	7.11	6.74	7.84	6	x	x	60	48

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

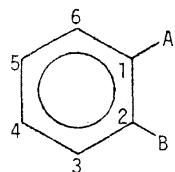


Table II

Entry No.	Molecular Formula	Name	A	B	δ_H^α				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Fred. (MHz)	Ref.
					3	4	5	6					
199	C ₉ H ₁₁ NO ₂	N-methyl- <i>o</i> -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 ₉ H ₁₂ O	<i>o</i> -isopropylphenol	OH	i-C ₃ H ₇	7.09	6.79	6.93	6.56	4	5	x	100	67
203	C ₉ H ₁₂ O	<i>o</i> -n-propylphenol	OH	n-C ₃ H ₇	7.00	6.75	6.94	6.59	4	5	x	100	67
204	C ₉ H ₁₃ N	N,N-dimethyl- <i>o</i> -toluidine	N(CH ₃) ₂	CH ₃	7.02	6.81	7.00	6.91	4	5	x	100	67
205	C ₁₀ H ₆ O ₂	1,4-naphthoquinone			8.218	7.905	7.905	8.218	3	15	x	100	5
206	C ₁₀ H ₈ D ₂ O	2,2-dideuterio- α -tetralone			7.876	7.148	7.297	7.098	4	15	32	100	83
207	C ₁₀ H ₈ D ₂ O	4,4-dideuterio- α -tetralone			7.870	7.150	7.300	7.100	4	15	32	100	83
208	C ₁₀ H ₈ O ₂	benzocyclohexene-1,4-dione			8.045	7.733	7.733	8.045	3	15	x	100	5

PROTON CHEMICAL SHIFTS, δ_H^a , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

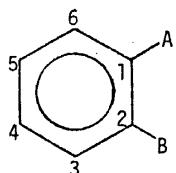


Table II

Entry No.	Molecular Formula	Name	δ_H^a				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.		
			A ^e	B ^e	3	4	5	6					
209	C ₁₀ H ₁₀ ⁰	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 α -methoxyphenylacetate	CH ₂ CO ₂ CH ₃	OCH ₃	6.929	7.224	6.875	7.174	8	1.0M	x	100	12
212	C ₁₀ H ₁₃ Br	α -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 ⁰	α -sec-butylphenol	OH	sec-C ₄ H ₉	7.05	6.79	6.93	6.58	4	5	x	100	67
214	C ₁₀ H ₁₄ ⁰	α -tert-butylphenol	OH	C(CH ₃) ₃	7.16	6.76	6.94	6.46	4	5	x	100	67
215	C ₁₂ H ₄ D ₅ Br	α -bromoperdeuteriophenylbenzene	C ₆ D ₅	Br	7.58	7.08	7.23	7.23	4	10	x	100	40
216	C ₁₂ H ₄ D ₅ Cl	α -chloroperdeuteriophenylbenzene	C ₆ D ₅	Cl	7.38	7.16	7.19	7.24	4	10	x	100	40
217	C ₁₂ H ₄ D ₅ F	α -fluoroperdeuteriophenylbenzene	C ₆ D ₅	F	7.04	7.17	7.07	7.33	4	10	x	100	40
218	C ₁₂ H ₄ D ₅ I	α -iodoperdeuteriophenylbenzene	C ₆ D ₅	I	7.87	6.92	7.27	7.21	4	10	x	100	40
219	C ₁₂ H ₄ D ₅ NO ₂	α -nitroperdeuteriophenylbenzene	C ₆ D ₅	NO ₂	7.71	7.36	7.48	7.33	4	10	x	100	40
220	C ₁₂ H ₅ D ₅ O	α -hydroxyperdeuteriophenylbenzene	C ₆ D ₅	OH	6.83	7.11	6.84	7.10	4	10	x	100	40
221	C ₁₂ H ₆ D ₅ N	α -aminoperdeuteriophenylbenzene	C ₆ D 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 ₈ Br ₂	α,α' -dibromobiphenyl	α -C ₆ H ₄ Br	Br	7.304	6.734	6.899	7.057	6	5	x	60	32

PROTON CHEMICAL SHIFTS, δ_H^a , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

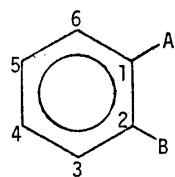
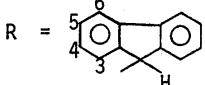


Table II

Entry No.	Molecular Formula	Name	A	<i>e</i>	B	δ_H^a				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
						3	4	5	6					
224	C ₁₂ H ₈ Cl ₂	o,o'-dichlorobiphenyl	o-C ₆ H ₄ Cl	Cl		7.155	6.815	6.874	7.138	6	5	x ^d	60	32
225	C ₁₂ H ₈ F ₂	o,o'-difluorobiphenyl	o-C ₆ H ₄ F	F		6.853	6.890	6.823	7.214	6	5	x	60	32
226	C ₁₂ H ₈ I ₂	o,o'-diiodobiphenyl	o-C ₆ H ₄ I	I		7.507	6.612	6.941	6.935	6	5	x	60	32
227	C ₁₂ H ₈ N ₂ O ₂ S	bis(o-nitrophenyl) sulfide	o-NO ₂ C ₆ H ₄ S	NO ₂		8.070	7.460	7.515	7.285	3	5-8	38	60	73
228	C ₁₂ H ₈ N ₂ O ₂ S ₂	bis(o-nitrophenyl) disulfide	o-NO ₂ C ₆ H ₄ S ₂	NO ₂		8.354	7.436	7.614	7.900	3	5-8	38	60	73
229	C ₁₂ H ₁₂ N ₂ S	bis(o-aminophenyl) sulfide	o-NH ₂ C ₆ H ₄ S	NH ₂		7.063	6.498	6.948	6.664	35	5-8	38	60	73
230	C ₁₂ H ₁₂ N ₂ S ₂	bis(o-aminophenyl) disulfide	o-NH ₂ C ₆ H ₄ S ₂	NH ₂		7.088	6.425	7.068	6.700	35	5-8	38	60	73
231	C ₁₃ H ₄ D ₅ N	o-cyanoperdeuteriophenylbenzene	C ₆ D ₅	CN		7.64	7.32	7.51	7.41	4	10	x	100	40
232	C ₁₃ H ₉ Br	9-bromofluorene		Br-R*		7.58	7.25	7.30	7.57	4	10	x	100	40
233	C ₁₃ H ₉ Cl	9-chlorofluorene		Cl-R*		7.54	7.22	7.27	7.52	4	10	x	100	40
234	C ₁₃ H ₉ I	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 ₈ Cl ₂	9-dichloromethylenefluorene	 ^e			8.22	7.20	7.27	7.54	4	10	x	100	40

* R =



PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

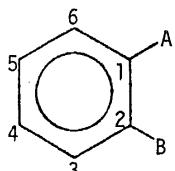
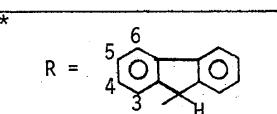


Table II

Entry No.	Molecular Formula	Name		A ^e	B ^e	δ_H^α				Solvent Code ^d	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
						3	4	5	6					
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 ₃ O-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	<u>o</u> -di- <i>t</i> -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	<u>o</u> -terphenyl		C ₆ H ₅	C ₆ H ₅	7.27	7.31	7.31	7.27	4	10	x	100	40
247	C ₂₀ H ₁₄	triptycene			CH ^e	7.228	6.855	6.855	7.228	7	2	29	60	6
248	C ₂₂ H ₂₂ O ₂ Te ₂	<u>o</u> -phenylene-bis[p-ethoxyphenyl-telluride]		A = B = p-C ₂ H ₅ OC ₆ H ₄ Te		7.255	6.902	6.902	7.255	3	1M	x	100	89



PROTON CHEMICAL SHIFTS, δ_H^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: ORTHO

Entry No.	Molecular Formula	Name
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249	$C_{26}H_{16}$	dibiphenylene ethylene
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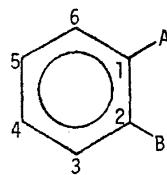
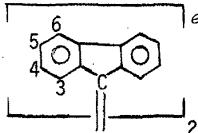


Table II

	A	e	B	δ_H^{α}				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				3	4	5	6					
				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.

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

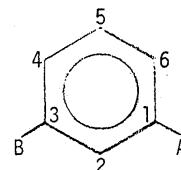


Table III

Entry No.	Molecular Formula	Name	A	B	δ_H^α				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2	4	5	6					
001	C ₆ H ₄ BrCl	m-bromochlorobenzene	Cl	Br	7.420	7.247	6.976	7.136	25	10	38	60	76
002	C ₆ H ₄ BrClMg	m-chlorophenylmagnesium bromide	MgBr	Cl	7.59	6.98	7.02	7.49	10	1M	x ^d	100	49
003	C ₆ H ₄ BrF	m-bromofluorobenzene	F	Br	7.141	7.163	7.032	6.856	25	10	38	60	31
004	C ₆ H ₄ BrFMg	m-fluorophenylmagnesium bromide	MgBr	F	7.41	6.67	7.06	7.34	10	1M	x	100	49
005	C ₆ H ₄ BrI	m-bromoiodobenzene	I	Br	7.771	7.312	6.767	7.481	25	10	38	60	76
006	C ₆ H ₄ BrNO 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 ₆ H ₄ Br ₂	m-dibromobenzene	Br	Br	7.581	7.292	6.916	7.292	25	10	38	60	76
020	C ₆ H ₄ ClF	m-chlorofluorobenzene	F	Cl	6.980	7.009	7.094	6.814	25	10	38	60	31

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

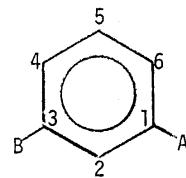
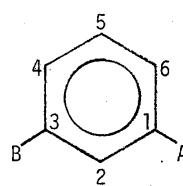


Table III

Entry No.	Molecular Formula	Name	A	B	δ_H^α				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2	4	5	6					
021	C ₆ H ₄ ClI	m-chloriodobenzene	I	Cl	7.626	7.170	6.836	7.454	25	10	38	60	76
022	C ₆ H ₄ ClLi	m-chlorophenyllithium	Li	Cl	7.90	6.94	6.97	7.81	10	1M	x ^d	100	49
023	C ₆ H ₄ ClNO ₂	m-chloronitrobenzene	NO ₂	Cl	8.076	7.532	7.368	7.997	25	10	38	60	76
024	C ₆ H ₄ Cl ₂	m-dichlorobenzene	Cl	Cl	7.270	7.104	7.051	7.104	25	10	38	60	76
025	C ₆ H ₄ FI	m-fluoroiodobenzene	I	F	7.337	6.884	6.881	7.362	25	10	38	60	31
026	C ₆ H ₄ F 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 ₆ H ₄ I ₂	m-diiodobenzene	I	I	8.001	7.537	6.648	7.537	25	10	38	60	76
029	C ₆ H ₄ Li ₂	m-dilithiobenzene	Li	Li	9.60	7.62	6.68	7.62	27	0.5M	x	60	37
030	C ₆ H ₄ N ₂ O 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	8.536	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	8.562	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^α , IN DISUBSTITUTED BENZENES

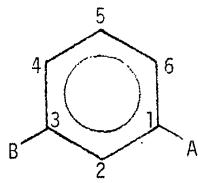
Substituent Arrangement: META

Entry No.	Molecular Formula	Name	A	B	δ_H^α				Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2	4	5	6					
041	C ₆ H ₆ N ₂ O ₂	m-nitroaniline	NH ₂	NO ₂	7.516	7.445	7.258	6.943	2	0 ^d	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 ₇ H ₄ BrF ₃ Mg	m-trifluoromethylmagnesium bromide	MgBr	CF ₃	7.98	7.24	7.28	7.90	10	1M	x ^d	100	49
051	C ₇ H ₄ F ₃ Li	m-trifluoromethylphenyllithium	Li	CF ₃	8.17	7.03	7.07	8.05	10	1M	x	100	49
052	C ₇ H ₅ BrO	m-bromobenzaldehyde	CHO	Br	7.720	7.478	7.196	7.596	1	90	x	60	59
053	C ₇ H ₅ BrO ₂	m-bromobenzoic acid	CO ₂ H	Br	8.104	7.806	7.480	7.991	5	10	x	60 or 100	75
054	C ₇ H ₅ ClO ₂	m-chlorobenzoic acid	CO ₂ H	Cl	7.955	7.667	7.543	7.949	5	10	x	60 or 100	75
055	C ₇ H ₅ FO	m-fluorobenzaldehyde	CHO	F	7.576	7.389	7.589	7.736	8	30	30	100	21
056	C ₇ H ₅ I0	m-iodobenzaldehyde	CHO	I	8.072	7.781	7.234	7.839	1	90	x	60	59
057	C ₇ H ₅ NO ₄	m-nitrobenzoic acid	CO ₂ H	NO ₂	8.626	8.449	7.819	8.354	5	10	x	60 or 100	75

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

Table III



Entry No.	Molecular Formula	Name	A	B	δ_H^α					Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2	4	5	6						
058	C ₇ H ₆ O ₃	m-hydroxybenzoic acid	CO ₂ H	OH	7.476	7.069	7.325	7.482	5	10	x ^d	60 or 100	75	
059			CO ₂ H	OH	7.572	7.123	7.347	7.576	8	1.0M	x	100	9	
060	C ₇ H ₇ Br	m-bromotoluene	CH ₃	Br	7.26	7.22	7.03	7.00	4	5	x	100	67	
061	C ₇ H ₇ BrMg	m-tolylmagnesium bromide	MgBr	CH ₃	7.45	6.79	6.93	7.39	10	1M	x	100	49	
062	C ₇ H ₇ BrMgO	m-anisylmagnesium bromide	MgBr	OCH ₃	7.22	6.57	7.02	7.21	10	1M	x	100	49	
063	C ₇ H ₇ Cl	m-chlorotoluene	CH ₃	Cl	7.10	7.06	7.09	6.95	4	5	x	100	67	
064	C ₇ H ₇ I	m-iodotoluene	CH ₃	I	7.48	7.42	6.90	7.03	4	5	x	100	67	
065	C ₇ H ₇ Li	m-tolyllithium	Li	CH ₃	7.86	6.80	6.95	7.80	10	1M	x	100	49	
066	C ₇ H ₇ LiO	m-anisyllithium	Li	OCH ₃	7.64	6.52	7.00	7.53	10	1M	x	100	49	
067	C ₇ H ₇ NO ₂	m-nitrotoluene	CH ₃	NO ₂	7.98	7.96	7.37	7.43	4	5	x	100	67	
068	C ₇ H ₈ O	m-cresol	OH	CH ₃	6.53	6.63	6.99	6.52	4	5	x	100	67	
069	C ₇ H ₉ N	m-toluidine	NH ₂	CH ₃	6.31	6.42	6.89	6.29	4	5	x	100	67	
070	C ₈ H ₇ Br	m-bromostyrene	CH=CH ₂	Br	7.415	7.248	7.073	7.183	7	5	x	100	62	
071	C ₈ H ₇ ClO	m-toluyl chloride	COCl	CH ₃	7.86	7.42	7.34	7.88	4	5	x	100	67	
072	C ₈ H ₇ N	m-tolunitrile	CN	CH ₃	7.41	7.34	7.31	7.39	4	5	x	100	67	
073	C ₈ H ₈ O	m-tolualdehyde	CHO	CH ₃	7.61	7.35	7.35	7.59	4	5	x	100	67	
074	C ₈ H ₈ O ₂	m-toluic acid	CO ₂ H	CH ₃	7.90	7.33	7.29	7.89	4	5	x	100	67	
075			CO ₂ H	CH ₃	7.831	7.417	7.385	7.810	5	10	x	60 or 100	75	

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

Entry No.	Molecular Formula	Name	A	B	δ_H^α					Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2	4	5	6						
076	C ₈ H ₈ O ₃	m-hydroxyphenylacetic acid	CH ₂ CO ₂ H	OH	6.818	6.724	7.109	6.766	8	1.0M	x ^d	100	12	
077	C ₈ H ₈ O ₃	m-methoxybenzoic acid	CO ₂ H	OCH ₃	7.531	7.193	7.425	7.610	5	10	x	60 or 100	75	
078	C ₈ H ₉ Br	m-bromoethylbenzene	C ₂ H ₅	Br	7.27	7.23	7.06	7.03	4	5	x	100	67	
079	C ₈ H ₉ NO ₂	m-nitroethylbenzene	C ₂ H ₅	NO ₂	8.00	7.98	7.40	7.46	4	5	x	100	67	
080	C ₈ H ₁₀ O	m-ethylphenol	OH	C ₂ H ₅	6.56	6.65	7.01	6.54	4	5	x	100	67	
081	C ₈ H ₁₀ O	m-methylanisole	OCH ₃	CH ₃	6.59	6.63	7.03	6.57	4	5	x	100	67	
082	C ₈ H ₁₁ N	m-ethylaniline	NH ₂	C ₂ H ₅	6.40	6.48	6.91	6.38	4	5	x	100	67	
083	C ₈ H 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 ₉ H ₁₀ O	m-methylacetophenone	COCH ₃	CH ₃	7.67	7.26	7.25	7.65	4	5	x	100	67	
085	C ₉ H 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 ₉ H ₁₀ O ₂	methyl m-toluate	CO ₂ CH ₃	CH ₃	7.78	7.26	7.24	7.75	4	5	x	100	67	
087	C ₉ H ₁₀ O ₃	m-methoxyphenylacetic acid	CH ₂ CO ₂ H	OCH ₃	6.893	6.805	7.206	6.875	8	1.0M	x	100	12	
088	C ₉ H ₁₀ O ₃	methyl m-methoxybenzoate	CO ₂ CH ₃	OCH ₃	7.518	7.171	7.396	7.583	8	1.0M	x	100	9	
089	C ₉ H 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 ₂ CH 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 ₂ CO ₂ CH 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 ₂ CO ₂ CH ₃	OCOCH ₃	7.055	7.012	7.321	7.156	8	1.0M	x	100	12	
093	C ₁₂ H ₈ Br ₂	m,m'-dibromobiphenyl	m-C ₆ H ₄ Br	Br	7.548	7.225	6.813	7.143	6	5	x	60	32	

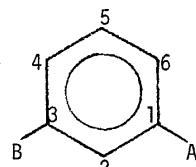


Table III

PROTON CHEMICAL SHIFTS, δ_H^a , IN DISUBSTITUTED BENZENES

Substituent Arrangement: META

Entry No.	Molecular Formula	Name	A	B	δ_H^a				Solvent Code ^b	Spect.			
					2	4	5	6		Concn. ^c (%)	Temp. (°C)	Freq. (MHz)	Ref.
094	C ₁₂ H ₈ Cl ₂	m,m'-dichlorobiphenyl	m-C ₆ H ₄ Cl	Cl	7.398	7.075	6.894	7.118	6	5	x ^d	60	32
095	C ₁₂ H ₈ F ₂	m,m'-difluorobiphenyl	m-C ₆ H ₄ F	F	7.097	6.774	6.970	7.067	6	5	x	60	32
096	C ₁₂ H ₈ I ₂	m,m'-diiodobiphenyl	m-C ₆ H ₄ I	I	7.751	7.427	6.691	7.185	6	5	x	60	32
097	C ₁₂ H ₁₈	m-tert-butylethylbenzene	C ₂ H ₅	C(CH ₃) ₃	6.76	6.85	7.04	6.55	4	5	x	100	67
098	C ₁₅ H ₁₂ N ₂ O ₂	cinnamaldehyde m-nitroanil	N=CHCH=CHC ₆ H ₅	NO ₂	7.98	7.99	7.46	7.35	4	x ^d	x	100	13
099			N=CHCH=CHC ₆ H ₅	NO ₂	7.82	7.72	6.81	7.10	6	x	x	100	13
100			N=CHCH=CHC ₆ H ₅	NO ₂	7.80	7.91	7.42	7.34	7	x	x	100	13

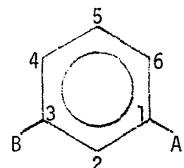
^a Usual δ -scale. See text, section 2, item 5.^b See Table V and text, section 2, item 6.^c Concentration is given in percent unless number is followed by "M", molarity. The designation "0" refers to the shift at "infinite dilution". See text, section 2, item 7.^d The designation "x" means unknown or unspecified.

Table III

PROTON CHEMICAL SHIFTS, δ_H^a , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

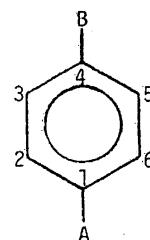


Table IV

Entry No.	Molecular Formula	Name	A	B	δ_H^a		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
001	C ₆ H ₄ BrCl	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 ₆ H ₄ BrClMg	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 ₆ H ₄ BrF	p-bromofluorobenzene	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 ₆ H ₄ BrFMg	p-fluorophenylmagnesium bromide	MgBr	F	7.62	6.88	10	1M	x	100	49
011	C ₆ H ₄ BrI	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 ₆ H ₄ BrNO 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 ₆ H ₄ Br 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^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

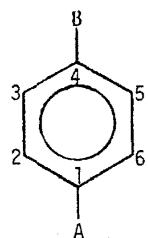


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^q	Concn. ^c (%)	Temp. ^b (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
019	C ₆ H ₄ Br 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 ₆ H ₄ Br ₂ Mg ₂	p-bis(bromomagnesio)benzene	MgBr	MgBr	7.70	7.70	27	0.5M	x ^d	60	37
022	C ₆ H ₄ ClF	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 ₆ H ₄ ClI	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 ₆ H ₄ ClLi	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 ₆ H ₄ ClNO ₂	p-chloronitrobenzene	NO ₂	Cl	8.29	7.71	8	8	25	60	78
030	C ₆ H ₄ Cl 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 ₆ H ₄ Cl ₂ FP	p-fluorophenyldichlorophosphine	PCl ₂	F	7.46	6.72	6	30	32	100	91
036	C ₆ H ₄ D ^b BrMg	p-deuteriophenylmagnesium bromide	MgBr	D	7.64	7.02	10	1.0M	33	60	36
037	C ₆ H ₄ DLi	p-deuteriophenyllithium	Li	D	8.02	7.02	10	1.0M	33	60	36

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

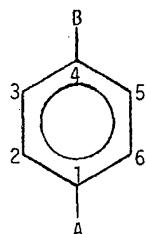


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
038	C ₆ H ₄ FI	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 ₆ H ₄ FLi	p-fluorophenyllithium	Li	F	7.98	6.85	10	1M	x ^d	100	49
041	C ₆ H ₄ FNO 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 ₆ H ₄ F 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 ₆ H ₄ INO 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 ₆ H ₄ I 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 ₆ H ₄ N ₂ O ₄	p-dinitrobenzene	NC ₂	NO ₂	8.34	8.34	3	x	x	x	2
050	C ₆ H ₅ BrO	p-bromophenol	OF	Br	6.60	7.25	3	x	x	x	2
051	C ₆ H ₅ ClNO ₂	p-chloronitrobenzene	NC ₂	Cl	8.11	7.45	3	x	x	x	2
052	C ₆ H ₅ ClO	p-chlorophenol	OF	Cl	6.64	7.12	3	x	x	x	2
053			OF	Cl	6.68	7.14	4	10	x	100	40
054			OF	Cl	6.87	7.17	8	25	25	60	78
055	C ₆ H ₅ FO	p-fluorophenol	OF	F	6.72	6.92	3	x	x	x	2
056	C ₆ H ₅ NO ₃	p-nitrophenol	OF	NO ₂	6.92	8.10	3	x	x	x	2

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

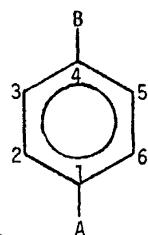


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
057	C ₆ H ₅ NO ₃	p-nitrophenol	OH	NO ₂	6.69	7.83	8	11	25	60	78
058	C ₆ H ₆ BrN	p-bromoaniline	NH ₂	Br	6.61	7.15	8	13	25	60	78
059	C ₆ H ₆ FN	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 ₆ H ₆ IN	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 ₆ H ₆ N ₂ O 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 ₆ H ₆ OS	p-hydroxybenzenethiol	SH	OH	7.066	6.644	3	1M	x	100	89
067	C ₆ H ₆ O ₂	p-hydroquinone	OH	OH	7.11	7.11	12	2	40	60	34
068	C ₇ H ₄ BrClO	p-bromobenzoyl chloride	COCl	Br	7.92	7.63	3	x	x	x	2
069	C ₇ H ₄ BrF ₃ Mg	p-trifluoromethylphenylmagnesium bromide	MgBr	CF ₃	7.82	7.30	10	1M	x	100	49
070	C ₇ H ₄ ClFO	p-fluorobenzoyl chloride	COCl	F	8.06	7.14	3	x	x	x	2
071	C ₇ H ₄ ClFO	p-chlorobenzoyl fluoride	COF	Cl	7.935	7.462	10	x	31	100	15
072	C ₇ H ₄ ClF ₃	p-trifluoromethylchlorobenzene	Cl	CF ₃	7.51	7.48	4	10	x	100	40
073	C ₇ H ₄ ClIO	p-iodobenzoyl chloride	COCl	I	7.78	7.78	3	x	x	x	2
074	C ₇ H ₄ CIN	p-chlorobenzonitrile	CN	Cl	7.56	7.43	3	x	x	x	2

PROTON CHEMICAL SHIFTS, δ_H^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

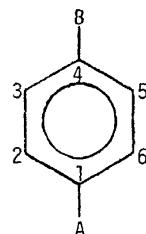


TABLE IV

Entry No.	Molecular Formula	Name			δ_H^{α}		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
			A	B	2,6	3,5					
075	C ₇ H ₄ ClNO 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 ₇ H ₄ Cl ₂ O	p-chlorobenzoyl chloride	COCl	Cl	7.94	7.41	3	x	x	x	2
078	C ₇ H ₄ Cl ₄	p-trichloromethylchlorobenzene	Cl	CCl ₃	7.36	7.86	4	10	x	100	40
079	C ₇ H ₄ FN	p-fluorobenzonitrile	CN	F	7.67	7.17	3	x	x	x	2
080	C ₇ H ₄ F ₃ Li	p-trifluoromethylphenyllithium	Li	CF ₃	8.05	7.23	10	1M	x	100	49
081	C ₇ H ₄ IN	p-iodobenzonitrile	CN	I	7.35	7.80	3	x	x	x	2
082	C ₇ H ₄ N ₂ O 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 ₇ H ₅ BrO ₂	p-bromobenzoic acid	CO ₂ H	Br	7.96	7.68	3	x	x	x	2
085			CO ₂ H	Br	7.925	7.707	5	10	x	60 or 100	75
086			CO ₂ H	Br	7.96	7.70	8	0.8	25	60	78
087	C ₇ H ₅ ClO ₂	p-chlorobenzoic acid	CO ₂ H	Cl	7.96	7.52	3	x	x	x	2
088			CO ₂ H	Cl	8.018	7.543	5	10	x	60 or 100	75
089	C ₇ H ₅ FO	p-fluorobenzaldehyde	CHO	F	7.976	7.289	8	30	30	100	21
090	C ₇ H ₅ FO ₂	p-fluorobenzoic acid	CO ₂ H	F	8.03	7.29	3	x	x	x	2
091			CO ₂ H	F	8.089	7.304	5	10	x	60 or 100	75

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

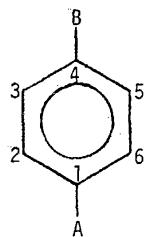


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^c	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
092	C ₇ H ₅ F ₂	p-fluorobenzoic acid	CO ₂ H	F	8.09	7.25	8	0.9	25	60	78
093	C ₇ H ₅ I ₂ O ₂	p-iodobenzoic acid	CO ₂ H	I	7.86	7.70	3	x ^d	x ^d	x ^d	2
094			CO ₂ H	I	7.898	7.765	5	10	x	60 or 100	75
095	C ₇ H ₅ NO	p-hydrcxybenzonitrile	CN	OH	7.51	6.95	3	x	x	x	2
096	C ₇ H ₅ N ₂ O ₃	p-nitrobenzaldehyde	CHO	NO ₂	8.22	8.44	8	7	25	60	78
097	C ₇ H ₆ N ₂	p-aminobenzonitrile	CN	NH ₂	7.30	6.57	3	x	x	x	2
098	C ₇ H ₆ O ₂	p-hydrcxybenzaldehyde	CHO	OH	7.82	7.04	8	9	25	60	78
099	C ₇ H ₆ O ₃	p-hydrcxybenzoic acid	CO ₂ H	OH	7.83	6.88	3	x	x	x	2
100			CO ₂ H	OH	7.889	6.904	5	10	x	60 or 100	75
101			CO ₂ H	OH	7.978	6.962	8	1.0M	x	100	9
102	C ₇ H ₇ Br	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 ₇ H ₇ BrMg	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^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

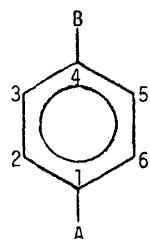


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
109	C ₇ H ₇ BrMg	p-tolylmagnesium bromide	MgBr	CH ₃	7.42	6.70	27	0.4M	x ^d	60	37
110	C ₇ H ₇ BrMgO	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 ₇ H ₇ BrO	p-bromoanisole	OCH ₃	Br	6.592	7.207	25	10	38	60	76
114	C ₇ H ₇ CaI	p-tolylicalcium iodide	CaI	CH ₃	8.24	6.96	27	0.5M	x	60	37
115	C ₇ H ₇ Cl	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 ₇ H ₇ ClO	p-chloroanisole	OCH ₃	Cl	6.65	7.09	1	100	25	60	78
120	C ₇ H ₇ Cl ₃ OSn	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 ₇ H ₇ Cl ₃ Si	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

Substituent Arrangement: PARA

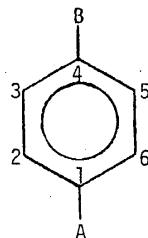


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^a		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
128	C ₇ H ₇ Cl ₃ Si	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 ₇ H ₇ Cl ₃ Sn	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 ₇ H ₇ F	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 ₇ H ₇ FO	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 ₇ H ₇ I	p-iodotoluene	CH ₃	I	6.86	7.54	3	x	x	x	2

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

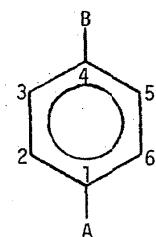


TABLE IV.

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
147	C ₇ H ₇ I	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 ₇ H ₇ IO	p-iodoanisole	OCH ₃	I	6.62	7.53	3	x ^d	x	x ^d	2
151	C ₇ H ₇ Li	p-tollyllithium	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 ₇ H ₇ LiO	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 ₇ H ₇ NO ₂	p-aminobenzoic acid	CO ₂ H	NH ₂	7.67	6.61	3	x	x	x	2
156			CO ₂ H	NH ₂	7.710	6.626	5	10	x	60 or 100	75
157	C ₇ H ₇ NO 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 ₇ H ₇ NO 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^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

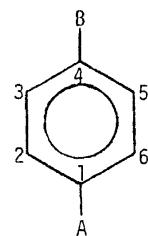


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^q	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
165	C ₇ H ₇ NO ₃	p-nitroanisole	OCH ₃	NO ₂	6.34	7.89	6	5	x	60	98
165			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 ₇ H ₈ O	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 ₇ H ₉ N	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
175			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 ₇ H ₉ NO	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 ₈ H ₅ NO ₂	p-cyano benzoic acid	CO ₂ H	CN	8.126	7.968	5	10	x	60 or 100	75
181	C ₈ H ₇ BrO ₂	methyl p-bromobenzoate	CO ₂ CH ₃	Br	7.82	7.52	3	x	x	x	2
182	C ₈ H ₇ ClO	p-tolyl chloride	COCl	CH ₃	7.91	7.22	3	x	x	x	2

PROTON CHEMICAL SHIFTS, δ_H^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

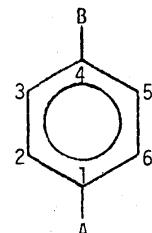


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^{α}		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
183	C ₈ H ₇ ClO	p-tolyl chloride	COCl	CH ₃	7.95	7.24	4	5	x ^d	100	67
184	C ₈ H ₇ ClO ₂	methyl p-chlorobenzoate	CO ₂ CH ₃	Cl	7.91	7.07	3	x ^d	x	x ^d	2
185	C ₈ H ₇ ClO ₂	p-methoxybenzoyl chloride	COCl	OCH ₃	7.94	6.89	3	x	x	x	2
186	C ₈ H ₇ F ₃	p-tolyl fluoride	COF	CH ₃	7.892	7.337	10	x	31	100	15
187	C ₈ H ₇ F ₃ O ₂	methyl p-fluorobenzoate	CO ₂ CH ₃	F	7.99	7.07	3	x	x	x	2
188	C ₈ H ₇ I ₂ O ₂	methyl p-iodobenzoate	CO ₂ CH ₃	I	7.70	7.70	3	x	x	x	2
189	C ₈ H ₇ LiN	p-dimethylaminophenyllithium	Li	N(CH ₃) ₂	7.91	6.69	10	0.5M	x	60	37
190	C ₈ H ₇ N	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 ₈ H ₇ NO	p-methoxybenzonitrile	CN	OCH ₃	7.56	6.97	3	x	x	x	2
195	C ₈ H ₇ NO ₂	p-nitrostyrene	CH=CH ₂	NO ₂	7.463	8.062	7	5	30	100	24
196	C ₈ H ₇ NO ₃	methyl p-nitrobenzoate	CO ₂ CH ₃	NO ₂	8.21	8.21	3	x	x	x	2
197	C ₈ H ₈ BrNO	p-bromoacetanilide	NHCOCH ₃	Br	7.77	7.39	3	x	x	x	2
198	C ₈ H ₈ ClNO	p-chloroacetanilide	NHCOCH ₃	Cl	7.80	7.23	3	x	x	x	2
199	C ₈ H ₈ FNO	p-fluoroacetanilide	NHCOCH ₃	F	7.60	6.93	3	x	x	x	2
200	C ₈ H ₈ INO	p-iodoacetanilide	NHCOCH ₃	I	7.58	7.58	3	x	x	x	2
201	C ₈ H ₈ O	p-tolualdehyde	CHO	CH ₃	7.69	7.25	4	5	x	100	67

PROTON CHEMICAL SHIFTS, δ_H^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

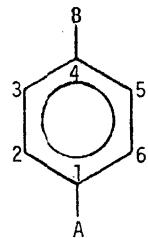


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^{α}		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
202	C ₈ H ₈ O ₂	p-hydroxyphenylacetic acid	CH ₂ CO ₂ H	OH	7.125	6.785	8	1.0M	x ^d	100	12
203	C ₈ H ₈ O ₂	p-methoxybenzaldehyde	CHO	OCH ₃	7.79	6.95	1	100	25	60	78
204	C ₈ H ₈ O ₂	p-toluic acid	CO ₂ H	CH ₃	7.88	7.30	3	x ^d	x	x ^d	2
205			CO ₂ H	CH ₃	7.98	7.20	4	5	x	100	67
206	C ₈ H ₈ O ₃	p-methoxybenzoic acid	CO ₂ H	OCH ₃	7.92	7.03	3	x	x	x	2
207			CO ₂ H	OCH ₃	7.964	7.026	5	10	x	60 or 100	75
208	C ₈ H ₈ O ₃	methyl p-hydroxybenzoate	CO ₂ CH ₃	OH	7.88	6.87	3	x	x	x	2
209	C ₈ H ₉ Br	p-methylbenzyl bromide	CH ₂ Br	CH ₃	7.12	7.00	7	11	x	60	92
210			CH ₂ Br	CH ₃	7.077	7.240	8	20	x	100	25
211	C ₈ H ₉ NC	p-aminoacetophenone	COCH ₃	NH ₂	7.77	6.71	8	13	25	60	78
212	C ₈ H ₉ NO ₂	p-ethylnitrobenzene	NO ₂	C ₂ H ₅	8.04	7.27	3	20	x	100	41
213			NO ₂	C ₂ H ₅	8.00	7.27	3	x	x	x	2
214	C ₈ H ₉ NO ₂	methyl p-aminobenzoate	CO ₂ CH ₃	NH ₂	7.79	6.61	3	x	x	x	2
215	C ₈ H 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^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

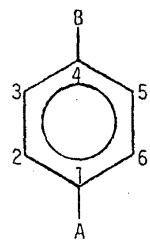


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
220	C ₈ H 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 ₈ H ₁₀ ClN	p-N,N-dimethylaminochlorobenzene	Cl	N(CH ₃) ₂	7.12	6.55	3	x	x	x	2
222	C ₈ H ₁₀ FN	p-N,N-dimethylaminofluorobenzene	F	N(CH ₃) ₂	6.86	6.55	3	x	x	x	2
223	C ₈ H ₁₀ IN	p-N,N-dimethylaminoiodobenzene	I	N(CH ₃) ₂	7.37	6.37	3	x	x	x	2
224	C ₈ H ₁₀ N ₂ O	N,N-dimethyl-p-nitrosoaniline*	N(CH ₃) ₂	NO	[*] s 7.01	^s 8.93	8	2	-56	60	68
					*a 6.71	a 6.62					
225			N(CH ₃) ₂	NO	^s 6.82	^s 8.91	3	2	-56(?)	60	69
					a 6.53	a 6.78					
226	C ₈ H ₁₀ N ₂ O 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 ₈ H 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 ₈ H ₁₁ N	N-methyl-p-toluidine	NHCH ₃	CH ₃	6.35	6.84	4	5	x	100	67
233	C ₉ H ₉ ClO	2-(p-chlorophenyl)oxetane	Cl CH ₂ O—CH ₂	Cl	7.28	7.28	4	2-5	x	300	81

*

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

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

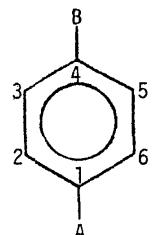


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
234	C ₉ H ₉ ClO	2-(<i>p</i> -chlorophenyl)oxetane	CH-CH ₂ O-CH ₂	C1	7.03	7.14	6	2-5	x ^d	300	81
235	C ₉ H ₉ ClO	<i>p</i> -ethylbenzoyl chloride	COCl	C ₂ H ₅	7.95	7.28	3	x ^d	x	x ^d	2
236	C ₉ H ₉ N	<i>p</i> -ethylbenzonitrile	CN	C ₂ H ₅	7.52	7.27	3	x	x	x	2
237	C ₉ H ₁₀ N ₂	<i>p</i> -N,N-dimethylaminobenzonitrile	CN	N(CH ₃) ₂	7.33	6.57	3	x	x	x	2
238	C ₉ H ₁₀ O	<i>p</i> -methoxystyrene	CH=CH ₂	OCH ₃	7.160	6.683	7	5	30	100	24
239	C ₉ H ₁₀ O	<i>p</i> -methylacetophenone	COCH ₃	CH ₃	7.75	7.16	4	5	x	100	67
240	C ₉ H ₁₀ O ₂	<i>p</i> -cresol acetate	OCOCH ₃	CH ₃	6.88	7.06	4	5	x	100	67
241	C ₉ H ₁₀ O ₂	<i>p</i> -ethylbenzoic acid	CO ₂ H	C ₂ H ₅	7.85	7.28	3	x	x	x	2
242	C ₉ H ₁₀ O ₂	methyl <i>p</i> -toluate	CO ₂ CH ₃	CH ₃	7.87	7.19	3	x	x	x	2
243			CO ₂ CH ₃	CH ₃	7.85	7.14	4	5	x	100	67
244			CO ₂ CH ₃	CH ₃	8.05	6.89	6	1-3	x	100	93
245			CO ₂ CH ₃	CH ₃	7.87	7.08	12	1-3	x	100	93
246	C ₉ H ₁₀ O ₃	<i>p</i> -methoxyphenylacetic acid	CH ₂ CO ₂ H	OCH ₃	7.208	6.853	8	1.0M	x	100	12
247	C ₉ H ₁₀ O ₃	methyl <i>p</i> -methoxybenzoate	CO ₂ CH ₃	OCH ₃	7.90	6.85	3	x	x	x	2
248			CO ₂ CH ₃	OCH ₃	7.952	6.999	8	1.0M	x	100	9
249	C ₉ H ₁₁ NO	N,N-dimethyl- <i>p</i> -aminobenzaldehyde	CHO	N(CH ₃) ₂	7.68	6.72	8	11	25	60	78
250	C ₉ H ₁₁ NO ₂	<i>p</i> -N,N-dimethylaminobenzoic acid	CO ₂ H	N(CH ₃) ₂	7.72	6.64	3	x	x	x	2
251	C ₉ H ₁₁ NO ₂	<i>p</i> -isopropylnitrobenzene	NO ₂	CH(CH ₃) ₂	8.13	7.38	3	20	x	100	41

PROTON CHEMICAL SHIFTS, δ_H^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

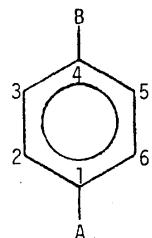


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^{α}		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
252	C ₉ H 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 ₉ H 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≡CH	6.985	7.341	6	5	30	100	24
257	C ₁₀ H ₁₀ O ₄	methyl p-acetoxybenzoate	CO ₂ CH 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 ₂ H	CH(CH ₃) ₂	7.88	7.33	3	x	x	x	2
261	C ₁₀ H ₁₂ O ₂	methyl p-ethylbenzoate	CO ₂ CH ₃	C ₂ H ₅	7.89	7.20	3	x	x	x	2
262	C ₁₀ H ₁₂ O ₃	methyl p-methoxyphenylacetate	CH ₂ CO ₂ CH 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 ₂ NS ₂ Sn	p-tolyldichlorotin N,N-dimethyl-dithiocarbamate	SnCl ₂ SCSN(CH ₃) ₂	CH ₃	7.80	7.36	2	x	21	60	87
266			SnCl ₂ SCSN(CH ₃) ₂	CH ₃	7.82	7.16	5	x	21	60	87
267			SnCl ₂ SCSN(CH ₃) ₂	CH ₃	7.78	7.39	8	x	21	60	87
268			SnCl ₂ SCSN(CH ₃) ₂	CH ₃	7.76	7.37	26	x	21	60	87
269			SnCl ₂ SCSN(CH ₃) ₂	CH ₃	7.57	7.17	27	x	21	60	87
270			SnCl ₂ SCSN(CH ₃) ₂	CH ₃	7.82	7.44	36	x	21	60	87

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

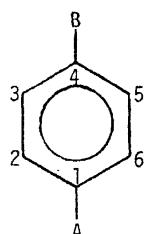


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Fred. (MHz)	Ref.
					2,6	3,5					
271	C ₁₀ H ₁₃ Cl ₃ Sn	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 ₂ O	N,N-diethyl-p-nitroaniline*	N(C ₂ H ₅) ₂	NO	^s 7.07 ^s 8.89 ^a 6.77 ^a 6.66		8	2	-56	60	68
281			N(C ₂ H ₅) ₂	NO	^s 6.83 ^s 8.86 ^a 6.54 ^a 6.84		3	2	-56(?)	60	69
282			N(C ₂ H ₅)	NO	^s 6.01 ^s 8.96 ^a 5.67 ^a 6.74		20	2	-56(?)	60	69
283	C ₁₁ H ₁₂ O ₄	methyl p-acetoxyphenylacetate	CH ₂ CO ₂ CH 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

Substituent Arrangement: PARA

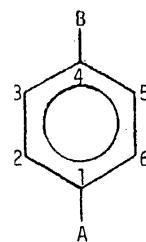


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^a		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
286	C ₁₁ H ₁₄ O ₂	p-tert-butylbenzoic acid	CO ₂ H	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 ₂ CH 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 ₃ H ₇	C ₂ H ₅	6.90	6.64	4	5	x	100	67
289	C ₁₂ H ₄ D ₅ C ₁	p-chloroperdeuteriophenylbenzene	C ₆ D ₅	Cl	7.39	7.30	4	10	x	100	40
290	C ₁₂ H ₄ D ₅ NO ₂	p-nitroperdeuterophenylbenzene	C ₆ D ₅	NO ₂	7.66	8.22	4	10	x	100	40
291	C ₁₂ H ₈ Br ₂	p,p'-dibromobiphenyl	p-C ₆ H ₄ Br	Br	7.057	7.304	6	1	x	60	32
292	C ₁₂ H ₈ C ₁ ₂	p,p'-dichlorobiphenyl	p-C ₆ H ₄ Cl	Cl	7.138	7.154	6	1	x	60	32
293	C ₁₂ H ₈ F ₂	p,p'-difluorobiphenyl	p-C ₆ H ₄ F	F	7.214	6.853	6	5	x	60	32
294			p-C ₆ H ₄ F	F	7.33	6.95	7	21	x	60	94
295	C ₁₂ H ₈ I ₂	p,p'-diiodobiphenyl	p-C ₆ H ₄ I	I	6.935	7.507	6	1	x	60	32
296	C ₁₂ H ₈ N ₂ O ₄ S	bis(p-nitrophenyl) sulfide	p-NO ₂ C ₆ H ₄ S	NO ₂	7.589	8.207	35	5-8	38	60	73
297	C ₁₂ H ₈ N ₂ O ₄ S ₂	bis(p-nitrophenyl) disulfide	p-NO ₂ C ₆ H ₄ S ₂	NO ₂	7.758	8.216	35	5-8	38	60	73
298	C ₁₂ H ₁₂ N ₂ S	bis(p-aminophenyl) sulfide	p-NH ₂ C ₆ H ₄ S	NH ₂	6.966	6.480	35	5-8	38	60	73
299	C ₁₂ H ₁₂ N ₂ S ₂	bis(p-aminophenyl) disulfide	p-NH ₂ C ₆ H ₄ S 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 ₂ CH ₃	C(CH ₃) ₃	7.89	7.39	3	x	x	x	2
301	C ₁₂ H ₁₈	p-sec-butylethylbenzene	C ₂ H ₅	sec-C ₄ H ₉	6.66	6.93	4	5	x	100	67
302	C ₁₂ H ₁₈	p-tert-butylethylbenzene	C ₂ H ₅	tert-C ₄ H ₉	6.66	7.13	4	5	x	100	67
303	C ₁₃ H ₁₁ NO ₂ S	p-tolylthio-p-nitrobenzene	NO ₂	p-CH ₃ C ₆ H ₄ S	8.02	7.83	3	x	x	60 or 100	80

PROTON CHEMICAL SHIFTS, δ_H^a , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

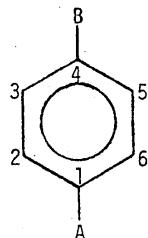
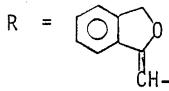


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^a		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
304	C ₁₄ H ₁₄ Cl ₂ Sn	di(p-tolyl)dichlorostannane	SnCl ₂ -p-CH ₃ C ₆ H ₄	CH ₃	7.54	7.33	2	x ^d	21	60	87
305			SnCl ₂ -p-CH ₃ C ₆ H ₄	CH ₃	7.77	7.14	5	x	21	60	87
306			SnCl ₂ -p-CH ₃ C ₆ H ₄	CH ₃	7.71	7.34	8	x	21	60	87
307			SnCl ₂ -p-CH ₃ C ₆ H ₄	CH ₃	7.46	7.18	12	x	21	60	87
308			SnCl ₂ -p-CH ₃ C ₆ H ₄	CH ₃	7.70	7.36	26	x	21	60	87
309			SnCl ₂ -p-CH ₃ C ₆ H ₄	CH ₃	7.65	7.41	36	x	21	60	87
310	C ₁₄ H ₁₄ N ₂ O ₃	p,p'-azoxyanisole (ring adjacent to NO)	p-CH ₃ O-C ₆ H ₄ -N-NO	OCH ₃	8.13	6.79	7	5	70	60	78
311	C ₁₄ H ₁₄ N ₂ O ₃	p,p'-azoxyanisole (ring remote from NO)	p-CH ₃ O-C ₆ H 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-bromophenyl)methylideneephthalide	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)methylideneephthalide	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 I ₂ O	3-(p-iodophenyl)methylideneephthalide	R*	I	7.84	7.63	8	.05M	24	80	84
318	C ₁₅ H ₁₁ I ₂ OS	3-(p-iodophenyl)thiomethylidene-phthalide	S-R*	I	7.37	7.79	8	.05M	24	80	84

*



PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

Entry No.	Molecular Formula	Name	R^*			δ_H^α		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
				A	B	2,6	3,5					
319	C ₁₅ H ₁₁ NO ₃	3-(<i>p</i> -nitrophenyl)methylidenephthalide	R [*]		NO ₂	8.32	8.08	8	.05M	24	80	84
320	C ₁₅ H ₁₁ NO ₃ S	3-(<i>p</i> -nitrophenyl)thiomethylidenephthalide	S-R [*]		NO ₂	7.80	8.27	8	.05M	24	80	84
321	C ₁₅ H ₁₂ BrN	cinnamaldehyde <i>p</i> -bromoanil	Br		N=CHCH=CHC ₆ H ₅	6.93	7.38	4	x ^d	x ^d	100	13
322			Br		N=CHCH=CHC ₆ H ₅	6.81	7.27	6	x	x	100	13
323			Br		N=CHCH=CHC ₆ H ₅	6.90	7.33	7	x	x	100	13
324	C ₁₅ H ₁₂ FN	cinnamaldehyde <i>p</i> -fluoroanil	F		N=CHCH=CHC ₆ H ₅	6.96	6.87	6	x	x	100	13
325	C ₁₅ H ₁₂ O ₂ S	3-(<i>p</i> -hydroxyphenyl)thiomethylidenephthalide	S-R [*]		OH	7.50	7.68	8	.05M	24	80	84
326	C ₁₅ H ₁₃ NO	3-(<i>p</i> -aminophenyl)methylidenephthalide	R [*]		NH ₂	7.61	6.72	8	.05M	24	80	84
327	C ₁₆ H ₁₄ O	3-(<i>p</i> -tolyl)methylidenephthalide	R [*]		CH ₃	7.75	7.25	8	.05M	24	80	84
328	C ₁₆ H ₁₄ OS	3-(<i>p</i> -tolyl)thiomethylidenephthalide	S-R [*]		CH ₃	7.23	7.45	8	.05M	24	80	84
329	C ₁₆ H ₁₄ O ₂	3-(<i>p</i> -anisyl)methylidenephthalide	R [*]		OCH ₃	7.83	7.02	8	.05M	24	80	84
330	C ₁₇ H ₁₅ NO	cinnamaldehyde <i>p</i> -acetylaniil	COCH ₃		N=CHCH=CHC ₆ H ₅	7.96	7.18	3	x	x	100	13
331			COCH ₃		N=CHCH=CHC ₆ H ₅	7.84	7.04	6	x	x	100	13
332	C ₁₇ H ₁₇ NO	cinnamaldehyde <i>p</i> -ethoxyaniil	OC ₂ H ₅		N=CHCH=CHC ₆ H ₅	6.75	7.02	4	x	x	100	13
333			OC ₂ H ₅		N=CHCH=CHC ₆ H ₅	6.83	7.22	6	x	x	100	13
334			OC ₂ H ₅		N=CHCH=CHC ₆ H ₅	6.40	6.66	7	x	x	100	13

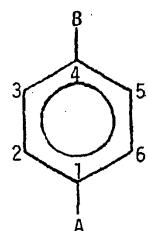
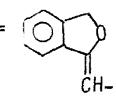
* *R* = 

TABLE IV

PROTON CHEMICAL SHIFTS, δ_H^α , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

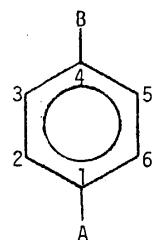


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^α		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
335	C ₁₈ H ₁₂ Br ₃ OP	tris-p-bromophenylphosphine oxide	PO(p-BrC ₆ H ₄) ₂	Br	7.50	7.64	2	0.5M	x ^d	60	44
336	C ₁₈ H ₁₂ Br ₃ P	tris-p-bromophenylphosphine	P(p-BrC ₆ H ₄) ₂	Br	7.14	7.47	x	0.5M	x	60	44
337	C ₁₈ H ₁₂ Br ₃ PS	tris-p-bromophenylphosphine sulfide	PS(p-BrC ₆ H ₄) ₂	Br	7.54	7.62	2	0.5M	x	60	44
338	C ₁₈ H ₁₂ C ₁₃ OP	tris-p-chlorophenylphosphine oxide	PO(p-ClC ₆ H ₄) ₂	Cl	7.59	7.47	3	0.5M	x	60	44
339	C ₁₈ H ₁₂ C ₁₃ P	tris-p-chlorophenylphosphine	P(p-ClC ₆ H ₄) ₂	Cl	7.19	7.30	3	0.5M	x	60	44
340	C ₁₈ H ₁₂ C ₁₃ PS	tris-p-chlorophenylphosphine sulfide	PS(p-ClC ₆ H ₄) ₂	Cl	7.63	7.44	2	0.5M	x	60	44
341	C ₁₈ H ₁₂ D ₃ OP	tris-p-deuteriophenylphosphine oxide	PO(p-DC ₆ H ₄) ₂	D	7.65	7.44	2	0.5M	x	60	44
342	C ₁₈ H ₁₂ D ₃ P	tris-p-deuteriophenylphosphine	P(p-DC ₆ H ₄) ₂	D	7.29	7.28	2	0.5M	x	60	44
343	C ₁₈ H ₁₂ D ₃ PS	tris-p-deuteriophenylphosphine sulfide	PS(p-DC ₆ H ₄) ₂	D	7.70	7.44	2	0.5M	x	60	44
344	C ₁₈ H ₁₂ F ₃ OP	tris(p-fluorophenyl)phosphine oxide	PO(p-FC ₆ H ₄) ₂	F	7.70	7.35	5	50	x	60	35
345	C ₁₈ H ₁₂ F ₃ P	tris-p-fluorophenylphosphine	P(p-FC ₆ H ₄) ₂	F	7.05	6.74	6	20	32	100	91
346	C ₁₈ H ₁₄	p-terphenyl	C ₆ H ₅	C ₆ H ₅	7.667	7.567	3	5	28	60	56
347	C ₁₉ H ₁₅ C ₁₃ IP	methyl(tris-p-chlorophenyl)phosphonium iodide	⁺ P(p-ClC ₆ H ₄) ₂ CH ₃ I ⁻	Cl	7.87	7.58	3	0.5M	x	60	44
348	C ₁₉ H ₁₅ D ₃ IP	methyl(tris-p-deuteriophenyl)phosphonium iodide	⁺ P(p-DC ₆ H ₄) ₂ CH ₃ I ⁻	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 ₂ H ₅	7.741	6.779	3	1M	x	100	89
350	C ₂₀ H ₁₈ F ₃ O ₃ P	dimethyl p-fluorophenylphosphonate	PO(OCH ₃) ₂ (p-FC ₆ H ₄) ₂	F	7.80	7.27	1	100	x	60	35
351			PO(OCH ₃) ₂ (p-FC ₆ H ₄) ₂	F	7.83	7.33	4	50	x	60	35

* R- = p-C₂H₅OC₆H₄Te-o-C₆H₄-Te-

PROTON CHEMICAL SHIFTS, δ_H^{α} , IN DISUBSTITUTED BENZENES

Substituent Arrangement: PARA

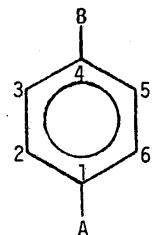


TABLE IV

Entry No.	Molecular Formula	Name	A	B	δ_H^{α}		Solvent Code ^b	Concn. ^c (%)	Temp. (°C)	Spect. Freq. (MHz)	Ref.
					2,6	3,5					
352	C ₂₁ H ₂₁ OP	tris-p-tolylphosphine oxide	PO(p-CH ₃ C ₆ H ₄) ₂	CH ₃	7.50	7.22	2	0.5M	x ^d	60	44
353	C ₂₁ H ₂₁ O ₃ P	tris-p-anisylphosphine	P(p-CH ₃ OC ₆ H ₄) ₂	OCH ₃	7.26	6.87	3	0.5M	x	60	44
354	C ₂₁ H ₂₁ O ₃ PS	tris-p-anisylphosphine sulfide	PS(p-CH ₃ OC ₆ H ₄) ₂	OCH ₃	7.62	6.92	3	0.5M	x	60	44
355	C ₂₁ H ₂₁ O ₄ P	tris-p-anisylphosphine oxide	PO(p-CH ₃ OC ₆ H 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-CH ₃ C ₆ H 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-CH ₃ C ₆ H ₄) ₂	CH ₃	7.56	7.18	2	1.0M	x	60	44
358	C ₂₂ H ₂₄ I ₀ ₃ P	methyl(tris-p-anisyl)phosphonium iodide	⁺ P(p-CH ₃ OC ₆ H ₄) ₂ CH ₃ I ⁻	OCH ₃	7.63	7.20	3	0.5M	x	60	44
359	C ₂₂ H ₂₄ IP	methyl(tris-p-tolyl)phosphonium iodide	⁺ P(p-CH ₃ C ₆ H ₄) ₂ CH ₃ I ⁻	CH ₃	7.62	7.53	2	0.5M	x	60	44
360	C ₂₄ H ₃₀ N ₃ OP	tris-p-dimethylaminophenylphosphine oxide	PO(p-(CH ₃) ₂ NC ₆ H 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

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

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