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Coal Liquefaction Process Streams Characterization and Evaluation

Estimation of Total Phenol Concentrations in Coal Liquefaction Resids by ^{31}P NMR Spectroscopy

Topical Report

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PROJECT ASSESSMENT

Introduction

Under subcontract from CONSOL Inc. (U.S. DOE Contract No. DE-AC22-89PC89883), Iowa State University used ^{31}P-tagged reagents for the speciation and quantification of the labile hydrogen functional groups, specifically the phenolic hydrogen, in tetrahydrofuran (THF)-soluble coal-derived samples. ^{31}P nuclear magnetic resonance (NMR) spectroscopy was used to analyze the derivatized samples. The full report authored by the Iowa State researchers is presented here. The following assessment briefly highlights the major findings of the project, and evaluates the potential of the method for application to coal derived materials. These results will be incorporated by CONSOL into a general overview of the application of novel analytical techniques to coal derived materials at the conclusion of this contract.

Summary

In this study, Iowa State University researchers used ^{31}P-tagged reagents to derivatize the labile hydrogen functional groups in the THF-soluble portion of $850°F^+$ distillation resid materials and the THF-soluble portion of process oils derived from direct coal liquefaction. ^{31}P-NMR was used to analyze the derivatized samples. NMR peak assignments can be made by comparison to model compounds similarly derivatized. Species can be quantified by integration of the NMR signals. Different ^{31}P-tagged reagents can be used to produce different degrees of peak resolution in the NMR spectrum. This, in turn, partially dictates the degree of speciation and/or quantification of species, or classes of compounds, that can be accomplished. Iowa State chose a ^{31}P-tagged reagent ($ClPOCMe_2CMe_2O$) which was shown previously to be particularly useful in the derivatization of phenols. The derivatized samples all exhibited a small group of peaks attributed to amines and a broad group of peaks in the phenol region. The presence of paramagnetic species in the samples caused the NMR signals to broaden. Electron paramagnetic resonance (EPR) spectra confirmed the presence of paramagnetic organic free radicals in selected samples. Various methods were employed to process the NMR data. The complexity and broadness of the phenol peak, however, made speciation of the phenols impractical. Quantification of

the total amount of phenol present in the sample was accomplished by integration. Values obtained agree well with Fourier transform infrared spectroscopic data obtained by CONSOL. Water in the samples also was derivatized by the ^{31}P reagent and quantified. Based on these results, further development of this analytical method as a process development tool may be justified if means are developed to improve resolution and speciate the component phenols.

Program Description

This report describes the work performed at Iowa State University under a subcontract from CONSOL Inc., Research and Development. CONSOL's prime contract to the U.S. Department of Energy (Contract No. DE-AC22-89PC89883, "Coal Liquefaction Process Streams Characterization and Evaluation") established a program for the analysis of direct coal liquefaction derived materials. The program involves a number of participating organizations whose analytical expertise is being applied to these materials. This Participants Program has two main objectives. The broad objective is to improve our understanding of fundamental coal liquefaction chemistry to facilitate process improvement and new process development. The specific approach to achieving this objective is to provide a bridge between direct coal liquefaction process development and analytical chemistry by demonstrating the application of various advanced analytical methods to coal liquefaction materials. The methodologies (or techniques) of interest are those which are novel in their application for the support of coal liquefaction and those which have not been fully demonstrated in this application. CONSOL is providing well-documented samples from different direct coal liquefaction production facilities to the program participants. The participants are required to interpret their analytical data in context to the processing conditions under which the samples were generated. The methodology employed is then evaluated for its usefulness in analyzing direct coal liquefaction derived materials.

Participant's Methodology

Iowa State University used ^{31}P-tagged reagents to speciate and quantify the labile hydrogen functional groups, specifically the phenolic hydrogen, present in the THF-soluble portion of (850°F^{+}) distillation resids and THF-soluble process oils. ^{31}P-NMR was used to analyze the derivatized samples. The samples were produced at the Wilsonville pilot plant. Two major processing parameters were varied among the Wilsonville runs. These were feed coal and reactor configuration (thermal/catalytic vs. catalytic/catalytic). Samples from Wilsonville were taken from three locations, between the first- and second-stage reactors, after the second-stage reactor, and at the recycle oil tank. These samples are expected to represent different extents of coal liquefaction. Ten of the samples were composites of samples taken over long periods of single runs. Five samples were obtained from single run periods. The experimental procedures are described on pages 24 through 27 of the attached report.

Participant's Major Findings

The following principal observations for the application of ^{31}P reagents and ^{31}P-NMR to coal liquefaction materials were reported by Iowa State. An expanded discussion can be found in the attached report, pages 3 through 15.

A curve-fitting program was applied to deconvolute the broad phenol region (138-144 ppm) of the spectra. Four different sets of parameters were used in the curve-fitting program: 1) line broadening parameter of 0.5 Hz, with no zero-filling factor; this resulted in approximately 100 peaks, making speciation impractical. 2) line-broadening parameter of 0.5 Hz and zero-filling factor; this resulted in narrow line widths, but a very large number of peaks (on the order of 150) in the phenol region. 3) line-broadening parameter of 2.5 Hz and no zero-filling factor; the number of phenol peaks was reduced by an order of magnitude, but the line widths were too broad to allow for speciation. 4) line-broadening parameter of 2.0 Hz and a zero-filling factor; this combination resulted in a small number of peaks that could be fitted; however, line widths were too broad for unambiguous identification of phenols. In all four cases, it was possible to quantify the total phenolic content, which was done by integration. An additional method, a Matched Filter Apodization (MPA) procedure with no zero-filling was used to process the NMR spectrum. This reduced the phenol region to, usually, one peak which was then quantified. Values obtained by the latter method agreed well with those obtained by CONSOL through the use of an FTIR method.

There appears to be four distinct sets of spectral groupings in the NMR spectra of the fifteen samples. These groups are defined by the presence (or absence) and intensity of peaks (or groups of peaks) at 139.2 ppm, 138.7 ppm, and 137.3 ppm. These four sets appear to correlate with the sampling location in the Wilsonville plant from which the samples were obtained. For example, of the six samples which fall into Group I, five were obtained from the interstage location. Similarly, three of the four samples in Group II were obtained from the second-stage product stream.

The presence of paramagnetic species in the coal-derived samples contributed to line broadening in the NMR spectra. EPR spectroscopy was used to examine the free radicals in the samples. The intensity of the organic free radical signal (at $g = 2.0036$) for different samples was found to correlate to the resolution of the ^{31}P-NMR spectra; the lower the intensity of the free radical signal, the better resolved was the NMR spectra. However, since the sample that was better resolved and had a lower free-radical content also had a lower boiling point, it may be that boiling point, and not free-radical content, primarily affected resolution.

The ^{31}P-tagged reagent used in this study forms an anhydride upon reaction with water. This compound has a distinct peak in the ^{31}P-NMR at 170 ppm. The small amount of water found in the samples most likely arises from adsorption from the atmosphere upon sample handling.

<u>CONSOL Evaluation</u>

The use of ^{31}P-tagged reagents to identify and quantify the labile hydrogen functionalities in coal-derived materials was demonstrated to a limited extent in this project. The total phenol contents determined by this method agree well with values obtained by an established FTIR method. It also is possible with this method to quantify water present in the samples. The method does show potential usefulness for the analysis of direct coal liquefaction resid samples. However, the appropriate choice of reagent and NMR data analysis technique must be further refined so that speciation of the phenolic groups can be made.

The NMR instrument used in this study cost about $300,000. Materials for reagent synthesis cost approximately $2.00 per sample. Approximately one week is required to synthesize enough reagent to perform fifty reactions. The ^{31}P NMR method is amenable to the use of a large variety of solvating agents for the samples, as long as they contain no labile hydrogen. Data manipulation with the MPA approach takes about 1 3/4 hr. Interpretation of the ^{31}P-NMR data requires a skilled professional.

Further Development

This technique appears to be a suitable means to quantify total phenols in coal liquids. However the possibility of phenol speciation was not realized. Future work should be directed toward that goal. Iowa State made the following recommendations for further work: 1) Utilization of different ^{31}P-tagged reagents that will allow for better differentiation of the amine and phenol region of the spectra, 2) Reduction of the free radical content of the samples (perhaps by hydrogenation) to reduce line broadening in the ^{31}P-NMR spectra. However, it would appear that this approach could reduce the phenols. 3) Further evaluation of the ^{31}P NMR spectral groupings in the phenolic region and their apparent correspondence to sampling location.

Participant's Statement of Work

Derivatization of labile hydrogen groups with phospholane reagents followed by analysis with ^{31}P-NMR spectroscopy is a method which has been used for the investigation of coal and coal pyrolysis products. However, it has not been widely applied to the analysis of direct coal liquefaction derived products, nor has it been demonstrated widely for its ability to answer questions pertaining to the chemistry of coal conversion. As such, it fits well within the scope of the participants program.

The application of phospholane derivatization/^{31}P-NMR spectroscopy to a sample set of 15 samples will allow a demonstration of the value of this technique for the speciation and quantitation of the labile hydrogen functional groups present in coal liquefaction-derived materials. These samples have been selected (see attached list) so that the utility of phospholane derivatization/^{31}P-NMR for characterizing coal liquefaction resids can be evaluated. Additionally, samples will be supplied so that the behavior of labile hydrogen groups can be evaluated as they pass through the direct coal liquefaction process. The samples will be supplied to the Iowa State University with the following information, as available: elemental analyses, phenolic -OH concentration by FTIR, calorific value, hydrogen classes by ^{1}H-NMR, and the full history of the sample (plant, process conditions, age, and storage conditions). Ten of the fifteen samples are tetrahydrofuran (THF)-soluble, non-distillable residual materials. Five of the samples will be the THF-soluble portion of whole process oils. Sample size will be at least 1 g. The resid samples will be brittle pitch-like materials that will be supplied as approximately minus 60 mesh powder. The whole process oils will be viscous liquids.

The phospholane reagents to be used will be selected by the Iowa State University researchers to provide the maximum qualitative and quantitative information on the labile hydrogen compound classes present in the resid samples. These compound classes will include phenols, alcohols, carboxylic acids, thiols and amines. Water content will be determined. Speciation and quantitation of individual compounds will be performed on Reference Nos. 10 and 11, which are distillable oils. Speciation and quantitation of individual compounds will be attempted on the other samples. Individual species or classes of labile hydrogen functional groups will be quantified by integration of the ^{31}P-NMR signals.

The sample set includes five samples (Reference Nos. 7-11) from Wilsonville Run 259G that represent all but one of the major product streams from both the first-stage and two-stage system. This set of samples will be analyzed to examine the behavior of the functional groups as they pass through the reactors in the two-stage liquefaction process.

Estimation of Total Phenol Concentrations in Coal Liquefaction Resids by ^{31}P NMR Spectroscopy

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Iowa State University

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Executive Summary

Fifteen coal liquefaction products are quantitatively analyzed for phenolics and moisture using the ^{31}P NMR tagging agent $\overline{ClPOCMe_2CMe_2O}$ (**1**). Despite the presence of organic free radicals in these resids, which contributed to the breadth of the derivatized phenolic ^{31}P resonances, excellent agreement with the phenolic contents obtained by FTIR spectroscopy[1a-c] was achieved. The best results were obtained by processing the ^{31}P NMR spectra with an NMR1 Matched Filter Apodization program.

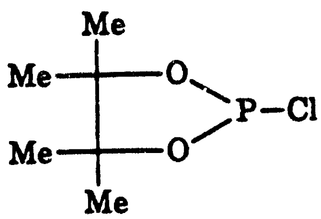
Thiols derivatized with **1** give rise to ^{31}P NMR peaks (209-218 ppm) well outside the range for phenolics (138-144 ppm,[9] and peaks for the former were not detected. Since the alcohol region with **1** (141-149 ppm,[9] overlaps slightly with the phenolic range, the presence of some alcohols such as Ph_3COH and pinacol cannot be ruled out. Aromatic and aliphatic carboxylic acids derivatized with **1** appear to give rise to ^{31}P NMR peaks in a very narrow range (135-136 ppm).[9] A small ^{31}P NMR peak at about 132 ppm appeared in all the samples except Nos. 10 and 11. This peak is probably due to amine (130-150 ppm).[9] The origin of the prominent ^{31}P NMR peak at 137 ppm in samples such as 10, 11 and 15 is not presently clear since it falls just outside the range of carboxylic acids and phenols. While the peak could be due to the presence of amines, it seems unlikely they would be present in such relatively high concentrations. Of course, the 137 ppm peak could be due to a phenols(s) we simply never measured as a model compound.

Background

Coal liquefaction processes require monitoring of process performance. One approach to accomplishing this goal is to selectively quantitate a chemical component such as phenolic OH. With the use of FTIR spectroscopy, the phenolic OH contents in a wide range of coal liquefaction samples were quantitatively assessed by employing THF as a solvent.[1a,b] Comparison of the FTIR results with those from similar studies using a ^{19}F NMR tagging reagent[2] revealed problematic discrepancies, however.[1c] Thus there was good agreement for many samples but substantial disagreement in samples containing high phenolic contents.[1d] On the other hand, quantitations of phenolic OH contents in a series of H-coal distillates and vacuum bottoms by three NMR tagging techniques (^{19}F, ^{29}Si and ^{31}P) compared favorably.[3] In that study, $Cl(O)PPh_2$ was concluded to be the reagent of choice because of the stability of its phenolic derivatives (compared with the instability over time of the corresponding derivatives of $F_3CC(O)Cl$) and the 100% natural abundance of ^{31}P compared with ^{29}Si (4.70%).

In previous publications[4-9] we have described a variety of NMR spectroscopic tagging reagents for the analysis and estimation of compounds containing labile hydrogen functional groups, and in particular the potential usefulness of reagents **1**[5,6,9] and **2**[7-9] in the quantitative estimation of phenols. Herein, we apply reagent **1** to the estimation of the phenol content in a series of fifteen coal liquefaction resids and we compare our results with those obtained for the same samples by FTIR spectroscopy.[1a,b] We also demonstrate the usefulness of reagent **1** in determining the moisture contents of these liquefaction resids. In the reaction associated with this analysis, the reagent **1** derivatizes water to form the anhydride of **1**, namely **3**.[9]

Although **2** provides more than twice the ^{31}P NMR dispersion for phenols, reagent **1** was chosen for this study since the peaks were too severely broadened by paramagnetic impurities for reagent **2** to be very useful.



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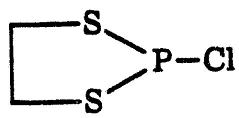

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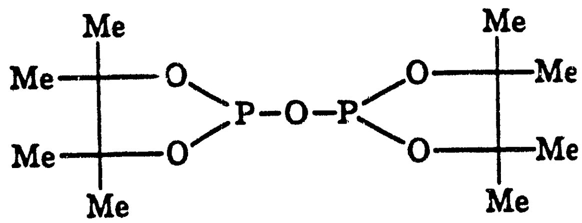

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Results and Discussion

To obtain reliable quantitative data from ^{31}P NMR spectroscopy, the following 5 conditions must be satisfied:

1. Complete derivatization with the NMR tagging reagent, as was shown earlier,[9] must be achieved.

2. Thermal equilibrium must be reached by the nuclei to be quantitated. This was accomplished by using relaxation delays at least five times greater than the longest T_1.[11] In the present study this delay was fixed at 3.0 s.

3. To reduce the relaxation time of the derivatized phenols to less than 0.5 s, 1 mole % of $Cr(acac)_3$ (based on reagent **1**) should be employed.

4. The recommended[11] signal-to-noise ratio of greater than 250 was achieved by optimizing the number of scans to 64 for the model phenol mixtures and 1000 scans for the derivatized coal product samples. In the case of some samples, signal-to-noise ratios of up to 5000 were achieved.

5. Broad band decoupling, should be employed to eliminate errors that are likely to arise from the nuclear Overhauser effect.

In this study, the concentration of each phenol in the model mixture was calculated as:

$$\frac{\text{meq phenolic O}}{\text{g coal material}} = \frac{I_{\text{derivatized phenol}}}{I_{\text{derivatized } l\text{-menthol}}} \times \frac{\text{meq } l\text{-menthol O}}{\text{g coal material}} \qquad (1)$$

where I refers to the relative intensity of the integral for the derivatized phenolic region and the meq of *l*-menthol oxygen is calculated from the weight of *l*-menthol used and its molecular weight. The meq values of amine nitrogen and moisture oxygen were calculated analogously, except in the last case where half of the corresponding integral was taken, since there are two replaceable hydrogens in H_2O and 3 is formed. The choice of *l*-menthol as the internal standard has been addressed earlier.[9]

A number of model mixtures containing different phenols were prepared in order to optimize the NMR parameters. The results obtained with an example of such a model mixture is tabulated in Table I. The use of more than 1 mole % of $Cr(acac)_3$ relative to 1 increased the linewidths of the individual signals, thereby introducing further error in the quantitative data.

The ^{31}P NMR spectra of the derivatized coal samples in Table II featured three predominating sharp peaks labelled A, B and D in Fig. 1, corresponding to excess reagent 1, at 179.5 ppm,[9] derivatized *l*-menthol at 146.6 ppm[9] and anhydride 3 at 132.9 ppm[9] arising from the moisture present in the coal sample, respectively. A broad signal C appeared in the derivatized phenolic region (138-144 ppm[9]). In Fig. 2 is shown an expansion of the latter set of signals. The ^{31}P NMR spectrum of this region after processing the FID with an apodization (line broadening) parameter of 0.5 Hz prior to Fourier transformation revealed the presence in this region of more than 100 peaks in the typical case. Application of the NMR1 curve-fitting program then gave rise to spectra resembling Fig. 3 in the typical case. However, the line widths of these signals varied from as low as 0.4

Table I. Quantitative ^{31}P NMR Analysis of Phenol Mixture Using Reagent 1.[a]

compound	mg	mmol (calcd)	$\delta^{31}P$ (ppm)	mmol found 0.5 Hz[b]	2.0 Hz[c]	MFA[d]
2,3,6-trimethylphenol	19.6	0.144	143.64	0.143	0.149	0.152
2,6-dimethylphenol	17.0	0.139	143.09	0.138	0.140	0.145
3,4-dimethylphenol	28.4	0.232	138.77	0.234	0.223	0.230

[a]*l*-menthol (18.7 mg, 0.120 mmol) was used as internal standard, 1 mol% (based on 1) of $Cr(acac)_3$ (9.6 mg) was used as relaxagent. [b]Calculated after processing with a line-broadening factor of 0.5 Hz. [c]Calculated after processing with a line broadening factor of 2.0 Hz. [d]Calculated after processing with Matched Filter Apodization.

Table II. Coal Liquefaction Samples[a] Studied Using NMR Tagging Reagent 1.

sample no.	run no.	sample designator	sampling point
1[b]	250[e]	R1236	interstage
2[b]	250[e]	V131B	recycle stream
3[b]	257[e]	R1235	interstage
4[b]	257[e]	V1067	2nd stage product
5[b]	257[e]	V131B	recycle stream
6[b]	255[f]	R1236	interstage
7[c]	259 G[g]	R1235	interstage
8[c]	259 G[g]	V1067	2nd stage product
9[c]	259 G[g]	V131B	recycle
10[d]	259 G[g]	V161 + V182	light net product
11[d]	259 G[g]	V164	interstage separator overhead
12[b]	260 ABC[h]	R1235	interstage
13[b]	260 ABC[h]	V1067	second stage product
14[b]	260 ABC[h]	V131B	recycle stream
15[b]	260 DEF[h]	R1235	interstage

[a]Wilsonville pilot plant samples provided by CONSOL Inc., 4000 Brownsville Road, Library, Pennsylvania 15129. [b]THF-soluble portions of solid 850 °F materials ("residue"). [c]THF-soluble portions of whole process oils. [d]Whole process oils. [e]Illinois No. 6 Burning Star No. 2 [f]Texas Lignite [g]Pittsburgh Seam Ireland Mine [h]Wyodak and Anderson Seam Black Thunder Mine

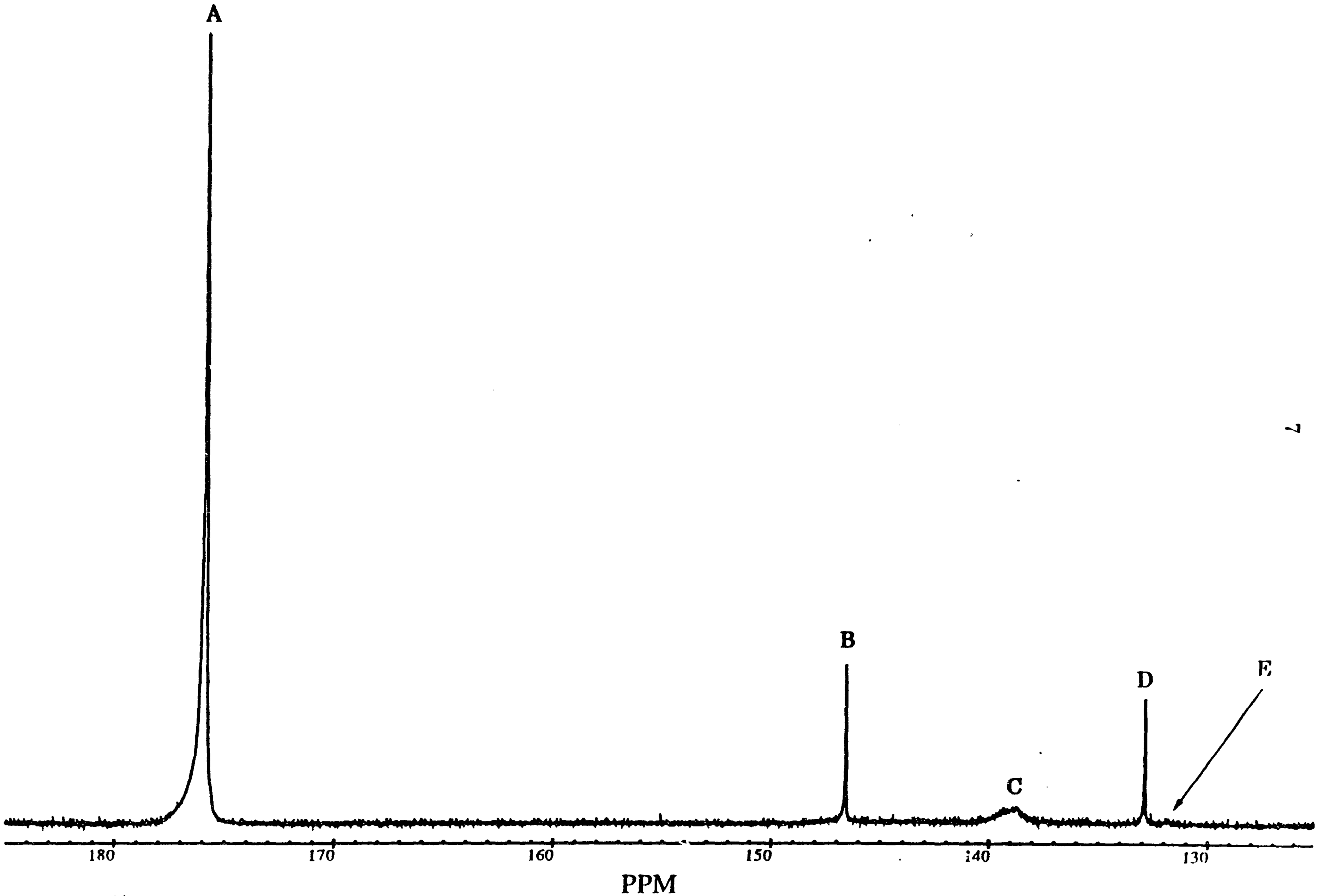

Fig. 1 ^{31}P NMR spectrum of a typical coal resid sample studied herein which was derivatized with 1. The letters A-D designate the resonances for 1, derivatized l-menthol, derivatized phenolics, derivatized water (3), respectively. The small resonances labelled E at 132 ppm are assigned to derivatized amines (see text).

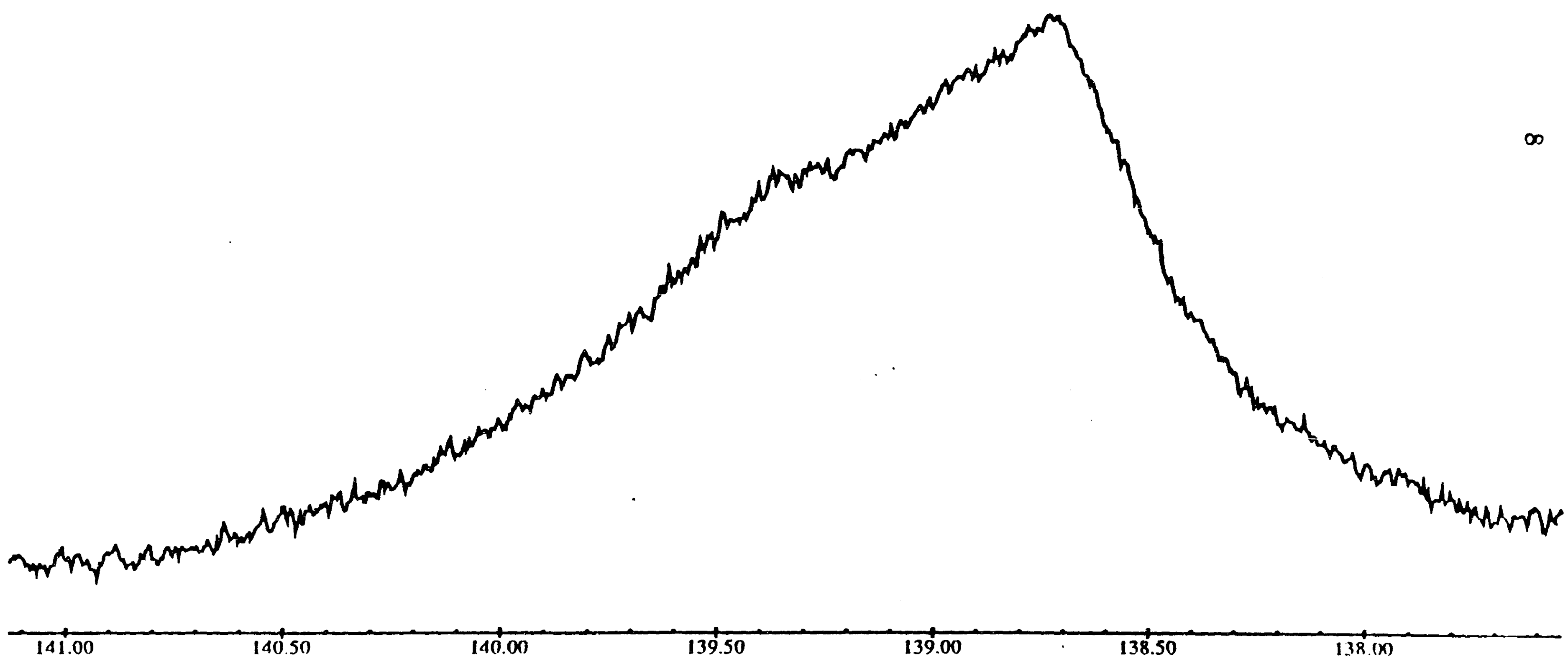

Fig. 2. An expansion of the ^{31}P region of the phenolics in a typical coal resid sample derivatized with 1.

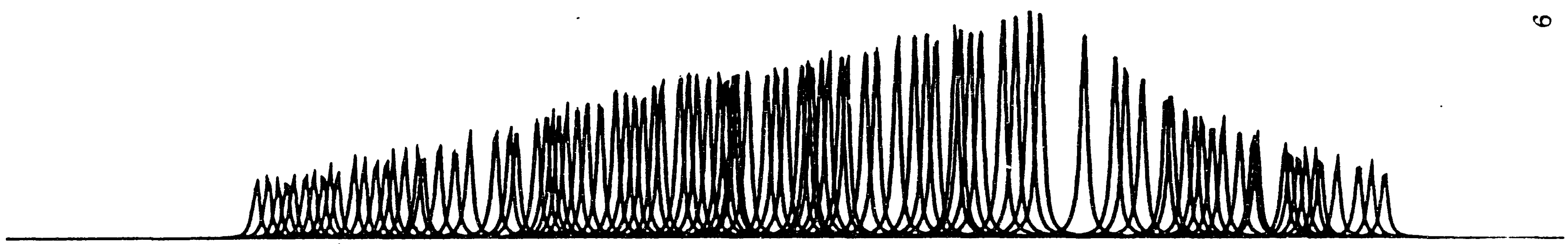

Fig. 3. The contributing peaks calculated by the NMR1 curve-fitting procedure for the phenolic region of a typical coal resid sample derivatized with 1, using a line-broadening factor of 0.5 Hz and zero-filling to achieve convergence.

Hz to as high as 197 Hz, which rendered the unequivocal identification of the phenols impractical. In about half of the samples, convergence could be achieved only by processing the FID with a zero-filling factor. In these cases, even though the line widths were small (0.81 Hz), the number of peaks was again unrealistically large (e.g., 148), making speciation impractical. Moreover, the FID of the two liquid samples examined (nos 10 and 11 in Table II) could be processed to a smooth curve only with a line broadening factor of 2.5 Hz although without zero filling. Here the number of peaks was found to be smaller (e.g., 13), but in view of their large line width, unequivocal assignments to specific derivatized phenols were not possible. However, total phenolic contents could be calculated from the integrals of the signals and they have been listed in Table III.

In view of the aforementioned difficulties, an attempt was made to reduce the number of peaks (and hence the iteration time) by processing the FID's of the coal product samples with a line-broadening factor of 2.0 Hz and zero filling. The curve-fitting was successfully achieved in all cases except the liquid samples 10 and 11. As expected, the number of peaks was reduced but the linewidths resulting from the curve-fitting procedure were found to be too large for unambiguous identification of phenol derivatives. As before, the total phenol contents could still be calculated and they are also collected in Table III.

A ^{31}P NMR spectrum obtained on the Unity 500 instrument at 202 MHz also failed to resolve the broad signal C adequately for speciation of phenolics. This prompted us to test for the presence of free radicals which are expected to broaden the signals. An EPR spectrum obtained on one such sample (No. 12) clearly indicated the presence of organic free radicals on the basis of the g factor (2.0036). The EPR spectrum of sample No. 11, a liquid, also revealed a signal at the same g value. The decreased intensity of the signal is in accord with the appearance of a better resolved ^{31}P NMR spectrum for this sample than for No. 12.

Table III. Phenolic, Amino and Moisture Contents[a] of Coal Liquefaction Samples.

sample no.	phenolic by FTIR[b]	by ^{31}P NMR phenolic	amino	moisture	phenolic error[g] excluding amino	including amino
1	1.07	1.02[c]	0.01[c]	0.13[c]	-0.05	-0.04
		1.13[d]	0.10[d]	0.13[d]	+0.06	+0.16
		1.07[e]	0[e]	0.12[e]	0	0
2	0.74	0.63[c]	0.03[c]	0.07[c]	-0.11	-0.08
		0.77[d]	0.01[d]	0.07[d]	+0.03	+0.04
		0.72[e]	0.02[e]	0.07[e]	-0.02	0
3	0.68	0.60[c]	0[c]	0.13[c]	-0.08	-0.08
		0.68[d]	0.02[d]	0.12[d]	-0.00	+0.02
		0.64[e]	0.02[e]	0.11[e]	-0.04	-0.02
4	0.57	0.43[c]	0.10[c]	0.06[c]	-0.14	-0.04
		0.40[d]	0.02[d]	0.09[d]	-0.17	-0.15
		0.42[e]	0.02[e]	0.08[e]	-0.15	-0.13
5	0.50	0.34[c]	0.03[c]	0.10[c]	-0.16	-0.13
		0.37[d]	0.04[d]	0.10[d]	-0.13	-0.09
		0.39[e]	0.04[e]	0.09[e]	-0.11	-0.07
6	1.04	0.85[c]	0.10[c]	0.10[c]	-0.19	-0.09
		1.00[d]	0.01[d]	0.10[d]	-0.04	-0.03
		0.98[e]	0[e]	0.10[e]	-0.06	-0.06
7	0.60	0.58[c]	0[c]	0.10[c]	-0.02	-0.02
		0.60[d]	0.01[d]	0.10[d]	0	+0.01
		0.57[e]	0[e]	0.09[e]	-0.03	-0.03
8	0.42	0.30[c]	0.03[c]	0.09[c]	-0.12	-0.09

		0.37[d]	0.01[d]	0.09[d]	-0.05	-0.04
		0.41[e]	0.02[e]	0.09[e]	-0.01	+0.01
9	0.60	0.48[c]	0.02[c]	0.11[c]	-0.12	-0.10
		0.30[d]	0.01[d]	0.11[d]	-0.30	-0.29
		0.28[e]	0[e]	0.10[e]	-0.32	-0.32
10	0.18	0.29[e]	0[e]	0.06[e]	+0.11	+0.11
		0.27[f]	0[f]	0.06[f]	+0.09	+0.09
11	0.27	0.33[e]	0[e]	0.09[e]	+0.05	+0.05
		0.51[f]	0[f]	0.05[f]	+0.24	+0.24
12	0.97	0.97[c]	0.08[c]	0.13[c]	0	+0.08
		0.90[d]	0.02[d]	0.13[d]	-0.07	-0.05
		0.84[e]	0[e]	0.12[e]	-0.13	-0.13
13	0.70	0.41[c]	0.21[c]	0.11[c]	-0.29	-0.08
		0.48[d]	0[d]	0.10[d]	-0.22	-0.22
		0.64[e]	0.01[e]	0.10[e]	-0.06	-0.05
14	0.71	0.69[c]	0.04[c]	0.17[c]	-0.02	+0.02
		0.44[d]	0.03[d]	0.10[d]	-0.27	-0.24
		0.60[e]	0.04[e]	0.09[e]	-0.11	-0.06
15	0.95	0.78[c]	0[c]	0.18[c]	-0.17	-0.17
		0.92[d]	0.03[d]	0.18[d]	-0.03	0
		1.00[e]	0.03[e]	0.17[e]	+0.05	+0.08

[a]meq/g. [b]See reference 1a,b. [c]FID processed with 0.5 Hz line-broadening factor. [d]FID processed with 2.0 Hz line-broadening factor. [e]FID processed with Matched Filter Apodization. [f]FID processed with 2.5 Hz line-broadening factor. [g]In meq/g of coal product sample.

This result strongly suggested that attempts to resolve the broad derivatized phenolic signal would be of little use for the speciation of derivatized phenols.

We then attempted to determine the total phenolic content using a simple function which processes the FID's by a Matched Filter Apodization procedure. Using this program (which required no zero filling), the broad signal C was generally identified by the program as a single peak (although in some cases as many as three or four peaks) and the phenolic contents were calculated after curve-fitting. The results are collected in Table III.

Table III summarizes the total phenolic contents calculated by the three different ^{31}P NMR analysis methods employed here, thus allowing a comparison with values reported for these samples by FTIR spectroscopy.[1a,b] The average error in the latter method was determined to be ± 0.1 meq/g coal product sample with a reproducibility of ± 0.09 meq/g.[1b] In Table IV are summarized the average errors (relative to the FTIR data) associated with the three line-broadening factor methods used in our ^{31}P NMR analyses. From this table it is seen that the average error decreases for all three line-broadening treatments when the amine contents are included. Since secondary amines (including pyrroles) also absorb in the phenolic OH region in the IR,[1a,b,d] we believe the amine contributions found in the present work should be included in the phenolic contents for comparison with the FTIR results. In that case, the average error for the MFA line-broadening analysis appears to match the FTIR results most closely.[13] The reproducibility of our technique was tested by using three separately weighed samples of sample No. 2. The average precisions using the 0.5 Hz, 2.0 Hz and MFA line broadening approaches are ±0.02, ±0.06 and ±0.05 meq/g.

We note here that the agreement between our ^{31}P NMR method with the FTIR technique on the present samples is much better than that found in a comparison of a ^{19}F NMR tagging approach[1c] with the FTIR method, for the analysis of phenolics in a series of distillates. Thus the ^{19}F NMR tagging method resulted in underestimates of the FTIR-determined phenolic contents, ranging from 0.07 to 1.12 meq/g,[1c] compound with *ca.* -0.04, -0.03 meq/g using the MFA approach (Table IV).

Moisture is reported not to interfere in the FTIR method for phenolics[1a,b] since the water peaks (when observed) are generally found to be 170 cm^{-1} or more to higher wave numbers.[1d] Because the preparation of the FTIR samples took place in air, some contamination of the samples by moisture is inevitable. Since our preparations rigorously excluded air, we believe the small rather constant H_2O contents observed in the samples studied here (Table III) strongly suggest the presence of moisture that is present in the liquefaction process and/or is absorbed by the sample during the preparation procedure. Interestingly, inclusion of both the amine and moisture contents with the phenolic analyses produce average errors of +0.05, +0.04 and +0.06 meq/g for our line-broadening treatments using 0.5 Hz, 2.0 Hz and MFA, respectively. It should be noted here that in contrast to the coal product samples for which the average error in the phenolic contents determined by ^{31}P NMR analysis decreased using a 0.5 Hz, then a 2.0 Hz and finally an MFA line-broadening factor, the same series of analyses for the model phenol mixture in Table IV gave an increase in average error from 0.00 to ± 0.03 to ± 0.13 meq/g of phenol mixture. We believe this result indicates that spectra consisting of non (paramagnetically) broadened, non overlapping peaks, wherein all the peaks are approximately equally sharp, are best analyzed with a small line-broadening factor (i.e., 0.5 Hz in the present instance).

Table IV. Average Errors[a] in Phenolic Contents by ^{31}P NMR.

line-broadening treatment	excluding amino	including amino
0.5 Hz	-0.11	-0.06
2.0 Hz	-0.09	-0.07
MFA	-0.04	-0.03

[a]In meq/g coal product samples.

Conclusions. From this study it can be concluded that: (1) Our ^{31}P NMR tagging method is applicable to the analysis of phenolic contents of coal products despite the relatively low concentrations of these compounds and despite the presence of organic free radicals which broaden the spectra. (2) The average errors for all three apodization methods employed here to analyze the derivatized phenolic region of the ^{31}P NMR spectra are at least as favorable as those for the FTIR method (± 0.1 meq/g), and by inclusion of the amine content found outside of this region, the NMR method using the MFA line-broadening approach appears to be somewhat better (-0.03 meq/g, Table IV). By comparison, the data given in the earlier report using $Cl(O)PPh_2$ as a ^{31}P NMR tagging reagent indicates that the agreement among the ^{31}P, ^{29}Si and ^{19}F NMR tagging results for five coal liquids averaged 0.15 meq/g.[3] (3) By also including the small intrinsic water contents found in the samples studied, the average error moves from slightly negative to slightly positive. (4) The ^{31}P NMR analysis reported here, which takes about 1 3/4 hours per sample when the MFA analysis approach is used, is not as rapid as the FTIR method which takes approximately 15 minutes per sample.[1a,b] However, our ^{31}P NMR approach is about as rapid as that reported with $Cl(O)PPh_2$.[3] (5) The ^{31}P NMR method described permits the simultaneous analysis of moisture, since interference of moisture is categorically absent, as is also the case for the reagent $Cl(O)PPh_2$.[3] (6) The ^{31}P NMR method is amenable to a large variety of solvents, including pyridine,[9] as long as they contain no labile hydrogen functional groups. With the reduction of the free radical concentration in coal resids, speciation of phenols could become feasible with reagent 2, which gives rise to more than twice the ^{31}P NMR peak dispersion for phenols than 1.[9]

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References

(1) (a) Robbins, G. A.; Winschel, R. A.; Burke, F. P. *Am. Chem. Soc. Div. Fuel Chem. Prepr.* **1985**, *30*, 155. (b) Winschel, R. A.; Robbins, G. A.; Burke, F. P. *Technical Progress Report, July 1-Sept. 1985, DOE/PC 70018-13*, December, 1985. (c) Burke, F. P.; Winschel, R. A. *Technical Report, Oct. 1, 1983-Mar. 31, 1984*, DOE Contract No. DE-AC22-80PC30027, March, 1985. (d) Robbins, G. A., private communication.

(2) (a) Winschel, R. A. and Burke, F. P. "Recycle Slurry Oil Characterization Report: 10/1/82-3/31/83", DOE Contract No. DE-AC22-80PC30027, February, 1984. (b) Winschel, R. A. and Burke, F. P. "Recycle Slurry Oil Characterization-Second Annual Report", DOE Contract No. DE-AC22-80-PC30027, August, 1983.

(3) E. J. Dadey, S. L. Smith, B. H. Davis *Energy Fuels* **1988**, *2*, 326.

(4) D. E. Schiff, J. G. Verkade, R. M. Metzler, T. G. Squires and C. G. Venier, *Appl. Spectrosc.* **1986**, *40*, 348.

(5) A. E. Wroblewski, R. Markuszweski and J. G. Verkade, *Prepr. Pap-Am. Chem. Soc.; Div. Fuel Chem.* **1987**, *32*, 302.

(6) A. E. Wroblewski, C. Lensink, R. Markuszweski and J. G. Verkade, *Energy Fuels*, **1988**, *2*, 765.

(7) C. Lensink and J. G. Verkade, *Prepr. Pap-Am. Chem. Soc., Div. Fuel Chem.* **1988**, *33*, 906.

(8) C. Lensink and J. G. Verkade, *Energy Fuels*, **1990**, *4*, 197.

(9) A. E. Wroblewski, C. Lensink and J. G. Verkade, *Energy Fuels*, **1991**, *5*, 491.

(10) A. Zwierzak, *Can. J. Chem.* **1961**, *45*, 2501.

(11) A. E. Derome, "Modern NMR Techniques for Chemistry Research", Pergamon: London, 1986.

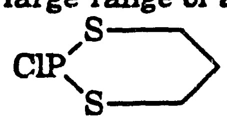
(12) In this procedure as many pseudo data points as the computer memory allows are introduced in order to achieve smooth curve fitting. This procedure did not adversely affect quantitation, however.

(13) It should be noted that we have not been able to identify the compounds responsible for the peaks in this portion of the amine region. Moreover, it cannot be concluded that the derivatized phenolic region in our spectra is uncontaminated by derivatized amines, since the derivatized amine region is large (130-150 ppm[3]).

Recommendations for Future Work

Although we were pleasantly surprised at how well our technique worked out, several problems remain to be solved:

1. There is a significant question raised by Gary Robbins in his FTIR work (reference 1) that we could only partially address quite completely. Apparently secondary amines and pyrroles contribute to the FTIR band associated with phenols. Although we indicate in th eppaer that we see an amine peak (whose integration in fact improves our data relative to Gary's) we also indicate that other amines derivatized with the reagent we used, resonate in the derivatized phenol region, thus perhaps contributing to that integral. In past work, however, we developed another reagent (see structure below) for which a large range of amine derivatives give a



dispersion of ^{31}P resonances which is over 55 ppm wide(!) and which is well away from the phenol region for this reagent (see ref. 7). Thus we should be able to integrate the derivatized amine region quite separately from the derivatized phenol region to gain a better measure of how badly the phenolic OH FTIR band may be contaminated by amine contributions. This reagent would also allow us to determine if the peak at 137 ppm in samples such as 10, 11 and 15 is due to amines or phenols. The 55 ppm wide dispersion may even allow us to speciate some of these amines despite paramagnetic impurity broadening.

2. We have shown that free radicals are present in two of the samples, and it is reasonable to surmise that they contribute to the severe broadening of the ^{31}P NMR spectra of all of the samples. Hydrogenation may reduce the concentrations of the free radicals to the point where sufficient resolution is

achieved for speciation of phenols using reagent **1** or reagent **2** which we have shown provides more than twice the dispersion of the ^{31}P chemical shifts of phenols derivatized with it.[7-9] Because of the severe broadening of the ^{31}P NMR spectra we encountered with **1**, there would have been virtually no gain in using **2** without first reducing the radical concentration. Such experiments would be accompanied by model compound derivatizations to expedite speciation.

3. It would be worthwhile using the reagent $Cl(O)PPh_2$ which Dadey et al. used to quantitate phenols in coal liquids[3] and which we have used to quantitate moisture in coal liquids and solids (*Energy and Fuels* **1991**, *5*, 786; *Energy Fuels* **1992**, *4*, 331). There are three reasons for this: First, Dadey et al. were troubled by an impurity in the reagent, and our preparation leads to pure material. With pure reagent, we can validly compare phenol analyses by ^{31}P NMR on a given set of coal liquids using reagent **1** and $Cl(O)PPh_2$. Secondly, this would give us a check on the moisture contents. Third, since Dadey et al. do not address the question of amine derivatization, we could have a look at where these resonate when derivatized with $Cl(O)PPh_2$ and perhaps gain additional valuable information on the FTIR/amine question.

4. A comparison of the ^{31}P NMR's of the phenolic regions for each of the 15 samples derivatized with **1** reveals four rather distinct "fingerprints" as shown in Table V and in the spectra in Appendix C. Three tentative conclusions worth further investigation are: (a) From our EPR results, it would appear that only the liquid samples have sufficiently

Table V. Grouping of Samples According to Spectral Appearance

		spectral appearance		
grouping	samples	139.2 ppm	138.7 ppm	137.3 ppm
I	1-3, 5, 7, 12	mod. intense sh.	mod. narrow	low intensity
II	4, 8, 9, 13	intense sh.	mod. narrow	mod. intensity
III	5, 14, 15	intense br. sh.	mod. narrow	high intensity
IV	10, 11	group of pks	group of pks	high intensity

low concentrations of radicals to give rise to distinct groupings of peaks at ~139.2 and ~138.7 ppm. Thus our technique gives a qualitative indication of relative radical concentrations. (b) Whole process oils such as samples 10 and 11 *may* be amenable to partial phenol speciation via reagent 2 without radical reduction. (c) There appears to be a partial correlation of spectral grouping with sampling point as shown in Table VI. Thus 5/6 of the samples in grouping I are from the interstage, 3/4 of the samples in grouping II are 2nd stage products, 2/3 of the samples from grouping III are from recycle streams and both light oils fall in grouping IV.

Table VI. Relationship of Spectral Grouping to Sampling Point.

grouping	samples	sampling point
I	1, 3, 6, 7, 12	interstage
	2	recycle stream
II	4, 8, 13	2nd stage product
	9	recycle
III	5, 14	recycle stream
	15	interstage
IV	10	light net product
	11	interstage separator overhead

Appendix A: Experimental Conditions

Reagents: Chloroform-d (Aldrich) was stored over activated molecular sieves before use. *l*-Menthol (Aldrich) was used as received. All the phenols used in this study were recrystallized from ethanol before use. Triethylamine (Kodak) was distilled over anhydrous KOH pellets and stored under nitrogen. 2-Chloro-4,4,5,5-tetramethyl-1,3,2-dioxaphospholane, **1**, was prepared according to a literature procedure[10] and was purified by distillation. Bp 39-41 °C at 0.04 mm (lit.[9] 81-82.5 °C at 15 mm; lit.[10] 77-78 °C at 12 mm).

Model Mixtures. Model mixtures of phenols were prepared by weighing the phenols directly into a 10 mm NMR tube together with a weighed amount of the internal standard, *l*-menthol and the relaxagent, $Cr(acac)_3$ (1 mole% based on reagent **1**). The mixture was dissolved in chloroform-d (4.0 mL) and after the addition of triethylamine (0.5 mL, 3.6 mmol), the phenols and *l*-menthol were reacted with reagent **1** (0.50 mL, 3.2 mmol) at 10 °C for about 1 h. The ^{31}P NMR spectrum was then obtained. Further data for a typical model phenol mixture are given in Table I.

Coal liquefaction products. The origins of the coal liquefaction samples employed in this study are listed in Table II. All the manipulations involving the coal samples were carried out in a dry boxy or a glove bag filled with dry nitrogen to avoid contamination with external moisture. The samples (280.5-650.9 mg) were weighed directly into previously weighed NMR tubes containing (13.5-33.4 mg) of *l*-menthol and 1 mole% (based on reagent **1**) of $Cr(acac)_3$. The contents were then dissolved in chloroform-d (4.0 mL), triethylamine was added (0.50 mL, 3.6 mmol) and then reagent **1** (0.50 mL, 3.2 mmol) was added to the sample after cooling it below 10 °C. After about 2 h at 10 °C, the NMR spectrum was obtained.

NMR Instrumentation and Processing. ^{31}P NMR spectra of the derivatized mixtures and coal liquefaction products were obtained on a Bruker WM-200 spectrometer operating at 81.0 MHz. The spectrometer was interfaced with an ASPECT 2000 computer. The following acquisition parameters were employed: broad band decoupling; pulse width, $\pi/2$, 26 μs; sweep width, 4864 Hz; memory size, 16K; relaxation delay, 3.0 s; acquisition time, 1.69 s; number of scans 64 for the model mixtures and 1000 in the case of coal samples.

Integrations were performed on a DEC Mini Computer using the NMR1 program. After base line correction and zero filling (if required - see later) the FID was processed three ways: using a line broadening factor of 0.5 Hz, 2.0 Hz and a factor automatically selected by the NMR1 Matched Filter Apodization (MFA) program. In the MFA program the line broadening factor is set equal to a calculated linewidth based on the equation of a theoretical Lorentzian line. The linewidth, and hence the line broadening factor is determined from the sum of all the frequencies in the FID. The MFA line broadening factors ranged from 2.5-8.3 Hz for the coal product samples and it was 6.6 Hz for the model phenol mixtures. After exponential multiplication, the FID was Fourier transformed and the resultant spectrum was interactively phased manually. Peak analysis was carried out after deleting extraneous peaks. The S/N ratio ranged from 500 to 5000 for the spectra of the coal product samples. The curve-fitting routine was then employed to obtain accurate integrations.

The broad derivatized phenolics region of the ^{31}P spectra of the coal product samples was curve-fitted in its entirety. With a line broadening factor of 0.5 Hz, zero filling[12] was required for about half of the samples in order to achieve convergence. The number of peaks at convergence ranged from 40-150. To reach convergence in samples not zero filled, it was necessary to delete peaks with large linewidths (>500 Hz) and no integral or intensity value. By employing a 2.0 Hz line broadening factor, the number of data points to process is diminished thus reducing the time required for iterations. Again, however, zero filling was always required to

sample no.	file name	sample wt. (g)	*l*-menthol (mg, mmol)
1	TCS01	0.4402	14.5, 0.0928
2	TCS2	0.4551	26.5, 0.170
3	TCS3	0.3618	20.8, 0.133
4	TCS4	0.4224	23.9, 0.153
5	TCS5	0.4842	23.4, 0.150
6	TCS6	0.5534	33.4, 0.214
7	TCS7	0.3549	20.3, 0.130
8	TCS8	0.5265	33.4, 0.214
9	TCS9	0.2795	23.2, 0.149
10	TCS10	0.3628	13.3, 0.0851
11	TCS11	0.6509	33.1, 0.212
12	TCS12	0.4538	24.5, 0.157
13	TCS13	0.3386	17.8, 0.114
14	TCS1.001	0.4065	16.0, 0.102
15	TCSI5	0.3740	28.8, 0.184

achieve convergence. Using MFA, convergence was reached more quickly and zero filling was never required.

The quantities of phenolics, amines and H_2O in meq/g of coal product relative to that of *l*-menthol present (in meq/g of coal product) were then calculated from the integrals (see Eq 1 in Results and Discussion).

EPR Instrumentation. EPR spectra were recorded at 292 K on a Bruker ER-200D spectrometer operating at a frequency of 9.45078 GHz and interfaced with an ASPECT 2000 computer. The sweep widths were maintained in the range 2700 to 3700 Gauss. The EPR spectrum of sample No. 11 as obtained as its solution in chloroform while that of sample No. 12 was obtained on the solution used for ^{31}P NMR spectroscopy. Both samples gave a single resonance at a g value of 2.0036, calculated by the relation $g = h\nu/\beta H_n$

Procedure for calculating the concentration of phenolic oxygen in the coal samples

The phenols (or the amines, if any) present in the coal samples were assumed to have only one labile hydrogen for the derivatization reaction. Hence the total concentration of phenols (or amines) calculated would be equal to the total concentration of phenolic oxygen (or amine nitrogen). Thus, for example, the amount of phenolic oxygen in mmol = amount of phenols in mmol, both of which are proportional to the ^{31}P NMR integral. Therefore:

$$\text{mmol O} = \frac{\text{Total integral of derivatized phenolic signals}}{\text{Total integral of derivatized } l\text{-menthol signal}} \times l\text{-menthol} \qquad (1)$$

The concentration of oxygen in meq/g can then be calculated as:

$$\frac{\text{meq O}}{\text{g coal sample}} \times \frac{\text{mmol O}}{\text{coal sample wt (g)}} \times \frac{\text{meq O}}{\text{mmol O}} \qquad (2)$$

Combining equations 1 and 2:

$$\frac{\text{meq O}}{\text{g coal sample}} = \frac{\text{Total integral of derivatized phenolic signals}}{\text{Total integral of derivatized-menthol signal}} \times \frac{\text{mmol } l\text{-menthol}}{\text{coal sample wt (g)}} \qquad (3)$$

An analogous procedure was used for the amine and moisture contents except that in the case of moisture, half the integral was used since there are two labile hydrogen functionalities that are derivatized, giving **3**.

Processing FID for integration using NMR1:

1. The desired data file (FID) is accessed and using the command BC the baseline is corrected.
2. Zero filling (if appropriate) is carried out at this stage.
3. The desired line broadening factor is entered manually (0.5 or 2.0 Hz; the command MF is used for Matched Filter Apodization Parameter which is set by the program automatically).
4. The FID is then subjected to exponential multiplication.
5. Fourier transformation is executed.
6. Using the commands Pf and PH→I, the spectrum is phased by manual interactive phasing.
7. Peak analysis is carried out. The spectrum may show many undesired peaks in any of the regions. By using the mouse correction threshold or manual deletion sub-routine the unwanted peaks are deleted. Because the process causes small shifts in the spectrum the standard is assigned to 175.9 ppm, thus resulting in the calibration of the rest of the spectrum. In many samples, peaks in the amine region are not revealed until that portion of the spectrum is enlarged. At this point the two peaks in this region can be identified manually by the appropriate sub-routines.
8. Using the function SN, the Signal/Noise factor is determined.
9. For curve fitting, the appropriate peaks are zoomed out using the function CF and by an automatic procedure, the peak is fitted to a Lorentzian shaped curve. The monitor displays the number of iterations performed by the program with the corresponding residual sum of the squares. For sharp peaks, the curve fitting is done within 3 to 20 iterations. The total time taken for even 20 iterations is less than 5 seconds.

Convergence in the broad phenolic region. Since the peaks in this region are not resolved, the entire region is zoomed out for curve fitting by the above procedure. The number of peaks shown by the program when processed with a line-broadening factor of 0.5 Hz ranges from 40 to 150. Thus the time taken for each iteration runs into several seconds. The program usually displays once in every 20 iterations whether convergence is achieved or not. In the case of many coal samples processed with a 0.5 Hz line-broadening, convergence is not achieved even after 300 iterations. At this stage the program will stop the iteration and request to do Peak Analysis. Without altering the peak information at this stage (i.e., after 300 iterations) the peaks with very large linewidth (>500 Hz) with no intensity or integral values may be deleted and the curve fitting procedure is continued. Depending on the sample, this procedure is repeated as many times as required to achieve convergence. The integrals and hence the quantities are then calculated.

The more data points present in the phenolic region, the more the number of iterations and the slower the rate of the whole process. The number of data points is decreased by processing the FID with a higher line-broadening factor, i.e., 2.0 Hz. Although the zero filling factor increases the number of data points, the linewidths are reduced. In the case of processing with 0.5 Hz, some FIDs are processable only by employing the zero filling factor. In these cases, convergence is achieved instantaneously. Hence a combination of a line-broadening factor of 2.0 Hz with zero filling was considered for processing the FID. However, convergence is generally achieved more slowly than for the 0.5 Hz plus zero filling treatment. The linewidths are generally more narrow than for the 0.5 Hz treatment alone but are broader than for the 0.5 Hz plus zero filling treatment. The linewidths are too broad to allow speciation of phenol compounds.

Matched Filter Apodization

In the light of the above problems, the matched filter apodization method was employed since the results were improved and since zero filling is not required or helpful.

To achieve the best resolution of the peaks and to interpret the fine structure in an FT-NMR spectrum, the following concepts and procedures were used.

The interval between the individual data points constituting the peak, called the digital resolution (Rd) is given by

$$Rd = \frac{1}{At}$$

where At is the acquisition time. Evidently, the smaller the value of Rd, the sharper the peaks will be. It is advantageous to have Rd smaller than the natural line width of the nuclei (eg. ≡ 0.1 Hz for protons and 2-3 Hz for other nuclei).

From the above equation, it is clear that Rd can be minimized by increasing the acquisition time, which consumes instrument time and is costly. Alternatively, the Zerofilling technique can be used, which utilizes the computer memory. This is a process by which zeros are appended to the data before Fourier transformation. This process increases the data points and reduces Rd without adding extra information to the spectrum. However, this method can be used only if the FID has already decayed close to zero.

If the acquisition time is short, the FID may not have decayed close to zero. Such decay can be achieved artificially by multiplying the FID by a smoothly decaying function (i.e., an exponential function ζ, called a window function) given by the equation

$$\zeta = e^{-t/a}$$

where a is a positive number, known as the apodization parameter (a line broadening factor that comes into play as the multiplication broadens the line in the frequency domain). Now the variable a has to be chosen carefully so that the process does not speed up the decay to zero.

The half width of the theoretical Lorentzian line ($\delta\nu$) is given by the relation

$$\delta\nu = \frac{1}{\pi T_2}$$

where T_2 is the decay time constant. Because of the exponential multiplcation, T_2 reduces to T_2', given by the equation

$$\frac{1}{T_2'} = \frac{1}{T_2} + \frac{1}{a}$$

Careful analyses of this problems shows that the sensitivity is decreased if a is too small or is not affected if a is too large. An optimum value of a is found to be $a = T_2$. This function is the "matched filter" which is matched to the decay envelope of the FID. Evidently, it doubles the natural line width in the frequency domain.

MFA line broadening factors selected by the NMR1 program for the coal samples.[a]

samples	Hz	samples	Hz
1	5.5957	9	6.6377
2	6.6594	10	7.4309
3	7.1300	11	6.5240
4	8.0180	12	8.3391
5	2.4994	13	5.5928
6	7.3726	14	6.2317
7	7.0401	15	3.4435
8	2.3367		

[a]The MFA factor for the model mixture was 6.6270 Hz.

Appendix B: Raw Data

This appendix contains the data resulting from processing the FIDs using 0.5 Hz and 2.0 Hz as line-broadening factors. Also included are data resulting from the Matched Filter Apodization technique which automatically applies an optimum line-broadening factor (2-8 Hz in the present samples) based on the shape of the FID.

^{31}P NMR spectral data of the coal samples, obtained by processing the FID's with a line-broadening factor of 0.5 Hz.

NMR1
****

Filename = TCSO1
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 3436.82

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14249.93	175.768	100.000	0.1197E+09	9.00
*	2	11877.29	146.502	13.359	0.1599E+08	2.30
*	3	11376.48	140.325	0.352	0.4214E+06	1.36
*	4	11374.03	140.294	0.377	0.4517E+06	1.36
*	5	11373.31	140.286	0.384	0.4592E+06	1.36
*	6	11371.21	140.260	0.401	0.4798E+06	1.36
*	7	11368.19	140.222	0.425	0.5082E+06	1.36
*	8	11367.05	140.208	0.465	0.5562E+06	1.36
*	9	11364.50	140.177	0.443	0.5300E+06	1.36
*	10	11362.68	140.154	0.463	0.5545E+06	1.36
*	11	11361.14	140.135	0.469	0.5609E+06	1.36
*	12	11360.26	140.125	0.462	0.5535E+06	1.36
*	13	11359.27	140.112	0.490	0.5868E+06	1.36
*	14	11357.60	140.092	0.474	0.5669E+06	1.36
*	15	11355.32	140.064	0.512	0.6134E+06	1.36
*	16	11353.55	140.042	0.519	0.6212E+06	1.36
*	17	11352.78	140.032	0.527	0.6308E+06	1.36
*	18	11351.63	140.018	0.519	0.6207E+06	1.36
*	19	11350.10	139.999	0.548	0.6564E+06	1.36
*	20	11348.60	139.981	0.576	0.6898E+06	1.36
*	21	11347.14	139.963	0.575	0.6888E+06	1.36
*	22	11346.48	139.955	0.584	0.6995E+06	1.36
*	23	11345.21	139.939	0.588	0.7035E+06	1.36
*	24	11343.30	139.915	0.601	0.7194E+06	1.36
*	25	11341.76	139.896	0.635	0.7605E+06	1.36
*	26	11339.98	139.874	0.610	0.7298E+06	1.36
*	27	11337.41	139.843	0.659	0.7884E+06	1.36
*	28	11336.45	139.831	0.665	0.7957E+06	1.36
*	29	11335.60	139.821	0.674	0.8071E+06	1.36
*	30	11333.81	139.798	0.695	0.8314E+06	1.36
*	31	11332.76	139.785	0.684	0.8191E+06	1.36
*	32	11331.64	139.772	0.713	0.8532E+06	1.36
*	33	11329.37	139.744	0.731	0.8747E+06	1.36
*	34	11327.78	139.724	0.757	0.9065E+06	1.36
*	35	11325.68	139.698	0.787	0.9421E+06	1.36
*	36	11323.96	139.677	0.802	0.9595E+06	1.36
*	37	11322.80	139.663	0.841	0.1006E+07	1.36
*	38	11322.02	139.653	0.836	0.1001E+07	1.36
*	39	11318.11	139.605	0.896	0.1072E+07	1.36
*	40	11316.06	139.579	0.933	0.1117E+07	1.36
*	41	11314.70	139.563	0.945	0.1131E+07	1.36
*	42	11312.01	139.529	0.972	0.1163E+07	1.36
*	43	11310.62	139.512	0.988	0.1183E+07	1.36
*	44	11305.68	139.451	1.111	0.1330E+07	1.36

*	45	11303.59	139.426	1.114	0.1333E+07	1.36
*	46	11302.56	139.413	1.118	0.1338E+07	1.36
*	47	11297.36	139.349	1.256	0.1503E+07	1.36
*	48	11292.77	139.292	1.338	0.1602E+07	1.36
*	49	11291.70	139.279	1.356	0.1624E+07	1.36
*	50	11290.14	139.260	1.356	0.1623E+07	1.36
*	51	11287.95	139.233	1.360	0.1628E+07	1.36
*	52	11287.15	139.223	1.369	0.1639E+07	1.36
*	53	11286.08	139.210	1.363	0.1631E+07	1.36
*	54	11285.06	139.197	1.380	0.1652E+07	1.36
*	55	11283.84	139.182	1.366	0.1635E+07	1.36
*	56	11282.59	139.167	1.392	0.1666E+07	1.36
*	57	11282.03	139.160	1.395	0.1669E+07	1.36
*	58	11281.04	139.148	1.399	0.1675E+07	1.36
*	59	11278.05	139.111	1.434	0.1717E+07	1.36
*	60	11275.67	139.081	1.435	0.1718E+07	1.36
*	61	11274.88	139.072	1.433	0.1716E+07	1.36
*	62	11274.25	139.064	1.440	0.1724E+07	1.36
*	63	11271.07	139.025	1.451	0.1737E+07	1.36
*	64	11269.30	139.003	1.472	0.1762E+07	1.36
*	65	11267.45	138.980	1.478	0.1769E+07	1.36
*	66	11266.58	138.969	1.506	0.1803E+07	1.36
*	67	11265.11	138.951	1.508	0.1805E+07	1.36
*	68	11263.63	138.933	1.529	0.1830E+07	1.36
*	69	11261.40	138.905	1.584	0.1896E+07	1.36
*	70	11259.76	138.885	1.552	0.1858E+07	1.36
*	71	11258.63	138.871	1.611	0.1928E+07	1.36
*	72	11257.19	138.853	1.607	0.1923E+07	1.36
*	73	11255.60	138.834	1.646	0.1970E+07	1.36
*	74	11254.46	138.820	1.657	0.1983E+07	1.36
*	75	11252.67	138.798	1.708	0.2044E+07	1.36
*	76	11251.44	138.782	1.725	0.2065E+07	1.36
*	77	11250.53	138.771	1.716	0.2054E+07	1.36
*	78	11247.88	138.738	1.753	0.2098E+07	1.36
*	79	11247.02	138.728	1.763	0.2111E+07	1.36
*	80	11243.52	138.685	1.869	0.2237E+07	1.36
*	81	11241.70	138.662	1.883	0.2254E+07	1.36
*	82	11240.75	138.651	1.880	0.2250E+07	1.36
*	83	11237.90	138.615	1.929	0.2309E+07	1.36
*	84	11234.93	138.579	1.873	0.2242E+07	1.36
*	85	11232.48	138.549	1.782	0.2133E+07	1.36
*	86	11231.01	138.530	1.748	0.2093E+07	1.36
*	87	11227.11	138.482	1.542	0.1845E+07	1.36
*	88	11225.33	138.460	1.496	0.1791E+07	1.36
*	89	11224.52	138.450	1.473	0.1763E+07	1.36
*	90	11215.29	138.336	1.076	0.1288E+07	1.36
*	91	11212.05	138.297	0.988	0.1182E+07	1.36
*	92	11209.42	138.264	0.916	0.1097E+07	1.36
*	93	11206.10	138.223	0.821	0.9824E+06	1.36
*	94	11203.77	138.194	0.755	0.9041E+06	1.36
*	95	11202.06	138.173	0.709	0.8492E+06	1.36
*	96	11201.23	138.163	0.699	0.8362E+06	1.36
*	97	11199.69	138.144	0.704	0.8426E+06	1.36
*	98	11197.66	138.119	0.658	0.7879E+06	1.36
*	99	11194.63	138.082	0.603	0.7218E+06	1.36
*	100	11193.42	138.067	0.571	0.6835E+06	1.36
*	101	11190.29	138.028	0.574	0.6870E+06	1.36
*	102	11188.43	138.005	0.517	0.6189E+06	1.36
*	103	11187.46	137.993	0.508	0.6080E+06	1.36
*	104	11186.96	137.987	0.514	0.6151E+06	1.36
*	105	11184.19	137.953	0.486	0.5812E+06	1.36
*	106	11181.25	137.917	0.442	0.5293E+06	1.36
*	107	11179.49	137.895	0.430	0.5149E+06	1.36
*	108	11178.49	137.883	0.425	0.5091E+06	1.36
*	109	11175.08	137.841	0.387	0.4632E+06	1.36
*	110	11173.07	137.816	0.383	0.4588E+06	1.36

*	111	11168.57	137.760	0.388	0.4649E+06	1.36
*	112	11166.11	137.730	0.399	0.4781E+06	1.36
*	113	10763.68	132.766	17.946	0.2148E+08	2.15
*	114	10682.37	131.763	0.307	0.3669E+06	3.88
*	115	10672.18	131.637	0.307	0.3677E+06	3.30

	Peak #	PPM	Relative integral	Absolute integral	Integral start(hz)	Integral end(hz)
*	1	175.768	100.000	0.4991E+10	14272.04	14227.05
*	2	146.502	3.418	0.1706E+09	11882.93	11871.42
*	3	140.325	0.053	0.2653E+07	11379.84	11373.05
*	4	140.294	0.057	0.2844E+07	11377.47	11370.68
*	5	140.286	0.058	0.2891E+07	11376.58	11369.79
*	6	140.260	0.061	0.3021E+07	11374.51	11367.72
*	7	140.222	0.064	0.3199E+07	11371.55	11364.76
*	8	140.208	0.070	0.3501E+07	11370.36	11363.57
*	9	140.177	0.067	0.3336E+07	11367.70	11360.91
*	10	140.154	0.070	0.3491E+07	11365.92	11359.13
*	11	140.135	0.071	0.3531E+07	11364.44	11357.65
*	12	140.125	0.070	0.3484E+07	11363.55	11356.76
*	13	140.112	0.074	0.3694E+07	11362.66	11355.87
*	14	140.092	0.071	0.3569E+07	11360.88	11354.09
*	15	140.064	0.077	0.3861E+07	11358.51	11351.72
*	16	140.042	0.078	0.3911E+07	11356.73	11349.94
*	17	140.032	0.080	0.3971E+07	11356.14	11349.35
*	18	140.018	0.078	0.3907E+07	11354.96	11348.17
*	19	139.999	0.083	0.4132E+07	11353.47	11346.68
*	20	139.981	0.087	0.4343E+07	11351.99	11345.20
*	21	139.963	0.087	0.4336E+07	11350.51	11343.72
*	22	139.955	0.088	0.4403E+07	11349.92	11343.13
*	23	139.939	0.089	0.4429E+07	11348.44	11341.65
*	24	139.915	0.091	0.4529E+07	11346.66	11339.87
*	25	139.896	0.096	0.4787E+07	11345.18	11338.39
*	26	139.874	0.092	0.4594E+07	11343.40	11336.61
*	27	139.843	0.099	0.4963E+07	11340.73	11333.94
*	28	139.831	0.100	0.5009E+07	11339.84	11333.05
*	29	139.821	0.102	0.5081E+07	11338.96	11332.17
*	30	139.798	0.105	0.5234E+07	11337.18	11330.39
*	31	139.785	0.103	0.5156E+07	11335.99	11329.20
*	32	139.772	0.108	0.5371E+07	11335.10	11328.31
*	33	139.744	0.110	0.5506E+07	11332.73	11325.94
*	34	139.724	0.114	0.5706E+07	11330.96	11324.17
*	35	139.698	0.119	0.5931E+07	11328.88	11322.09
*	36	139.677	0.121	0.6041E+07	11327.40	11320.61
*	37	139.663	0.127	0.6335E+07	11326.22	11319.43
*	38	139.653	0.126	0.6299E+07	11325.33	11318.54
*	39	139.605	0.135	0.6750E+07	11321.48	11314.69
*	40	139.579	0.141	0.7030E+07	11319.40	11312.61
*	41	139.563	0.143	0.7122E+07	11317.92	11311.13
*	42	139.529	0.147	0.7323E+07	11315.25	11308.46
*	43	139.512	0.149	0.7447E+07	11314.07	11307.28
*	44	139.451	0.168	0.8370E+07	11309.03	11302.24
*	45	139.426	0.168	0.8393E+07	11306.96	11300.17
*	46	139.413	0.169	0.8423E+07	11305.77	11298.98
*	47	139.349	0.190	0.9464E+07	11300.74	11293.95
*	48	139.292	0.202	0.1008E+08	11295.99	11289.20
*	49	139.279	0.205	0.1022E+08	11295.11	11288.32
*	50	139.260	0.205	0.1021E+08	11293.33	11286.54
*	51	139.233	0.205	0.1025E+08	11291.25	11284.46
*	52	139.223	0.207	0.1032E+08	11290.37	11283.58
*	53	139.210	0.206	0.1027E+08	11289.48	11282.69
*	54	139.197	0.208	0.1040E+08	11288.29	11281.50

*	55	139.182	0.206	0.1029E+08	11287.11	11280.32
*	56	139.167	0.210	0.1049E+08	11285.92	11279.13
*	57	139.160	0.211	0.1051E+08	11285.33	11278.54
*	58	139.148	0.211	0.1054E+08	11284.44	11277.65
*	59	139.111	0.216	0.1081E+08	11281.48	11274.69
*	60	139.081	0.217	0.1081E+08	11279.11	11272.32
*	61	139.072	0.216	0.1080E+08	11278.22	11271.43
*	62	139.064	0.217	0.1085E+08	11277.63	11270.83
*	63	139.025	0.219	0.1093E+08	11274.37	11267.58
*	64	139.003	0.222	0.1109E+08	11272.59	11265.80
*	65	138.980	0.223	0.1113E+08	11270.81	11264.02
*	66	138.969	0.227	0.1135E+08	11269.92	11263.13
*	67	138.951	0.228	0.1137E+08	11268.44	11261.65
*	68	138.933	0.231	0.1152E+08	11266.96	11260.17
*	69	138.905	0.239	0.1194E+08	11264.59	11257.80
*	70	138.885	0.234	0.1169E+08	11263.11	11256.32
*	71	138.871	0.243	0.1214E+08	11261.92	11255.13
*	72	138.853	0.243	0.1211E+08	11260.44	11253.65
*	73	138.834	0.249	0.1240E+08	11258.96	11252.17
*	74	138.820	0.250	0.1248E+08	11257.77	11250.98
*	75	138.798	0.258	0.1287E+08	11256.00	11249.21
*	76	138.782	0.260	0.1300E+08	11254.81	11248.02
*	77	138.771	0.259	0.1293E+08	11253.92	11247.13
*	78	138.738	0.265	0.1321E+08	11251.25	11244.46
*	79	138.728	0.266	0.1329E+08	11250.37	11243.58
*	80	138.685	0.282	0.1408E+08	11246.81	11240.02
*	81	138.662	0.284	0.1419E+08	11245.03	11238.24
*	82	138.651	0.284	0.1416E+08	11244.14	11237.35
*	83	138.615	0.291	0.1453E+08	11241.18	11234.39
*	84	138.579	0.283	0.1412E+08	11238.22	11231.43
*	85	138.549	0.269	0.1343E+08	11235.85	11229.06
*	86	138.530	0.264	0.1317E+08	11234.37	11227.58
*	87	138.482	0.233	0.1162E+08	11230.52	11223.72
*	88	138.460	0.226	0.1127E+08	11228.74	11221.95
*	89	138.450	0.222	0.1110E+08	11227.85	11221.06
*	90	138.336	0.162	0.8107E+07	11218.66	11211.87
*	91	138.297	0.149	0.7442E+07	11215.40	11208.61
*	92	138.264	0.138	0.6904E+07	11212.74	11205.95
*	93	138.223	0.124	0.6184E+07	11209.48	11202.69
*	94	138.194	0.114	0.5692E+07	11207.11	11200.32
*	95	138.173	0.107	0.5346E+07	11205.33	11198.54
*	96	138.163	0.105	0.5264E+07	11204.44	11197.65
*	97	138.144	0.106	0.5304E+07	11202.96	11196.17
*	98	138.119	0.099	0.4960E+07	11200.89	11194.10
*	99	138.082	0.091	0.4544E+07	11197.92	11191.13
*	100	138.067	0.086	0.4303E+07	11196.74	11189.95
*	101	138.028	0.087	0.4325E+07	11193.48	11186.69
*	102	138.005	0.078	0.3896E+07	11191.70	11184.91
*	103	137.993	0.077	0.3828E+07	11190.81	11184.02
*	104	137.987	0.078	0.3872E+07	11190.22	11183.43
*	105	137.953	0.073	0.3659E+07	11187.55	11180.76
*	106	137.917	0.067	0.3332E+07	11184.59	11177.80
*	107	137.895	0.065	0.3241E+07	11182.81	11176.02
*	108	137.883	0.064	0.3205E+07	11181.92	11175.13
*	109	137.841	0.058	0.2916E+07	11178.37	11171.58
*	110	137.816	0.058	0.2888E+07	11176.29	11169.50
*	111	137.760	0.059	0.2926E+07	11171.85	11165.06
*	112	137.730	0.060	0.3010E+07	11169.48	11162.69
*	113	132.766	4.280	0.2137E+09	10769.09	10758.36
*	114	131.763	0.132	0.6598E+07	10691.95	10672.55
*	115	131.637	0.113	0.5627E+07	10680.43	10663.92

(*) Peaks 1 to 115 are fitted to Lorentzian

NMR1
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Filename = TCS2
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 654.061

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14260.86	175.902	100.000	0.5260E+08	8.92
*	2	11889.81	146.656	64.531	0.3394E+08	4.68
*	3	11388.81	140.477	1.300	0.6837E+06	1.25
*	4	11387.63	140.462	1.253	0.6592E+06	1.25
*	5	11386.20	140.445	1.246	0.6554E+06	1.25
*	6	11384.84	140.428	1.265	0.6655E+06	1.25
*	7	11383.09	140.406	1.431	0.7525E+06	1.25
*	8	11381.16	140.382	1.310	0.6891E+06	1.25
*	9	11378.97	140.355	1.301	0.6845E+06	1.25
*	10	11378.09	140.345	1.352	0.7113E+06	1.25
*	11	11375.32	140.310	1.404	0.7387E+06	1.25
*	12	11374.04	140.295	1.435	0.7550E+06	1.25
*	13	11372.18	140.272	1.430	0.7524E+06	1.25
*	14	11370.57	140.252	1.448	0.7615E+06	1.25
*	15	11367.94	140.219	1.657	0.8713E+06	1.25
*	16	11366.80	140.205	1.572	0.8267E+06	1.25
*	17	11366.07	140.196	1.557	0.8187E+06	1.25
*	18	11365.12	140.185	1.612	0.8478E+06	1.25
*	19	11363.88	140.169	1.712	0.9006E+06	1.25
*	20	11362.71	140.155	1.589	0.8356E+06	1.25
*	21	11360.97	140.133	1.763	0.9271E+06	1.25
*	22	11358.28	140.100	1.894	0.9962E+06	1.25
*	23	11354.37	140.052	1.914	0.1007E+07	1.25
*	24	11352.83	140.033	1.951	0.1026E+07	1.25
*	25	11351.74	140.019	2.083	0.1095E+07	1.25
*	26	11350.42	140.003	2.108	0.1109E+07	1.25
*	27	11349.41	139.991	2.115	0.1112E+07	1.25
*	28	11348.41	139.978	2.154	0.1133E+07	1.25
*	29	11346.66	139.957	2.198	0.1156E+07	1.25
*	30	11345.53	139.943	2.240	0.1178E+07	1.25
*	31	11344.65	139.932	2.364	0.1243E+07	1.25
*	32	11343.51	139.918	2.424	0.1275E+07	1.25
*	33	11340.23	139.878	2.443	0.1285E+07	1.25
*	34	11339.39	139.867	2.473	0.1301E+07	1.25
*	35	11336.65	139.833	2.615	0.1375E+07	1.25
*	36	11334.89	139.812	2.883	0.1516E+07	1.25
*	37	11331.17	139.766	2.984	0.1569E+07	1.25
*	38	11328.66	139.735	3.029	0.1593E+07	1.25
*	39	11328.06	139.727	3.036	0.1597E+07	1.25
*	40	11327.39	139.719	3.059	0.1609E+07	1.25
*	41	11325.57	139.697	3.080	0.1620E+07	1.25
*	42	11324.70	139.686	3.166	0.1665E+07	1.25
*	43	11322.69	139.661	3.400	0.1788E+07	1.25
*	44	11321.72	139.649	3.352	0.1763E+07	1.25

*	45	11320.83	139.638	3.315	0.1743E+07	1.25
*	46	11317.96	139.603	3.545	0.1865E+07	1.25
*	47	11317.03	139.591	3.520	0.1851E+07	1.25
*	48	11315.04	139.567	3.688	0.1940E+07	1.25
*	49	11313.49	139.548	3.705	0.1949E+07	1.25
*	50	11311.30	139.521	4.090	0.2151E+07	1.25
*	51	11307.89	139.479	4.087	0.2149E+07	1.25
*	52	11306.08	139.456	4.312	0.2268E+07	1.25
*	53	11305.21	139.446	4.425	0.2327E+07	1.25
*	54	11303.47	139.424	4.491	0.2362E+07	1.25
*	55	11302.29	139.410	4.369	0.2298E+07	1.25
*	56	11300.86	139.392	4.342	0.2284E+07	1.25
*	57	11298.40	139.362	4.420	0.2325E+07	1.25
*	58	11296.61	139.340	4.509	0.2371E+07	1.25
*	59	11295.57	139.327	4.520	0.2378E+07	1.25
*	60	11294.43	139.313	4.613	0.2426E+07	1.25
*	61	11292.14	139.284	4.578	0.2408E+07	1.25
*	62	11290.98	139.270	4.576	0.2407E+07	1.25
*	63	11290.01	139.258	4.667	0.2455E+07	1.25
*	64	11286.91	139.220	4.580	0.2409E+07	1.25
*	65	11285.05	139.197	4.719	0.2482E+07	1.25
*	66	11283.31	139.175	4.616	0.2428E+07	1.25
*	67	11282.44	139.165	4.569	0.2403E+07	1.25
*	68	11281.57	139.154	4.616	0.2428E+07	1.25
*	69	11280.36	139.139	4.733	0.2489E+07	1.25
*	70	11277.01	139.098	4.756	0.2502E+07	1.25
*	71	11274.99	139.073	4.810	0.2530E+07	1.25
*	72	11274.11	139.062	4.939	0.2598E+07	1.25
*	73	11273.17	139.050	4.892	0.2573E+07	1.25
*	74	11270.95	139.023	5.134	0.2700E+07	1.25
*	75	11269.46	139.005	5.049	0.2656E+07	1.25
*	76	11268.14	138.988	5.191	0.2730E+07	1.25
*	77	11266.36	138.966	5.111	0.2688E+07	1.25
*	78	11265.04	138.950	5.174	0.2722E+07	1.25
*	79	11263.42	138.930	5.203	0.2737E+07	1.25
*	80	11262.32	138.917	5.284	0.2779E+07	1.25
*	81	11260.28	138.891	5.400	0.2840E+07	1.25
*	82	11259.65	138.884	5.408	0.2844E+07	1.25
*	83	11256.82	138.849	5.559	0.2924E+07	1.25
*	84	11254.36	138.818	5.618	0.2955E+07	1.25
*	85	11252.92	138.801	5.747	0.3023E+07	1.25
*	86	11252.19	138.792	5.740	0.3019E+07	1.25
*	87	11251.51	138.783	5.770	0.3035E+07	1.25
*	88	11248.55	138.747	5.954	0.3132E+07	1.25
*	89	11247.73	138.737	5.947	0.3128E+07	1.25
*	90	11245.73	138.712	5.741	0.3019E+07	1.25
*	91	11244.49	138.697	5.801	0.3051E+07	1.25
*	92	11242.94	138.678	5.491	0.2888E+07	1.25
*	93	11240.97	138.653	5.378	0.2829E+07	1.25
*	94	11240.36	138.646	5.386	0.2833E+07	1.25
*	95	11237.96	138.616	5.209	0.2740E+07	1.25
*	96	11234.79	138.577	4.727	0.2486E+07	1.25
*	97	11233.82	138.565	4.656	0.2449E+07	1.25
*	98	11232.67	138.551	4.462	0.2347E+07	1.25
*	99	11228.90	138.504	3.932	0.2068E+07	1.25
*	100	11227.13	138.483	3.596	0.1892E+07	1.25
*	101	11225.88	138.467	3.463	0.1821E+07	1.25
*	102	11222.15	138.421	3.077	0.1619E+07	1.25
*	103	11220.73	138.404	3.031	0.1594E+07	1.25
*	104	11218.93	138.381	2.895	0.1523E+07	1.25
*	105	11215.54	138.340	2.642	0.1390E+07	1.25
*	106	11213.85	138.319	2.582	0.1358E+07	1.25
*	107	11212.05	138.296	2.363	0.1243E+07	1.25
*	108	11210.39	138.276	2.327	0.1224E+07	1.25
*	109	11209.24	138.262	2.235	0.1175E+07	1.25
*	110	11205.64	138.217	2.060	0.1084E+07	1.25

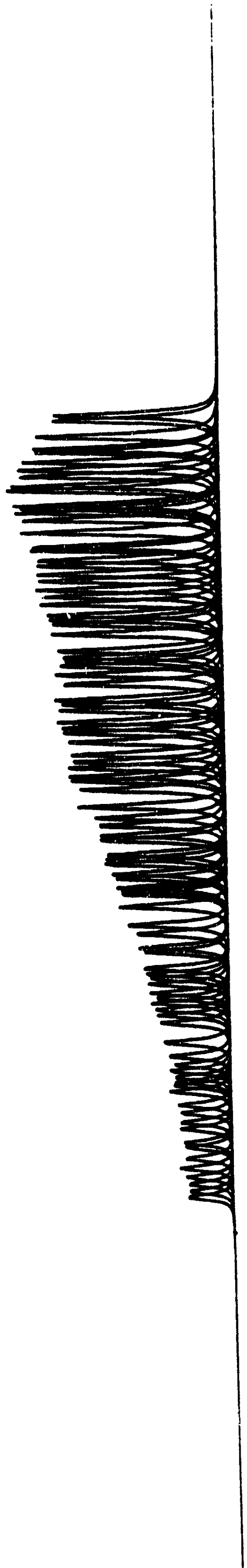
*	111	11204.49	138.203	1.934	0.1017E+07	1.25
*	112	11203.26	138.188	1.820	0.9571E+06	1.25
*	113	11202.20	138.175	1.773	0.9324E+06	1.25
*	114	11200.33	138.152	1.808	0.9508E+06	1.25
*	115	11199.19	138.138	1.640	0.8627E+06	1.25
*	116	11197.76	138.120	1.713	0.9009E+06	1.25
*	117	11196.56	138.105	1.687	0.8872E+06	1.25
*	118	11194.68	138.082	1.545	0.8126E+06	1.25
*	119	11193.97	138.074	1.597	0.8399E+06	1.25
*	120	11191.75	138.046	1.484	0.7804E+06	1.25
*	121	11190.00	138.024	1.363	0.7168E+06	1.25
*	122	11189.10	138.013	1.330	0.6995E+06	1.25
*	123	11187.85	137.998	1.371	0.7209E+06	1.25
*	124	11186.95	137.987	1.399	0.7360E+06	1.25
*	125	11185.70	137.972	1.418	0.7456E+06	1.25
*	126	11184.54	137.957	1.282	0.6740E+06	1.25
*	127	11182.89	137.937	1.287	0.6771E+06	1.25
*	128	11181.98	137.926	1.316	0.6924E+06	1.25
*	129	11179.88	137.900	1.277	0.6717E+06	1.25
*	130	10774.84	132.904	34.689	0.1824E+08	3.40
*	131	10735.68	132.421	0.396	0.2083E+06	33.34
*	132	10693.30	131.898	1.215	0.6389E+06	3.44
*	133	10682.63	131.766	1.208	0.6353E+06	3.63

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.902	100.000	0.1244E+10	14265.04	14256.12
*	2	146.656	33.861	0.4211E+09	11892.03	11887.35
*	3	140.477	0.182	0.2264E+07	11389.29	11388.04
*	4	140.462	0.176	0.2183E+07	11388.11	11386.86
*	5	140.445	0.175	0.2171E+07	11386.63	11385.38
*	6	140.428	0.177	0.2204E+07	11385.44	11384.19
*	7	140.406	0.200	0.2492E+07	11383.66	11382.41
*	8	140.382	0.184	0.2283E+07	11381.59	11380.34
*	9	140.355	0.182	0.2267E+07	11379.51	11378.27
*	10	140.345	0.189	0.2356E+07	11378.63	11377.38
*	11	140.310	0.197	0.2447E+07	11375.9[illegible]	11374.71
*	12	140.295	0.201	0.2501E+07	11374.4[illegible]	11373.23
*	13	140.272	0.200	0.2492E+07	11372.70	11371.45
*	14	140.252	0.203	0.2522E+07	11371.22	11369.97
*	15	140.219	0.232	0.2886E+07	11368.55	11367.30
*	16	140.205	0.220	0.2738E+07	11367.37	11366.12
*	17	140.196	0.218	0.2712E+07	11366.48	11365.23
*	18	140.185	0.226	0.2808E+07	11365.59	11364.34
*	19	140.169	0.240	0.2983E+07	11364.40	11363.16
*	20	140.155	0.223	0.2768E+07	11363.22	11361.97
*	21	140.133	0.247	0.3071E+07	11361.44	11360.19
*	22	140.100	0.265	0.3300E+07	11358.77	11357.53
*	23	140.052	0.268	0.3334E+07	11354.92	11353.67
*	24	140.033	0.273	0.3399E+07	11353.44	11352.19
*	25	140.019	0.292	0.3628E+07	11352.26	11351.01
*	26	140.003	0.295	0.3673E+07	11351.07	11349.82
*	27	139.991	0.296	0.3684E+07	11349.89	11348.64
*	28	139.978	0.302	0.3753E+07	11349.00	11347.75
*	29	139.957	0.308	0.3829E+07	11347.22	11345.97
*	30	139.943	0.314	0.3903E+07	11346.03	11344.79
*	31	139.932	0.331	0.4119E+07	11345.15	11343.90
*	32	139.918	0.340	0.4223E+07	11343.96	11342.71
*	33	139.878	0.342	0.4257E+07	11340.70	11339.45
*	34	139.867	0.346	0.4309E+07	11339.81	11338.56
*	35	139.833	0.366	0.4555E+07	11337.15	11335.90
*	36	139.812	0.404	0.5023E+07	11335.37	11334.12

*	37	139.766	0.418	0.5198E+07	11331.81	11330.56
*	38	139.735	0.424	0.5276E+07	11329.15	11327.90
*	39	139.727	0.425	0.5289E-07	11328.55	11327.30
*	40	139.719	0.428	0.5329E+07	11327.96	11326.71
*	41	139.697	0.431	0.5367E+07	11326.18	11324.93
*	42	139.686	0.443	0.5515E+07	11325.29	11324.04
*	43	139.661	0.476	0.5923E+07	11323.22	11321.97
*	44	139.649	0.470	0.5839E+07	11322.33	11321.08
*	45	139.638	0.464	0.5774E+07	11321.44	11320.19
*	46	139.603	0.497	0.6176E+07	11318.48	11317.23
*	47	139.591	0.493	0.6132E+07	11317.59	11316.34
*	48	139.567	0.517	0.6425E+07	11315.52	11314.27
*	49	139.548	0.519	0.6455E+07	11314.04	11312.79
*	50	139.521	0.573	0.7126E+07	11311.96	11310.71
*	51	139.479	0.572	0.7119E+07	11308.41	11307.16
*	52	139.456	0.604	0.7512E+07	11306.63	11305.38
*	53	139.446	0.620	0.7709E+07	11305.74	11304.49
*	54	139.424	0.629	0.7823E+07	11303.96	11302.71
*	55	139.410	0.612	0.7611E+07	11302.78	11301.53
*	56	139.392	0.608	0.7564E+07	11301.29	11300.05
*	57	139.362	0.619	0.7700E+07	11298.92	11297.68
*	58	139.340	0.632	0.7855E+07	11297.15	11295.90
*	59	139.327	0.633	0.7875E+07	11296.26	11295.01
*	60	139.313	0.646	0.8037E+07	11295.07	11293.82
*	61	139.284	0.641	0.7975E+07	11292.70	11291.45
*	62	139.270	0.641	0.7971E+07	11291.52	11290.27
*	63	139.258	0.654	0.8130E+07	11290.63	11289.38
*	64	139.220	0.642	0.7979E+07	11287.37	11286.12
*	65	139.197	0.661	0.8221E+07	11285.59	11284.34
*	66	139.175	0.647	0.8041E+07	11283.81	11282.56
*	67	139.165	0.640	0.7959E+07	11282.93	11281.68
*	68	139.154	0.647	0.8042E+07	11282.04	11280.79
*	69	139.139	0.663	0.8245E+07	11280.85	11279.60
*	70	139.098	0.666	0.8286E+07	11277.59	11276.34
*	71	139.073	0.674	0.8380E+07	11275.52	11274.27
*	72	139.062	0.692	0.8605E+07	11274.63	11273.38
*	73	139.050	0.685	0.8523E+07	11273.74	11272.49
*	74	139.023	0.719	0.8945E+07	11271.37	11270.12
*	75	139.005	0.707	0.8797E+07	11269.89	11268.64
*	76	138.988	0.727	0.9043E+07	11268.70	11267.45
*	77	138.966	0.716	0.8905E+07	11266.93	11265.68
*	78	138.950	0.725	0.9014E+07	11265.74	11264.49
*	79	138.930	0.729	0.9064E+07	11263.96	11262.71
*	80	138.917	0.740	0.9206E+07	11262.78	11261.53
*	81	138.891	0.756	0.9407E+07	11260.70	11259.45
*	82	138.884	0.758	0.9421E+07	11260.11	11258.86
*	83	138.849	0.779	0.9685E+07	11257.44	11256.20
*	84	138.818	0.787	0.9787E+07	11254.78	11253.53
*	85	138.801	0.805	0.1001E+08	11253.59	11252.34
*	86	138.792	0.804	0.9999E+07	11252.70	11251.46
*	87	138.783	0.808	0.1005E+08	11252.11	11250.86
*	88	138.747	0.834	0.1037E+08	11249.15	11247.90
*	89	138.737	0.833	0.1036E+08	11248.26	11247.01
*	90	138.712	0.804	0.1000E+08	11246.19	11244.94
*	91	138.697	0.813	0.1011E+08	11245.00	11243.75
*	92	138.678	0.769	0.9566E+07	11243.52	11242.27
*	93	138.653	0.753	0.9369E+07	11241.45	11240.20
*	94	138.646	0.754	0.9382E+07	11240.85	11239.60
*	95	138.616	0.730	0.9074E+07	11238.48	11237.23
*	96	138.577	0.662	0.8235E+07	11235.22	11233.97
*	97	138.565	0.652	0.8112E+07	11234.33	11233.08
*	98	138.551	0.625	0.7774E+07	11233.15	11231.90
*	99	138.504	0.551	0.6850E+07	11229.59	11228.34
*	100	138.483	0.504	0.6266E+07	11227.82	11226.57
*	101	138.467	0.485	0.6032E+07	11226.33	11225.08
*	102	138.421	0.431	0.5361E+07	11222.78	11221.53

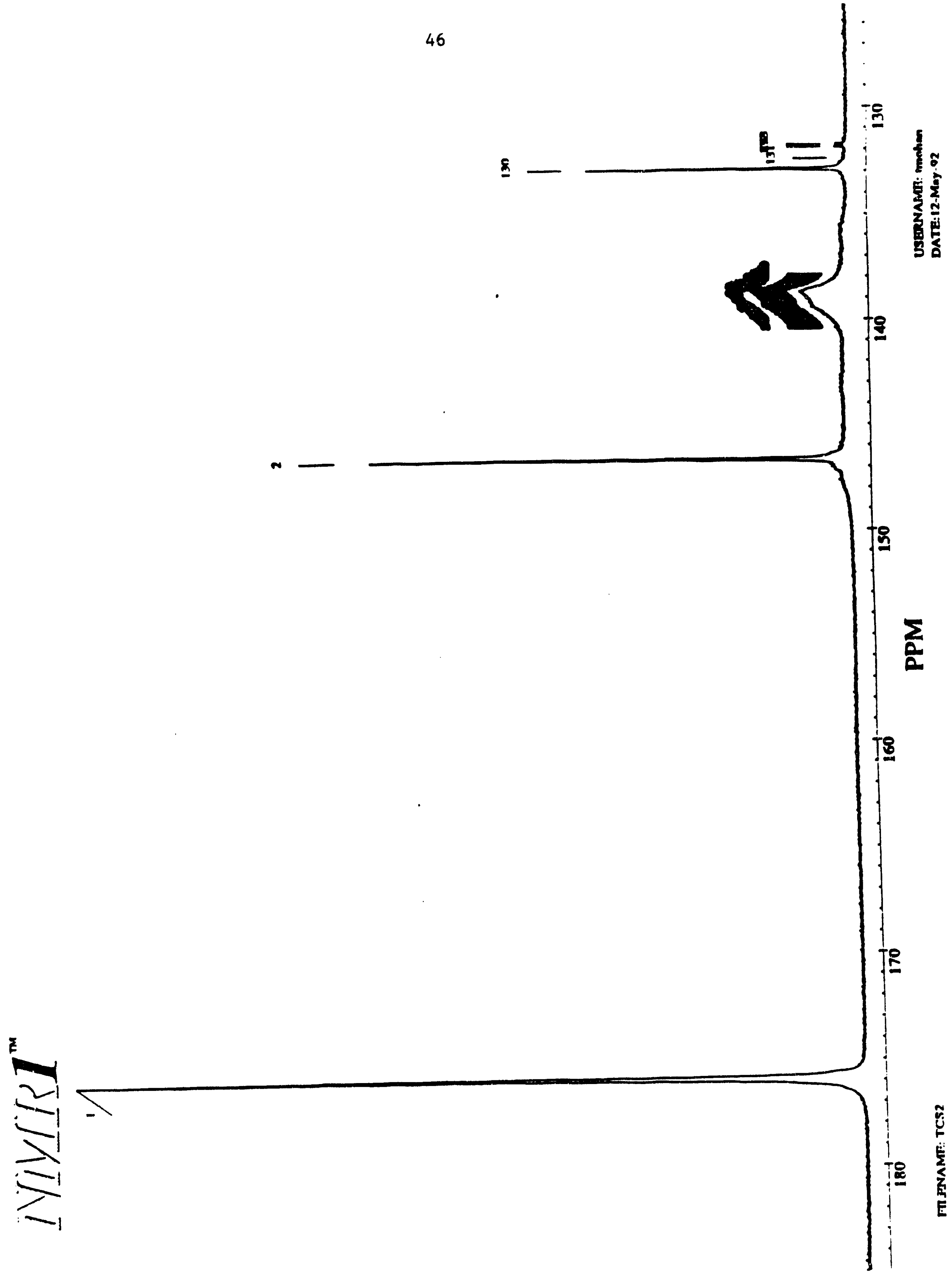
*	103	138.404	0.425	0.5280E+07	11221.30	11220.05
*	104	138.381	0.406	0.5044E+07	11219.52	11218.27
*	105	138.340	0.370	0.4603E+07	11215.96	11214.71
*	106	138.319	0.362	0.4498E+07	11214.48	11213.23
*	107	138.296	0.331	0.4116E+07	11212.71	11211.46
*	108	138.276	0.326	0.4054E+07	11210.93	11209.68
*	109	138.262	0.313	0.3893E+07	11209.74	11208.49
*	110	138.217	0.289	0.3589E+07	11206.19	11204.94
*	111	138.203	0.271	0.3369E+07	11205.00	11203.75
*	112	138.188	0.255	0.3170E+07	11203.82	11202.57
*	113	138.175	0.248	0.3088E+07	11202.63	11201.38
*	114	138.152	0.253	0.3149E+07	11200.85	11199.60
*	115	138.138	0.230	0.2858E+07	11199.67	11198.42
*	116	138.120	0.240	0.2984E+07	11198.19	11196.94
*	117	138.105	0.236	0.2939E+07	11197.00	11195.75
*	118	138.082	0.216	0.2692E+07	11195.22	11193.97
*	119	138.074	0.224	0.2782E+07	11194.63	11193.38
*	120	138.046	0.208	0.2585E+07	11192.26	11191.01
*	121	138.024	0.191	0.2374E+07	11190.48	11189.23
*	122	138.013	0.186	0.2317E+07	11189.59	11188.35
*	123	137.998	0.192	0.2388E+07	11188.41	11187.16
*	124	137.987	0.196	0.2438E+07	11187.52	11186.27
*	125	137.972	0.199	0.2469E+07	11186.34	11185.09
*	126	137.957	0.180	0.2233E+07	11185.15	11183.90
*	127	137.937	0.180	0.2243E+07	11183.37	11182.12
*	128	137.926	0.184	0.2293E+07	11182.48	11181.23
*	129	137.900	0.179	0.2225E+07	11180.41	11179.16
*	130	132.904	13.219	0.1644E+09	10776.46	10773.06
*	131	132.421	1.480	0.1840E+08	10752.32	10718.98
*	132	131.898	0.469	0.5828E+07	10695.00	10691.56
*	133	131.766	0.492	0.6117E+07	10684.43	10680.80

(*) Peaks 1 to 133 are fitted to Lorentzian



USERNAME: tmohan

NMR1™



130
2
1
130
140
150
160
170
180
PPM
DATE:12-May-92
FILENAME: TCS2

NMR1
****

Filename = TCS3
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 3262.34

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14248.80	175.754	100.000	0.1251E+09	9.35
*	2	11876.97	146.498	13.761	0.1721E+08	3.69
*	3	11316.79	139.589	0.072	0.9024E+05	5.35
*	4	11327.02	139.715	0.161	0.2012E+06	34.00
*	5	11379.11	140.357	0.064	0.7979E+05	130.70
*	6	11280.23	139.137	0.009	0.1097E+05	18.27
*	7	11309.19	139.495	0.164	0.2053E+06	12.88
*	8	11299.45	139.375	0.156	0.1951E+06	10.96
*	9	11291.39	139.275	0.138	0.1725E+06	11.62
*	10	11298.10	139.358	0.051	0.6411E+05	48.37
*	11	11352.50	140.029	0.105	0.1312E+06	52.68
*	12	11278.28	139.113	0.011	0.1314E+05	8.40
*	13	11282.81	139.169	0.106	0.1323E+06	15.33
*	14	11240.92	138.653	0.027	0.3400E+05	141.39
*	15	11291.69	139.279	0.042	0.5310E+05	28.14
*	16	11285.22	139.199	0.107	0.1344E+06	16.74
*	17	11499.22	141.839	0.034	0.4311E+05	115.45
*	18	11278.13	139.112	0.123	0.1542E+06	13.06
*	19	11218.08	138.371	0.003	3506.	128.74
*	20	11272.25	139.039	0.058	0.7205E+05	6.62
*	21	11272.66	139.044	0.051	0.6420E+05	14.56
*	22	11271.35	139.028	0.024	0.2971E+05	19.38
*	23	11267.61	138.982	0.139	0.1734E+06	14.69
*	24	10767.80	132.817	0.034	0.4261E+05	85.29
*	25	11262.06	138.913	0.111	0.1386E+06	16.41
*	26	11261.06	138.901	0.104	0.1299E+06	13.73
*	27	11259.96	138.887	0.027	0.3341E+05	9.88
*	28	11253.91	138.813	0.084	0.1048E+06	7.80
*	29	11256.40	138.844	0.067	0.8399E+05	10.42
*	30	11249.83	138.762	0.034	0.4201E+05	1.79
*	31	11238.01	138.617	0.064	0.8062E+05	1.44
*	32	11250.45	138.770	0.178	0.2229E+06	11.99
*	33	11243.99	138.690	0.202	0.2532E+06	10.93
*	34	11238.96	138.628	0.111	0.1383E+06	12.71
*	35	11242.05	138.667	0.092	0.1154E+06	9.63
*	36	11234.63	138.575	0.217	0.2719E+06	11.39
*	37	11229.50	138.512	0.230	0.2882E+06	12.98
*	38	11224.81	138.454	0.139	0.1735E+06	13.86
*	39	11529.70	142.215	0.003	3770.	143.22
*	40	11219.00	138.382	0.105	0.1317E+06	15.26
*	41	11213.20	138.311	0.093	0.1162E+06	25.15
*	42	11201.46	138.166	0.196	0.2445E+06	51.62
*	43	10762.99	132.757	10.105	0.1264E+08	3.44

Peak #	PPM	Relative integral	Absolute integral	Integral start(hz)	Integral end(hz)
* 1	175.754	100.000	0.1550E+10	14252.74	14243.39
* 2	146.498	5.438	0.8427E+08	11878.43	11874.73
* 3	139.589	0.041	0.6400E+06	11319.27	11313.92
* 4	139.715	0.585	0.9068E+07	11343.67	11309.67
* 5	140.357	0.892	0.1382E+08	11444.17	11313.47
* 6	139.137	0.017	0.2656E+06	11288.99	11270.72
* 7	139.495	0.226	0.3504E+07	11315.33	11302.46
* 8	139.375	0.183	0.2832E+07	11304.89	11293.94
* 9	139.275	0.172	0.2658E+07	11296.93	11285.31
* 10	139.358	0.265	0.4110E+07	11322.42	11274.04
* 11	140.029	0.591	0.9158E+07	11378.49	11325.81
* 12	139.113	0.009	0.1464E+06	11282.28	11273.88
* 13	139.169	0.173	0.2687E+07	11290.49	11275.16
* 14	138.653	0.411	0.6371E+07	11311.44	11170.05
* 15	139.279	0.128	0.1981E+07	11305.78	11277.64
* 16	139.199	0.192	0.2981E+07	11293.56	11276.82
* 17	141.839	0.426	0.6596E+07	11556.84	11441.39
* 18	139.112	0.172	0.2669E+07	11284.61	11271.55
* 19	138.371	0.039	0.5981E+06	11282.60	11153.86
* 20	139.039	0.041	0.6321E+06	11275.46	11268.85
* 21	139.044	0.080	0.1239E+07	11280.03	11265.47
* 22	139.028	0.049	0.7631E+06	11280.66	11261.28
* 23	138.982	0.218	0.3376E+07	11274.76	11260.07
* 24	132.817	0.311	0.4818E+07	10810.52	10725.23
* 25	138.913	0.195	0.3016E+07	11270.29	11253.88
* 26	138.901	0.153	0.2364E+07	11267.76	11254.03
* 27	138.887	0.028	0.4376E+06	11264.65	11254.77
* 28	138.813	0.070	0.1084E+07	11257.69	11249.89
* 29	138.844	0.075	0.1159E+07	11261.36	11250.95
* 30	138.762	0.006	0.9977E+05	11250.53	11248.74
* 31	138.617	0.010	0.1537E+06	11238.51	11237.07
* 32	138.770	0.229	0.3542E+07	11256.23	11244.24
* 33	138.690	0.237	0.3666E+07	11249.17	11238.25
* 34	138.628	0.150	0.2330E+07	11245.33	11232.62
* 35	138.667	0.095	0.1473E+07	11246.75	11237.12
* 36	138.575	0.265	0.4104E+07	11239.93	11228.54
* 37	138.512	0.320	0.4958E+07	11235.98	11223.00
* 38	138.454	0.206	0.3186E+07	11231.68	11217.82
* 39	142.215	0.046	0.7156E+06	11600.94	11457.72
* 40	138.382	0.172	0.2665E+07	11226.45	11211.19
* 41	138.311	0.250	0.3875E+07	11225.47	11200.32
* 42	138.166	1.080	0.1673E+08	11226.86	11175.24
* 43	132.757	3.716	0.5759E+08	10764.85	10761.42

*) Peaks 1 to 43 are fitted to Lorentzian

NMR1
****

Filename = TCS4
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 1705.98

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14254.34	175.822	100.000	0.1096E+09	9.93
*	2	11879.64	146.531	13.613	0.1492E+08	4.08
*	3	11877.98	146.511	5.232	0.5735E+07	1.17
*	4	11272.39	139.041	0.065	0.7113E+05	2.53
*	5	11291.05	139.271	0.024	0.2677E+05	0.52
*	6	11301.67	139.402	0.308	0.3371E+06	98.20
*	7	11289.72	139.255	0.137	0.1497E+06	88.52
*	8	11294.53	139.314	0.025	0.2703E+05	5.52
*	9	11298.57	139.364	0.028	0.3019E+05	4.53
*	10	11821.64	145.816	0.001	1317.	4.99
*	11	11036.88	136.136	0.020	0.2165E+05	33.46
*	12	11291.87	139.281	0.049	0.5341E+05	10.42
*	13	11286.88	139.219	0.017	0.1830E+05	5.27
*	14	11285.47	139.202	0.068	0.7445E+05	2.15
*	15	11283.52	139.178	0.063	0.6930E+05	0.88
*	16	11282.04	139.160	0.097	0.1065E+06	1.03
*	17	11280.58	139.142	0.065	0.7114E+05	1.08
*	18	11278.89	139.121	0.121	0.1328E+06	1.51
*	19	11276.81	139.095	0.066	0.7218E+05	1.24
*	20	11274.83	139.071	0.109	0.1195E+06	2.15
*	21	11271.65	139.032	0.014	0.1489E+05	0.83
*	22	11270.75	139.021	0.091	0.9933E+05	0.40
*	23	11269.09	139.000	0.081	0.8891E+05	2.26
*	24	11265.52	138.956	0.146	0.1600E+06	6.96
*	25	11261.79	138.910	0.039	0.4323E+05	2.90
*	26	11347.09	139.962	0.014	0.1520E+05	6.08
*	27	11236.91	138.603	0.006	6375.	195.73
*	28	11258.53	138.870	0.096	0.1054E+06	5.59
*	29	11251.63	138.785	0.163	0.1783E+06	9.93
*	30	12372.32	152.608	0.010	0.1130E+05	4.19
*	31	11246.33	138.719	0.048	0.5297E+05	1.14
*	32	11245.28	138.706	0.071	0.7807E+05	6.00
*	33	11242.17	138.668	0.040	0.4402E+05	1.04
*	34	11296.11	139.333	0.001	1151.	10.17
*	35	11318.37	139.608	0.006	6184.	49.08
*	36	11237.37	138.609	0.239	0.2623E+06	13.66
*	37	11243.30	138.682	0.051	0.5548E+05	0.20
*	38	11227.02	138.481	0.089	0.9775E+05	15.43
*	39	11225.05	138.457	0.273	0.2993E+06	56.46
*	40	11240.77	138.651	0.039	0.4221E+05	0.70
*	41	10767.49	132.813	6.069	0.6652E+07	2.92
*	42	10765.48	132.788	4.827	0.5291E+07	2.28
*	43	10680.87	131.745	0.309	0.3388E+06	16.45

	Peak #	PPM	Relative integral	Absolute integral	Integral start(hz)	Integral end(hz)
*	1	175.822	100.000	0.1442E+10	14258.96	14249.03
*	2	146.531	5.597	0.8074E+08	11881.59	11877.50
*	3	146.511	0.616	0.8889E+07	11878.35	11877.18
*	4	139.041	0.017	0.2383E+06	11273.42	11270.89
*	5	139.271	0.001	0.1862E+05	11291.38	11290.86
*	6	139.402	3.041	0.4387E+08	11350.88	11252.68
*	7	139.255	1.218	0.1756E+08	11333.60	11245.08
*	8	139.314	0.014	0.1977E+06	11297.43	11291.91
*	9	139.364	0.013	0.1811E+06	11300.49	11295.97
*	10	145.816	0.001	8717.	11823.97	11818.97
*	11	136.136	0.067	0.9599E+06	11053.63	11020.17
*	12	139.281	0.051	0.7379E+06	11296.92	11286.50
*	13	139.219	0.009	0.1279E+06	11289.61	11284.33
*	14	139.202	0.015	0.2124E+06	11286.27	11284.12
*	15	139.178	0.006	0.8092E+05	11283.86	11282.97
*	16	139.160	0.010	0.1455E+06	11282.15	11281.12
*	17	139.142	0.007	0.1022E+06	11280.99	11279.91
*	18	139.121	0.018	0.2653E+06	11279.43	11277.92
*	19	139.095	0.008	0.1183E+06	11277.51	11276.28
*	20	139.071	0.024	0.3405E+06	11275.60	11273.45
*	21	139.032	0.001	0.1641E+05	11271.98	11271.15
*	22	139.021	0.004	0.5286E+05	11270.58	11270.18
*	23	139.000	0.018	0.2661E+06	11270.32	11268.06
*	24	138.956	0.102	0.1475E+07	11269.12	11262.16
*	25	138.910	0.012	0.1660E+06	11262.94	11260.04
*	26	139.962	0.008	0.1225E+06	11349.86	11343.78
*	27	138.603	0.115	0.1654E+07	11334.46	11138.74
*	28	138.870	0.054	0.7818E+06	11261.32	11255.73
*	29	138.785	0.163	0.2347E+07	11256.38	11246.45
*	30	152.608	0.004	0.6267E+05	12374.07	12369.88
*	31	138.719	0.006	0.7997E+05	11246.65	11245.51
*	32	138.706	0.043	0.6212E+06	11247.90	11241.90
*	33	138.668	0.004	0.6083E+05	11242.46	11241.41
*	34	139.333	0.001	0.1551E+05	11300.94	11290.78
*	35	139.608	0.028	0.4022E+06	11342.92	11293.84
*	36	138.609	0.329	0.4748E+07	11244.02	11230.37
*	37	138.682	0.001	0.1498E+05	11243.22	11243.02
*	38	138.481	0.139	0.1999E+07	11234.83	11219.41
*	39	138.457	1.553	0.2240E+08	11252.98	11196.52
*	40	138.651	0.003	0.3898E+05	11241.10	11240.40
*	41	132.813	1.786	0.2576E+08	10768.74	10765.82
*	42	132.788	1.106	0.1596E+08	10766.64	10764.37
*	43	131.745	0.512	0.7385E+07	10688.99	10672.54

(*) Peaks 1 to 43 are fitted to Lorentzian

NMR1
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Filename = TCS5
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 2965.44

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14260.90	175.903	100.000	0.1069E+09	8.58
*	2	11884.98	146.597	26.988	0.2885E+08	1.82
*	3	11353.15	140.037	0.027	0.2886E+05	3.48
*	4	10853.39	133.873	0.188	0.2007E+06	13.91
*	5	11313.21	139.544	0.021	0.2237E+05	20.65
*	6	11306.93	139.467	0.072	0.7647E+05	16.53
*	7	11311.06	139.518	0.219	0.2342E+06	82.50
*	8	11278.83	139.120	0.027	0.2933E+05	6.23
*	9	11299.44	139.374	0.063	0.6777E+05	6.35
*	10	11132.96	137.321	0.138	0.1477E+06	0.65
*	11	11238.75	138.626	0.014	0.1540E+05	3.31
*	12	11269.86	139.010	0.010	0.1064E+05	1.98
*	13	11293.88	139.306	0.056	0.5987E+05	7.04
*	14	10238.94	126.294	0.199	0.2124E+06	26.52
*	15	11286.73	139.218	0.042	0.4541E+05	0.88
*	16	11285.23	139.199	0.245	0.2615E+06	24.44
*	17	11278.56	139.117	0.003	2755.	7.21
*	18	11283.64	139.180	0.005	5593.	0.88
*	19	11319.88	139.627	0.026	0.2751E+05	46.55
*	20	11276.23	139.088	0.068	0.7313E+05	4.56
*	21	11275.32	139.077	0.018	0.1913E+05	3.09
*	22	11272.70	139.045	0.066	0.7048E+05	5.19
*	23	11269.06	139.000	0.121	0.1297E+06	7.76
*	24	11264.63	138.945	0.164	0.1756E+06	5.45
*	25	11262.25	138.916	0.047	0.5042E+05	1.78
*	26	11260.33	138.892	0.080	0.8564E+05	2.15
*	27	11257.25	138.854	0.079	0.8493E+05	3.70
*	28	11252.54	138.796	0.155	0.1655E+06	12.75
*	29	11253.35	138.806	0.136	0.1456E+06	15.14
*	30	11248.71	138.749	0.026	0.2828E+05	5.20
*	31	11245.12	138.704	0.150	0.1604E+06	9.52
*	32	11241.64	138.661	0.059	0.6264E+05	9.72
*	33	11235.62	138.587	0.249	0.2658E+06	16.17
*	34	11226.61	138.476	0.153	0.1635E+06	34.14
*	35	11228.16	138.495	0.021	0.2228E+05	0.52
*	36	10772.86	132.879	17.846	0.1908E+08	1.71
*	37	10691.94	131.881	1.100	0.1176E+07	2.20
*	38	10681.74	131.755	1.076	0.1151E+07	2.10

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)

*	1	175.903	100.000	0.2126E+10	14281.99	14239.10
*	2	146.597	5.725	0.1217E+09	11889.47	11880.37
*	3	140.037	0.011	0.2325E+06	11361.48	11344.09
*	4	133.873	0.304	0.6472E+07	10888.02	10818.46
*	5	139.544	0.050	0.1070E+07	11364.70	11261.47
*	6	139.467	0.138	0.2929E+07	11347.88	11265.25
*	7	139.518	2.107	0.4478E+08	11516,97	11104.45
*	8	139.120	0.020	0.4234E+06	11294.28	11263.14
*	9	139.374	0.047	0.9967E+06	11315.32	11283.59
*	10	137.321	0.010	0.2224E+06	11134.56	11131.32
*	11	138.626	0.006	0.1182E+06	11246.69	11230.14
*	12	139.010	0.002	0.4884E+05	11274.77	11264.87
*	13	139.306	0.046	0.9774E+06	11311.14	11275.92
*	14	126.294	0.614	0.1305E+08	10305.05	10172.44
*	15	139.218	0.004	0.9215E+05	11288.60	11284.23
*	16	139.199	0.697	0.1482E+08	11346.34	11224.12
*	17	139.117	0.002	0.4603E+05	11296.73	11260.69
*	18	139.180	0.001	0.1141E+05	11285.65	11281.25
*	19	139.627	0.140	0.2968E+07	11435.98	11203.22
*	20	139.088	0.036	0.7737E+06	11287.75	11264.93
*	21	139.077	0.006	0.1371E+06	11282.89	11267.42
*	22	139.045	0.040	0.8483E+06	11285.77	11259.80
*	23	139.000	0.110	0.2333E+07	11288.05	11249.23
*	24	138.945	0.104	0.2219E+07	11278.12	11250.86
*	25	138.916	0.010	0.2082E+06	11266.58	11257.67
*	26	138.892	0.020	0.4272E+06	11265.72	11254.96
*	27	138.854	0.034	0.7275E+06	11266.62	11248.14
*	28	138.796	0.230	0.4890E+07	11284.52	11220.76
*	29	138.806	0.240	0.5107E+07	11291.07	11215.39
*	30	138.749	0.016	0.3409E+06	11261.49	11235.49
*	31	138.704	0.167	0.3540E+07	11268.74	11221.13
*	32	138.661	0.066	0.1412E+07	11265.69	11217.07
*	33	138.587	0.469	0.9960E+07	11275.88	11195.03
*	34	138.476	0.609	0.1294E+08	11311.91	11141.22
*	35	138.495	0.001	0.2696E+05	11229.06	11226.45
*	36	132.879	3.561	0.7570E+08	10776.93	10768.37
*	37	131.881	0.283	0.6006E+07	10697.57	10686.56
*	38	131.755	0.263	0.5588E+07	10686.64	10676.16

(*) Peaks 1 to 38 are fitted to Lorentzian

NMR1
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Filename = TCS6
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 756.611

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14261.07	175.905	100.000	0.6886E+08	10.12
*	2	11885.30	146.601	47.850	0.3295E+08	5.43
*	3	11375.59	140.314	1.345	0.9258E+06	1.31
*	4	11374.33	140.298	1.360	0.9366E+06	1.31
*	5	11370.87	140.255	1.360	0.9365E+06	1.31
*	6	11368.41	140.225	1.539	0.1060E+07	1.31
*	7	11366.62	140.203	1.438	0.9901E+06	1.31
*	8	11365.63	140.191	1.467	0.1010E+07	1.31
*	9	11364.36	140.175	1.557	0.1072E+07	1.31
*	10	11363.29	140.162	1.545	0.1064E+07	1.31
*	11	11361.53	140.140	1.556	0.1072E+07	1.31
*	12	11359.47	140.115	1.573	0.1083E+07	1.31
*	13	11356.88	140.083	1.810	0.1246E+07	1.31
*	14	11356.14	140.074	1.818	0.1252E+07	1.31
*	15	11353.13	140.037	1.884	0.1297E+07	1.31
*	16	11350.57	140.005	2.077	0.1430E+07	1.31
*	17	11349.77	139.995	2.020	0.1391E+07	1.31
*	18	11348.77	139.983	1.945	0.1339E+07	1.31
*	19	11347.02	139.961	2.124	0.1463E+07	1.31
*	20	11344.79	139.934	2.249	0.1549E+07	1.31
*	21	11343.06	139.912	2.335	0.1608E+07	1.31
*	22	11340.02	139.875	2.558	0.1762E+07	1.31
*	23	11338.09	139.851	2.673	0.1841E+07	1.31
*	24	11335.36	139.817	2.703	0.1861E+07	1.31
*	25	11334.21	139.803	2.735	0.1883E+07	1.31
*	26	11333.17	139.790	2.716	0.1870E+07	1.31
*	27	11331.27	139.767	2.874	0.1979E+07	1.31
*	28	11329.14	139.741	3.100	0.2135E+07	1.31
*	29	11326.76	139.711	3.201	0.2204E+07	1.31
*	30	11325.57	139.697	3.295	0.2269E+07	1.31
*	31	11324.21	139.680	3.231	0.2225E+07	1.31
*	32	11321.16	139.642	3.536	0.2435E+07	1.31
*	33	11320.55	139.635	3.516	0.2421E+07	1.31
*	34	11319.02	139.616	3.621	0.2493E+07	1.31
*	35	11317.31	139.595	3.595	0.2476E+07	1.31
*	36	11316.36	139.583	3.759	0.2588E+07	1.31
*	37	11314.83	139.564	3.889	0.2678E+07	1.31
*	38	11314.07	139.555	3.888	0.2677E+07	1.31
*	39	11312.89	139.540	3.939	0.2712E+07	1.31
*	40	11312.03	139.530	4.059	0.2795E+07	1.31
*	41	11310.18	139.507	4.172	0.2873E+07	1.31
*	42	11309.32	139.496	4.187	0.2883E+07	1.31
*	43	11306.96	139.467	4.407	0.3034E+07	1.31
*	44	11304.17	139.433	4.582	0.3155E+07	1.31

*	45	11301.27	139.397	4.737	0.3262E+07	1.31
*	46	11299.03	139.369	4.960	0.3415E+07	1.31
*	47	11296.29	139.336	4.926	0.3392E+07	1.31
*	48	11293.83	139.305	4.886	0.3364E+07	1.31
*	49	11292.42	139.288	4.962	0.3417E+07	1.31
*	50	11291.28	139.274	4.987	0.3434E+07	1.31
*	51	11289.80	139.256	5.023	0.3459E+07	1.31
*	52	11289.18	139.248	5.032	0.3464E+07	1.31
*	53	11287.32	139.225	5.095	0.3508E+07	1.31
*	54	11285.41	139.201	5.174	0.3562E+07	1.31
*	55	11284.15	139.186	5.077	0.3496E+07	1.31
*	56	11281.82	139.157	5.190	0.3574E+07	1.31
*	57	11280.26	139.138	5.286	0.3639E+07	1.31
*	58	11278.85	139.120	5.228	0.3600E+07	1.31
*	59	11277.24	139.101	5.348	0.3683E+07	1.31
*	60	11276.10	139.087	5.327	0.3668E+07	1.31
*	61	11274.88	139.072	5.430	0.3739E+07	1.31
*	62	11274.13	139.062	5.425	0.3735E+07	1.31
*	63	11272.91	139.047	5.371	0.3698E+07	1.31
*	64	11270.79	139.021	5.533	0.3810E+07	1.31
*	65	11269.36	139.003	5.585	0.3845E+07	1.31
*	66	11268.14	138.988	5.589	0.3849E+07	1.31
*	67	11266.72	138.971	5.737	0.3950E+07	1.31
*	68	11265.74	138.959	5.725	0.3942E+07	1.31
*	69	11263.97	138.937	5.854	0.4031E+07	1.31
*	70	11263.21	138.928	5.898	0.4061E+07	1.31
*	71	11261.74	138.909	5.925	0.4080E+07	1.31
*	72	11260.12	138.889	5.952	0.4098E+07	1.31
*	73	11259.15	138.877	6.103	0.4202E+07	1.31
*	74	11256.87	138.849	6.297	0.4336E+07	1.31
*	75	11255.28	138.830	6.159	0.4241E+07	1.31
*	76	11254.22	138.817	6.290	0.4331E+07	1.31
*	77	11252.56	138.796	6.327	0.4356E+07	1.31
*	78	11251.78	138.787	6.329	0.4358E+07	1.31
*	79	11248.90	138.751	6.630	0.4565E+07	1.31
*	80	11247.42	138.733	6.663	0.4588E+07	1.31
*	81	11244.61	138.698	6.565	0.4520E+07	1.31
*	82	11243.38	138.683	6.584	0.4534E+07	1.31
*	83	11240.67	138.650	6.317	0.4349E+07	1.31
*	84	11239.43	138.634	6.211	0.4276E+07	1.31
*	85	11237.03	138.605	5.914	0.4072E+07	1.31
*	86	11233.56	138.562	5.449	0.3752E+07	1.31
*	87	11229.87	138.516	4.992	0.3437E+07	1.31
*	88	11225.68	138.465	4.372	0.3010E+07	1.31
*	89	11219.36	138.387	3.751	0.2583E+07	1.31
*	90	11216.43	138.350	3.354	0.2309E+07	1.31
*	91	11213.38	138.313	3.176	0.2187E+07	1.31
*	92	11212.03	138.296	3.166	0.2180E+07	1.31
*	93	11210.05	138.272	2.906	0.2001E+07	1.31
*	94	11209.02	138.259	2.842	0.1957E+07	1.31
*	95	11206.32	138.226	2.762	0.1902E+07	1.31
*	96	11203.00	138.185	2.386	0.1643E+07	1.31
*	97	11201.99	138.172	2.408	0.1658E+07	1.31
*	98	11200.75	138.157	2.356	0.1622E+07	1.31
*	99	11198.85	138.134	2.308	0.1589E+07	1.31
*	100	11197.43	138.116	2.260	0.1556E+07	1.31
*	101	11195.08	138.087	2.091	0.1439E+07	1.31
*	102	11192.95	138.061	2.120	0.1460E+07	1.31
*	103	11191.65	138.045	2.133	0.1469E+07	1.31
*	104	11190.29	138.028	2.065	0.1422E+07	1.31
*	105	11187.85	137.998	1.895	0.1305E+07	1.31
*	106	11186.94	137.987	1.891	0.1302E+07	1.31
*	107	11184.69	137.959	1.767	0.1217E+07	1.31
*	108	11183.46	137.944	1.763	0.1214E+07	1.31
*	109	11181.72	137.922	1.787	0.1230E+07	1.31
*	110	11180.14	137.903	1.666	0.1147E+07	1.31

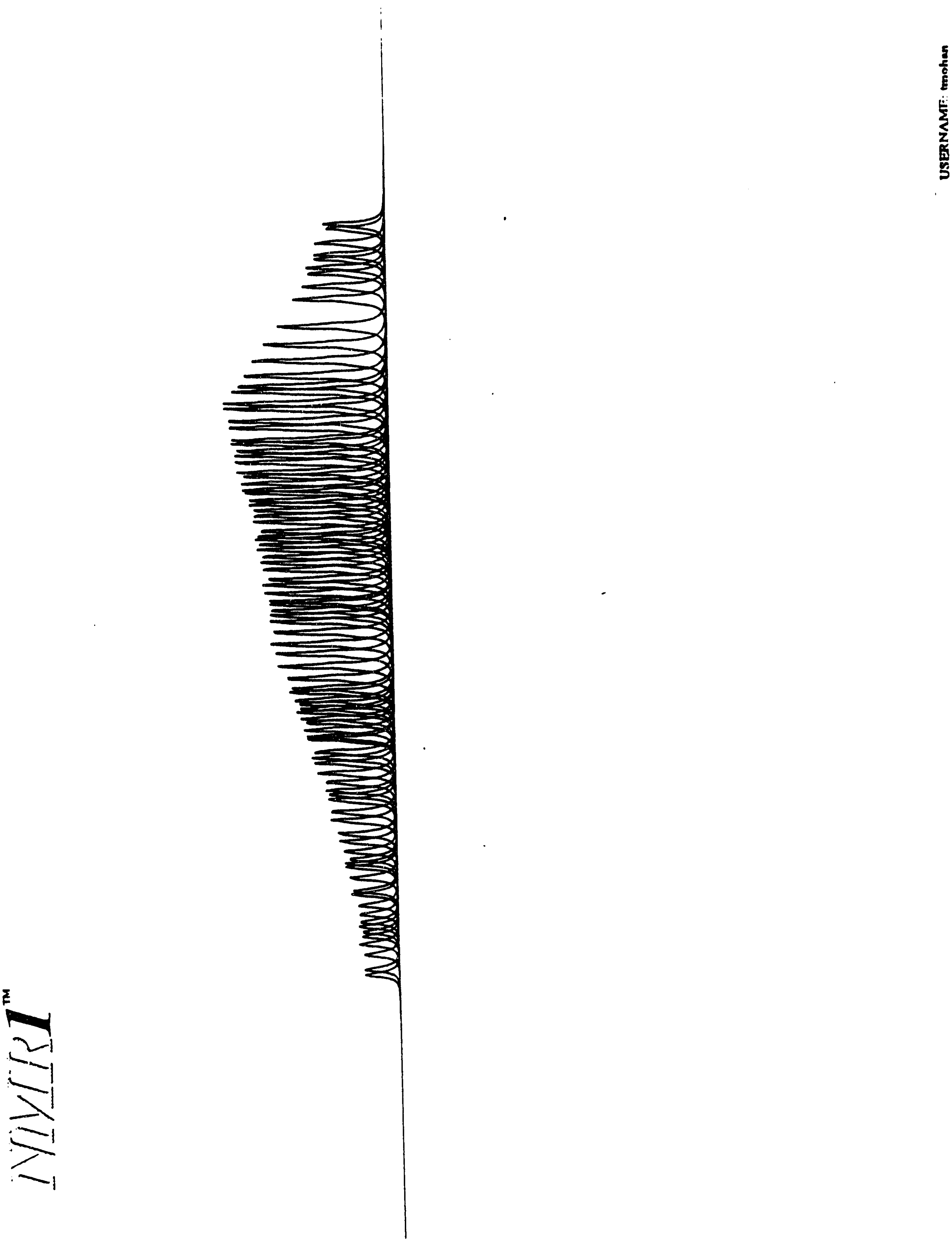
* 111	11179.21	137.891	1.738	0.1197E+07	1.31
* 112	11177.25	137.867	1.651	0.1137E+07	1.31
* 113	11175.25	137.843	1.622	0.1117E+07	1.31
* 114	11173.19	137.817	1.596	0.1099E+07	1.31
* 115	11172.08	137.804	1.613	0.1111E+07	1.31
* 116	11170.39	137.783	1.358	0.9353E+06	1.31
* 117	11168.45	137.759	1.494	0.1029E+07	1.31
* 118	11167.39	137.746	1.441	0.9920E+06	1.31
* 119	11163.92	137.703	1.440	0.9915E+06	1.31
* 120	11162.59	137.686	1.334	0.9182E+06	1.31
* 121	11162.10	137.680	1.380	0.9500E+06	1.31
* 122	11160.83	137.665	1.347	0.9273E+06	1.31
* 123	10791.32	133.107	0.733	0.5050E+06	4.19
* 124	10772.67	132.877	28.474	0.1961E+08	4.60
* 125	10760.86	132.731	0.279	0.1919E+06	1.67
* 126	10759.20	132.711	0.073	0.5000E+05	1.04
* 127	10757.68	132.692	0.256	0.1763E+06	2.58
* 128	10611.05	130.883	2.274	0.1566E+07	23.20
* 129	10748.21	132.575	0.784	0.5397E+06	19.47

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
* 1	175.905	100.000	0.1848E+10	14265.87	14255.74
* 2	146.601	25.660	0.4741E+09	11887.89	11882.46
* 3	140.314	0.175	0.3224E+07	11376.22	11374.90
* 4	140.298	0.177	0.3261E+07	11375.03	11373.72
* 5	140.255	0.177	0.3261E+07	11371.48	11370.16
* 6	140.225	0.200	0.3691E+07	11369.11	11367.79
* 7	140.203	0.187	0.3448E+07	11367.33	11366.02
* 8	140.191	0.190	0.3516E+07	11366.14	11364.83
* 9	140.175	0.202	0.3734E+07	11364.96	11363.65
* 10	140.162	0.200	0.3704E+07	11363.77	11362.46
* 11	140.140	0.202	0.3731E+07	11362.00	11360.68
* 12	140.115	0.204	0.3771E+07	11359.92	11358.61
* 13	140.083	0.235	0.4340E+07	11357.55	11356.24
* 14	140.074	0.236	0.4360E+07	11356.66	11355.35
* 15	140.037	0.244	0.4517E+07	11353.70	11352.39
* 16	140.005	0.270	0.4981E+07	11351.03	11349.72
* 17	139.995	0.262	0.4843E+07	11350.44	11349.13
* 18	139.983	0.252	0.4665E+07	11349.26	11347.94
* 19	139.961	0.276	0.5094E+07	11347.48	11346.17
* 20	139.934	0.292	0.5394E+07	11345.40	11344.09
* 21	139.912	0.303	0.5598E+07	11343.63	11342.31
* 22	139.875	0.332	0.6134E+07	11340.66	11339.35
* 23	139.851	0.347	0.6410E+07	11338.59	11337.28
* 24	139.817	0.351	0.6482E+07	11335.92	11334.61
* 25	139.803	0.355	0.6557E+07	11334.74	11333.42
* 26	139.790	0.352	0.6512E+07	11333.85	11332.54
* 27	139.767	0.373	0.6891E+07	11331.78	11330.46
* 28	139.741	0.402	0.7434E+07	11329.70	11328.39
* 29	139.711	0.415	0.7676E+07	11327.33	11326.02
* 30	139.697	0.428	0.7900E+07	11326.15	11324.83
* 31	139.680	0.419	0.7748E+07	11324.66	11323.35
* 32	139.642	0.459	0.8479E+07	11321.70	11320.39
* 33	139.635	0.456	0.8431E+07	11321.11	11319.79
* 34	139.616	0.470	0.8682E+07	11319.63	11318.31
* 35	139.595	0.467	0.8621E+07	11317.85	11316.54
* 36	139.583	0.488	0.9014E+07	11316.96	11315.65
* 37	139.564	0.505	0.9324E+07	11315.48	11314.17
* 38	139.555	0.505	0.9324E+07	11314.59	11313.28
* 39	139.540	0.511	0.9446E+07	11313.41	11312.09
* 40	139.530	0.527	0.9733E+07	11312.52	11311.20

•	41	139.507	0.542	0.1000E+08	11310.74	11309.42
•	42	139.496	0.543	0.1004E+08	11309.85	11308.54
•	43	139.467	0.572	0.1057E+08	11307.48	11306.17
*	44	139.433	0.595	0.1099E+08	11304.81	11303.50
*	45	139.397	0.615	0.1136E+08	11301.85	11300.54
*	46	139.369	0.644	0.1189E+08	11299.48	11298.17
*	47	139.336	0.639	0.1181E+08	11296.81	11295.50
*	48	139.305	0.634	0.1171E+08	11294.44	11293.13
*	49	139.288	0.644	0.1190E+08	11292.96	11291.65
*	50	139.274	0.647	0.1196E+08	11291.78	11290.46
*	51	139.256	0.652	0.1205E+08	11290.29	11288.98
*	52	139.248	0.653	0.1206E+08	11289.70	11288.39
*	53	139.225	0.661	0.1222E+08	11287.92	11286.61
*	54	139.201	0.671	0.1241E+08	11285.85	11284.54
*	55	139.186	0.659	0.1217E+08	11284.67	11283.35
*	56	139.157	0.674	0.1245E+08	11282.29	11280.98
*	57	139.138	0.686	0.1267E+08	11280.81	11279.50
*	58	139.120	0.679	0.1254E+08	11279.33	11278.02
*	59	139.101	0.694	0.1282E+08	11277.85	11276.54
*	60	139.087	0.691	0.1277E+08	11276.67	11275.35
*	61	139.072	0.705	0.1302E+08	11275.48	11274.17
*	62	139.062	0.704	0.1301E+08	11274.59	11273.28
*	63	139.047	0.697	0.1288E+08	11273.41	11272.09
*	64	139.021	0.718	0.1327E+08	11271.33	11270.02
*	65	139.003	0.725	0.1339E+08	11269.85	11268.54
*	66	138.988	0.725	0.1340E+08	11268.67	11267.35
*	67	138.971	0.745	0.1376E+08	11267.18	11265.87
*	68	138.959	0.743	0.1373E+08	11266.30	11264.98
*	69	138.937	0.760	0.1404E+08	11264.52	11263.20
*	70	138.928	0.766	0.1414E+08	11263.93	11262.61
*	71	138.909	0.769	0.1421E+08	11262.44	11261.13
*	72	138.889	0.772	0.1427E+08	11260.67	11259.35
*	73	138.877	0.792	0.1463E+08	11259.78	11258.46
*	74	138.849	0.817	0.1510E+08	11257.41	11256.09
*	75	138.830	0.799	0.1477E+08	11255.93	11254.61
*	76	138.817	0.816	0.1508E+08	11254.74	11253.43
*	77	138.796	0.821	0.1517E+08	11253.26	11251.95
*	78	138.787	0.821	0.1517E+08	11252.37	11251.06
*	79	138.751	0.861	0.1590E+08	11249.41	11248.09
*	80	138.733	0.865	0.1598E+08	11247.93	11246.61
*	81	138.698	0.852	0.1574E+08	11245.26	11243.95
*	82	138.683	0.855	0.1579E+08	11244.07	11242.76
*	83	138.650	0.820	0.1515E+08	11241.41	11240.09
*	84	138.634	0.806	0.1489E+08	11239.93	11238.61
*	85	138.605	0.768	0.1418E+08	11237.56	11236.24
*	86	138.562	0.707	0.1307E+08	11234.00	11232.69
*	87	138.516	0.648	0.1197E+08	11230.45	11229.13
*	88	138.465	0.567	0.1048E+08	11226.30	11224.98
*	89	138.387	0.487	0.8995E+07	11220.07	11218.76
*	90	138.350	0.435	0.8041E+07	11217.11	11215.80
*	91	138.313	0.412	0.7616E+07	11213.85	11212.54
*	92	138.296	0.411	0.7590E+07	11212.67	11211.35
*	93	138.272	0.377	0.6968E+07	11210.59	11209.28
*	94	138.259	0.369	0.6814E+07	11209.71	11208.39
*	95	138.226	0.359	0.6623E+07	11207.04	11205.72
*	96	138.185	0.310	0.5722E+07	11203.48	11202.17
*	97	138.172	0.313	0.5775E+07	11202.59	11201.28
*	98	138.157	0.306	0.5650E+07	11201.41	11200.09
*	99	138.134	0.300	0.5534E+07	11199.33	11198.02
*	100	138.116	0.293	0.5420E+07	11198.15	11196.84
*	101	138.087	0.271	0.5013E+07	11195.78	11194.47
*	102	138.061	0.275	0.5084E+07	11193.41	11192.10
*	103	138.045	0.277	0.5115E+07	11192.22	11190.91
*	104	138.028	0.268	0.4951E+07	11190.74	11189.43
*	105	137.998	0.246	0.4545E+07	11188.37	11187.06
*	106	137.987	0.245	0.4535E+07	11187.48	11186.17

*	107	137.959	0.229	0.4236E+07	11185.41	11184.10
*	108	137.944	0.229	0.4228E+07	11183.93	11182.61
*	109	137.922	0.232	0.4284E+07	11182.45	11181.13
*	110	137.903	0.216	0.3994E+07	11180.67	11179.36
*	111	137.891	0.226	0.4167E+07	11179.78	11178.47
*	112	137.867	0.214	0.3959E+07	11177.71	11176.39
*	113	137.843	0.211	0.3890E+07	11175.93	11174.61
*	114	137.817	0.207	0.3826E+07	11173.85	11172.54
*	115	137.804	0.209	0.3868E+07	11172.67	11171.36
*	116	137.783	0.176	0.3257E+07	11170.89	11169.58
*	117	137.759	0.194	0.3582E+07	11169.11	11167.80
*	118	137.746	0.187	0.3455E+07	11167.93	11166.61
*	119	137.703	0.187	0.3453E+07	11164.37	11163.06
*	120	137.686	0.173	0.3198E+07	11163.19	11161.87
*	121	137.680	0.179	0.3308E+07	11162.59	11161.28
*	122	137.665	0.175	0.3229E+07	11161.41	11160.10
*	123	133.107	0.303	0.5606E+07	10793.3[illegible]	10789.19
*	124	132.877	12.944	0.2391E+09	10774.92	10770.32
*	125	132.731	0.046	0.8489E+06	10761.60	10759.93
*	126	132.711	0.007	0.1383E+06	10759.81	10758.76
*	127	132.692	0.065	0.1208E+07	10758.80	10756.21
*	128	130.883	5.212	0.9630E+08	10622.74	10599.54
*	129	132.575	1.508	0.2786E+08	10757.76	10738.29

(*) Peaks 1 to 129 are fitted to Lorentzian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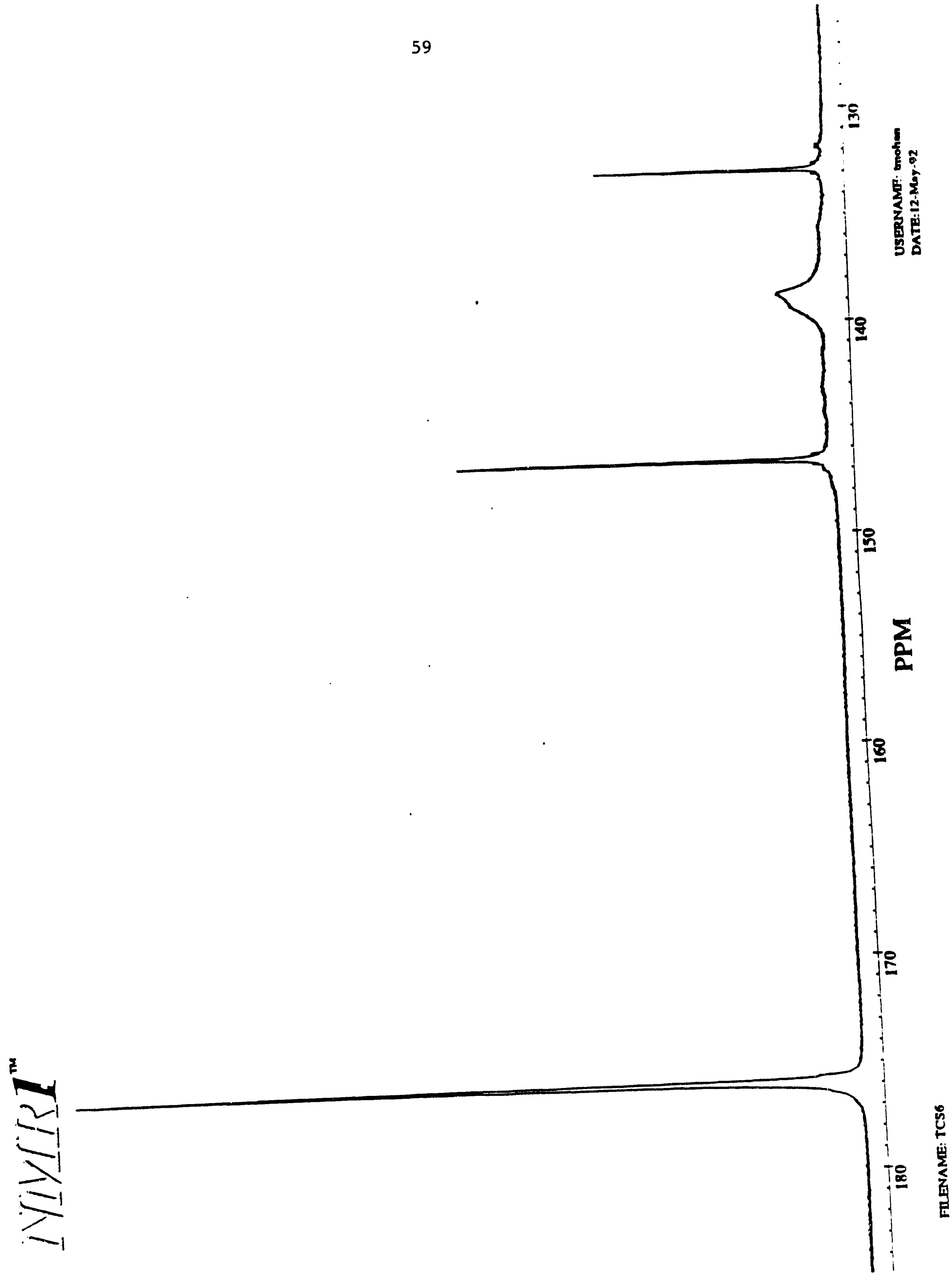

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USERNAME: tmohan
DATE:12-May-92
PPM
130
140
150
160
170
180

NMR1
****

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Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 2918.78

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
	1	14260.66	175.900	100.000	0.1038E+09	10.15
*	2	11886.91	146.621	13.843	0.1437E+08	2.98
*	3	11346.28	139.952	0.257	0.2672E+06	0.87
*	4	11345.09	139.937	0.258	0.2673E+06	0.87
*	5	11343.50	139.918	0.288	0.2993E+06	0.87
*	6	11342.22	139.902	0.329	0.3414E+06	0.87
*	7	11341.00	139.887	0.329	0.3414E+06	0.87
*	8	11339.78	139.872	0.300	0.3112E+06	0.87
*	9	11337.84	139.848	0.304	0.3150E+06	0.87
*	10	11336.76	139.835	0.353	0.3663E+06	0.87
*	11	11335.65	139.821	0.327	0.3395E+06	0.87
*	12	11334.47	139.806	0.346	0.3595E+06	0.87
*	13	11333.89	139.799	0.355	0.3684E+06	0.87
*	14	11332.51	139.782	0.375	0.3887E+06	0.87
*	15	11331.05	139.764	0.394	0.4086E+06	0.87
*	16	11330.64	139.759	0.396	0.4110E+06	0.87
*	17	11329.67	139.747	0.377	0.3917E+06	0.87
*	18	11328.45	139.732	0.405	0.4200E+06	0.87
*	19	11326.92	139.713	0.439	0.4561E+06	0.87
*	20	11325.83	139.700	0.408	0.4233E+06	0.87
*	21	11323.74	139.674	0.445	0.4616E+06	0.87
*	22	11323.10	139.666	0.445	0.4618E+06	0.87
*	23	11322.42	139.658	0.424	0.4400E+06	0.87
*	24	11321.08	139.641	0.499	0.5180E+06	0.87
*	25	11319.61	139.623	0.487	0.5051E+06	0.87
*	26	11318.70	139.612	0.501	0.5197E+06	0.87
*	27	11318.01	139.604	0.528	0.5484E+06	0.87
*	28	11316.31	139.582	0.517	0.5366E+06	0.87
*	29	11315.74	139.576	0.520	0.5402E+06	0.87
*	30	11314.56	139.561	0.553	0.5744E+06	0.87
*	31	11312.46	139.535	0.571	0.5932E+06	0.87
*	32	11310.17	139.507	0.628	0.6518E+06	0.87
*	33	11308.93	139.491	0.595	0.6181E+06	0.87
*	34	11307.49	139.474	0.621	0.6443E+06	0.87
*	35	11304.82	139.441	0.676	0.7016E+06	0.87
*	36	11304.08	139.432	0.684	0.7098E+06	0.87
*	37	11303.49	139.424	0.699	0.7254E+06	0.87
*	38	11302.93	139.417	0.685	0.7107E+06	0.87
*	39	11301.13	139.395	0.675	0.7002E+06	0.87
*	40	11300.54	139.388	0.671	0.6970E+06	0.87
*	41	11299.92	139.380	0.676	0.7019E+06	0.87
*	42	11299.14	139.371	0.691	0.7174E+06	0.87
*	43	11297.60	139.352	0.669	0.6945E+06	0.87
*	44	11295.93	139.331	0.679	0.7050E+06	0.87

* 45	11295.25	139.323	0.688	0.7136E+06	0.87
* 46	11294.02	139.308	0.699	0.7261E+06	0.87
* 47	11293.23	139.298	0.709	0.7363E+06	0.87
* 48	11292.39	139.287	0.700	0.7264E+06	0.87
* 49	11290.55	139.265	0.710	0.7367E+06	0.87
* 50	11289.42	139.251	0.704	0.7310E+06	0.87
* 51	11288.82	139.243	0.699	0.7253E+06	0.87
* 52	11288.00	139.233	0.687	0.7135E+06	0.87
* 53	11286.91	139.220	0.741	0.7689E+06	0.87
* 54	11285.34	139.201	0.732	0.7603E+06	0.87
* 55	11283.57	139.179	0.699	0.7260E+06	0.87
* 56	11282.27	139.163	0.740	0.7686E+06	0.87
* 57	11281.60	139.154	0.724	0.7513E+06	0.87
* 58	11280.91	139.146	0.722	0.7490E+06	0.87
* 59	11279.28	139.126	0.729	0.7571E+06	0.87
* 60	11278.37	139.115	0.729	0.7571E+06	0.87
* 61	11277.28	139.101	0.752	0.7805E+06	0.87
* 62	11274.84	139.071	0.762	0.7906E+06	0.87
* 63	11274.07	139.062	0.752	0.7808E+06	0.87
* 64	11272.08	139.037	0.792	0.8223E+06	0.87
* 65	11271.16	139.026	0.758	0.7871E+06	0.87
* 66	11270.24	139.014	0.780	0.8098E+06	0.87
* 67	11269.54	139.006	0.787	0.8171E+06	0.87
* 68	11268.30	138.990	0.783	0.8130E+06	0.87
* 69	11266.84	138.972	0.801	0.8316E+06	0.87
* 70	11265.42	138.955	0.818	0.8490E+06	0.87
* 71	11263.96	138.937	0.841	0.8731E+06	0.87
* 72	11262.56	138.920	0.823	0.8543E+06	0.87
* 73	11261.74	138.909	0.841	0.8725E+06	0.87
* 74	11260.55	138.895	0.828	0.8599E+06	0.87
* 75	11259.64	138.883	0.835	0.8663E+06	0.87
* 76	11258.10	138.865	0.868	0.9015E+06	0.87
* 77	11257.00	138.851	0.848	0.8807E+06	0.87
* 78	11256.19	138.841	0.842	0.8736E+06	0.87
* 79	11255.45	138.832	0.844	0.8758E+06	0.87
* 80	11253.41	138.807	0.920	0.9549E+06	0.87
* 81	11252.56	138.796	0.917	0.9522E+06	0.87
* 82	11251.26	138.780	0.925	0.9600E+06	0.87
* 83	11250.39	138.769	0.916	0.9504E+06	0.87
* 84	11248.71	138.749	0.970	0.1007E+07	0.87
* 85	11247.95	138.739	0.960	0.9967E+06	0.87
* 86	11246.96	138.727	0.950	0.9859E+06	0.87
* 87	11245.69	138.711	0.946	0.9823E+06	0.87
* 88	11244.95	138.702	0.951	0.9877E+06	0.87
* 89	11244.35	138.695	0.954	0.9900E+06	0.87
* 90	11243.79	138.688	0.951	0.9868E+06	0.87
* 91	11240.71	138.650	0.895	0.9292E+06	0.87
* 92	11239.92	138.640	0.927	0.9620E+06	0.87
* 93	11238.33	138.621	0.854	0.8861E+06	0.87
* 94	11237.14	138.606	0.855	0.8875E+06	0.87
* 95	11235.08	138.581	0.795	0.8253E+06	0.87
* 96	11233.57	138.562	0.764	0.7928E+06	0.87
* 97	11231.77	138.540	0.736	0.7635E+06	0.87
* 98	11229.93	138.517	0.708	0.7350E+06	0.87
* 99	11229.17	138.508	0.698	0.7249E+06	0.87
* 100	11226.95	138.480	0.606	0.6289E+06	0.87
* 101	11225.32	138.460	0.577	0.5987E+06	0.87
* 102	11224.37	138.448	0.534	0.5544E+06	0.87
* 103	11223.45	138.437	0.531	0.5513E+06	0.87
* 104	11222.50	138.425	0.504	0.5227E+06	0.87
* 105	11221.62	138.415	0.486	0.5049E+06	0.87
* 106	11219.44	138.388	0.458	0.4751E+06	0.87
* 107	11218.26	138.373	0.456	0.4733E+06	0.87
* 108	11217.26	138.361	0.438	0.4551E+06	0.87
* 109	11216.03	138.346	0.404	0.4197E+06	0.87
* 110	11214.61	138.328	0.415	0.4308E+06	0.87

*	111	11212.63	138.304	0.398	0.4130E+06	0.87
*	112	11211.50	138.290	0.377	0.3918E+06	0.87
*	113	11210.34	138.275	0.341	0.3536E+06	0.87
*	114	11209.39	138.264	0.349	0.3626E+06	0.87
*	115	11208.16	138.249	0.350	0.3633E+06	0.87
*	116	11207.26	138.237	0.340	0.3531E+06	0.87
*	117	11205.50	138.216	0.326	0.3388E+06	0.87
*	118	11204.75	138.206	0.310	0.3213E+06	0.87
*	119	11203.48	138.191	0.295	0.3063E+06	0.87
*	120	11201.94	138.172	0.326	0.3382E+06	0.87
*	121	11200.05	138.149	0.307	0.3185E+06	0.87
*	122	11198.33	138.127	0.283	0.2940E+06	0.87
*	123	11196.90	138.110	0.265	0.2754E+06	0.87
*	124	11196.19	138.101	0.269	0.2787E+06	0.87
*	125	11195.14	138.088	0.276	0.2866E+06	0.87
*	126	10773.60	132.888	7.986	0.8290E+07	2.82

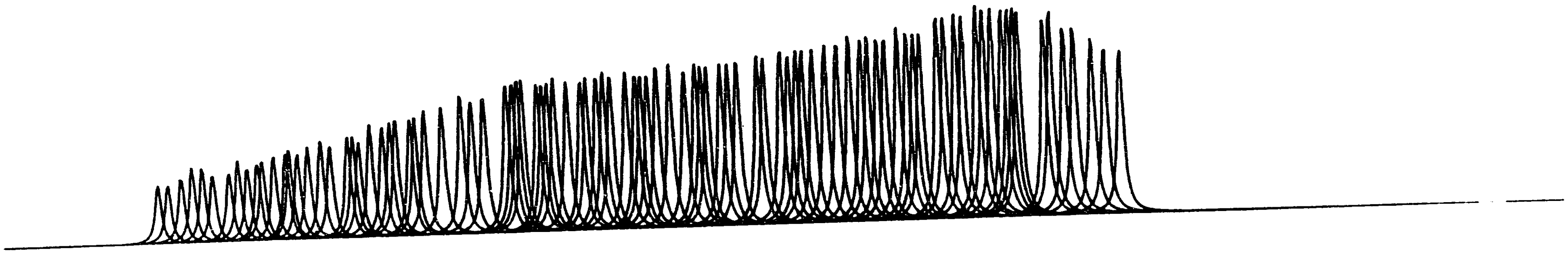
	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
	1	175.900	100.000	0.1407E+11	14430.43	14179.48
*	2	146.621	1.612	0.2268E+09	11888.30	11885.32
*	3	139.952	0.009	0.1229E+07	11346.67	11345.80
*	4	139.937	0.009	0.1230E+07	11345.48	11344.61
*	5	139.918	0.010	0.1377E+07	11343.85	11342.98
*	6	139.902	0.011	0.1571E+07	11342.67	11341.80
*	7	139.887	0.011	0.1570E+07	11341.33	11340.47
*	8	139.872	0.010	0.1432E+07	11340.15	11339.28
*	9	139.848	0.010	0.1449E+07	11338.22	11337.36
*	10	139.835	0.012	0.1685E+07	11337.19	11336.32
*	11	139.821	0.011	0.1562E+07	11336.00	11335.13
*	12	139.806	0.012	0.1654E+07	11334.82	11333.95
*	13	139.799	0.012	0.1695E+07	11334.22	11333.36
*	14	139.782	0.013	0.1788E+07	11332.89	11332.02
*	15	139.764	0.013	0.1880E+07	11331.41	11330.54
*	16	139.759	0.013	0.1891E+07	11331.11	11330.24
*	17	139.747	0.013	0.1802E+07	11330.08	11329.21
*	18	139.732	0.014	0.1932E+07	11328.89	11328.02
*	19	139.713	0.015	0.2098E+07	11327.26	11326.39
*	20	139.700	0.014	0.1947E+07	11326.22	11325.36
*	21	139.674	0.015	0.2124E+07	11324.15	11323.28
*	22	139.666	0.015	0.2124E+07	11323.56	11322.69
*	23	139.658	0.014	0.2024E+07	11322.82	11321.95
*	24	139.641	0.017	0.2383E+07	11321.48	11320.62
*	25	139.623	0.017	0.2324E+07	11320.00	11319.13
*	26	139.612	0.017	0.2391E+07	11319.11	11318.25
*	27	139.604	0.018	0.2523E+07	11318.37	11317.50
*	28	139.582	0.018	0.2469E+07	11316.74	11315.88
*	29	139.576	0.018	0.2485E+07	11316.15	11315.28
*	30	139.561	0.019	0.2642E+07	11314.96	11314.10
*	31	139.535	0.019	0.2729E+07	11312.89	11312.02
*	32	139.507	0.021	0.2998E+07	11310.52	11309.65
*	33	139.491	0.020	0.2843E+07	11309.33	11308.47
*	34	139.474	0.021	0.2964E+07	11307.85	11306.99
*	35	139.441	0.023	0.3227E+07	11305.19	11304.32
*	36	139.432	0.023	0.3265E+07	11304.45	11303.58
*	37	139.424	0.024	0.3337E+07	11303.85	11302.99
*	38	139.417	0.023	0.3269E+07	11303.26	11302.39
*	39	139.395	0.023	0.3221E+07	11301.48	11300.62
*	40	139.388	0.023	0.3206E+07	11300.89	11300.02
*	41	139.380	0.023	0.3229E+07	11300.30	11299.43
*	42	139.371	0.023	0.3300E+07	11299.56	11298.69
*	43	139.352	0.023	0.3195E+07	11297.93	11297.06

*	44	139.331	0.023	0.3243E+07	11296.30	11295.43
*	45	139.323	0.023	0.3283E+07	11295.71	11294.84
*	46	139.308	0.024	0.3340E+07	11294.37	11293.50
*	47	139.298	0.024	0.3387E+07	11293.63	11292.76
*	48	139.287	0.024	0.3341E+07	11292.74	11291.88
*	49	139.265	0.024	0.3389E+07	11290.96	11290.10
*	50	139.251	0.024	0.3363E+07	11289.78	11288.91
*	51	139.243	0.024	0.3336E+07	11289.19	11288.32
*	52	139.233	0.023	0.3282E+07	11288.45	11287.58
*	53	139.220	0.025	0.3537E+07	11287.26	11286.39
*	54	139.201	0.025	0.3497E+07	11285.78	11284.91
*	55	139.179	0.024	0.3340E+07	11284.00	11283.13
*	56	139.163	0.025	0.3536E+07	11282.67	11281.80
*	57	139.154	0.025	0.3456E+07	11281.93	11281.06
*	58	139.146	0.024	0.3446E+07	11281.34	11280.47
*	59	139.126	0.025	0.3483E+07	11279.71	11278.84
*	60	139.115	0.025	0.3483E+07	11278.82	11277.95
*	61	139.101	0.026	0.3590E+07	11277.63	11276.76
*	62	139.071	0.026	0.3637E+07	11275.26	11274.39
*	63	139.062	0.026	0.3592E+07	11274.52	11273.65
*	64	139.037	0.027	0.3783E+07	11272.45	11271.58
*	65	139.026	0.026	0.3621E+07	11271.56	11270.69
*	66	139.014	0.026	0.3725E+07	11270.67	11269.80
*	67	139.006	0.027	0.3759E+07	11269.93	11269.06
*	68	138.990	0.027	0.3740E+07	11268.74	11267.88
*	69	138.972	0.027	0.3825E+07	11267.26	11266.39
*	70	138.955	0.028	0.3906E+07	11265.78	11264.91
*	71	138.937	0.029	0.4016E+07	11264.30	11263.43
*	72	138.920	0.028	0.3930E+07	11262.97	11262.10
*	73	138.909	0.029	0.4013E+07	11262.08	11261.21
*	74	138.895	0.028	0.3956E+07	11260.89	11260.02
*	75	138.883	0.028	0.3985E+07	11260.00	11259.14
*	76	138.865	0.029	0.4147E+07	11258.52	11257.65
*	77	138.851	0.029	0.4051E+07	11257.34	11256.47
*	78	138.841	0.029	0.4019E+07	11256.60	11255.73
*	79	138.832	0.029	0.4029E+07	11255.86	11254.99
*	80	138.807	0.031	0.4393E+07	11253.78	11252.91
*	81	138.796	0.031	0.4380E+07	11252.89	11252.02
*	82	138.780	0.031	0.4416E+07	11251.71	11250.84
*	83	138.769	0.031	0.4372E+07	11250.82	11249.95
*	84	138.749	0.033	0.4632E+07	11249.04	11248.17
*	85	138.739	0.033	0.4585E+07	11248.30	11247.43
*	86	138.727	0.032	0.4535E+07	11247.41	11246.54
*	87	138.711	0.032	0.4519E+07	11246.08	11245.21
*	88	138.702	0.032	0.4543E+07	11245.34	11244.47
*	89	138.695	0.032	0.4554E+07	11244.74	11243.88
*	90	138.688	0.032	0.4539E+07	11244.15	11243.28
*	91	138.650	0.030	0.4275E+07	11241.04	11240.17
*	92	138.640	0.031	0.4425E+07	11240.30	11239.43
*	93	138.621	0.029	0.4076E+07	11238.67	11237.80
*	94	138.606	0.029	0.4082E+07	11237.49	11236.62
*	95	138.581	0.027	0.3796E+07	11235.41	11234.54
*	96	138.562	0.026	0.3647E+07	11233.93	11233.06
*	97	138.540	0.025	0.3512E+07	11232.15	11231.28
*	98	138.517	0.024	0.3381E+07	11230.37	11229.51
*	99	138.508	0.024	0.3335E+07	11229.63	11228.77
*	100	138.480	0.021	0.2893E+07	11227.41	11226.54
*	101	138.460	0.020	0.2754E+07	11225.78	11224.91
*	102	138.448	0.018	0.2550E+07	11224.75	11223.88
*	103	138.437	0.01[illegible]	0.2536E+07	11223.86	11222.99
*	104	138.425	0.017	0.2405E+07	11222.97	11222.10
*	105	138.415	0.017	0.2322E+07	11222.08	11221.21
*	106	138.388	0.016	0.2185E+07	11219.86	11218.99
*	107	138.373	0.015	0.2177E+07	11218.67	11217.80
*	108	138.361	0.015	0.2093E+07	11217.63	11216.77
*	109	138.346	0.014	0.1931E+07	11216.45	11215.58

* 110	138.328	0.014	0.1982E+07	11214.97	11214.10
* 111	138.304	0.014	0.1900E+07	11213.04	11212.17
* 112	138.290	0.013	0.1802E+07	11211.86	11210.99
* 113	138.275	0.012	0.1627E+07	11210.67	11209.80
* 114	138.264	0.012	0.1668E+07	11209.78	11208.92
* 115	138.249	0.012	0.1671E+07	11208.60	11207.73
* 116	138.237	0.012	0.1624E+07	11207.71	11206.84
* 117	138.216	0.011	0.1559E+07	11205.93	11205.06
* 118	138.206	0.011	0.1478E+07	11205.19	11204.32
* 119	138.191	0.010	0.1409E+07	11203.86	11202.99
* 120	138.172	0.011	0.1556E+07	11202.38	11201.51
* 121	138.149	0.010	0.1465E+07	11200.45	11199.58
* 122	138.127	0.010	0.1353E+07	11198.67	11197.80
* 123	138.110	0.009	0.1267E+07	11197.34	11196.47
* 124	138.101	0.009	0.1282E+07	11196.60	11195.73
* 125	138.088	0.009	0.1318E+07	11195.56	11194.69
* 126	132.888	0.881	0.1239E+09	10774.92	10772.10

(*) Peaks 2 to 126 are fitted to Lorentzian

NMR1™



USERNAME: tmohan

NMR1
****

Filename = TCS8
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 2701.34

Peak Analysis

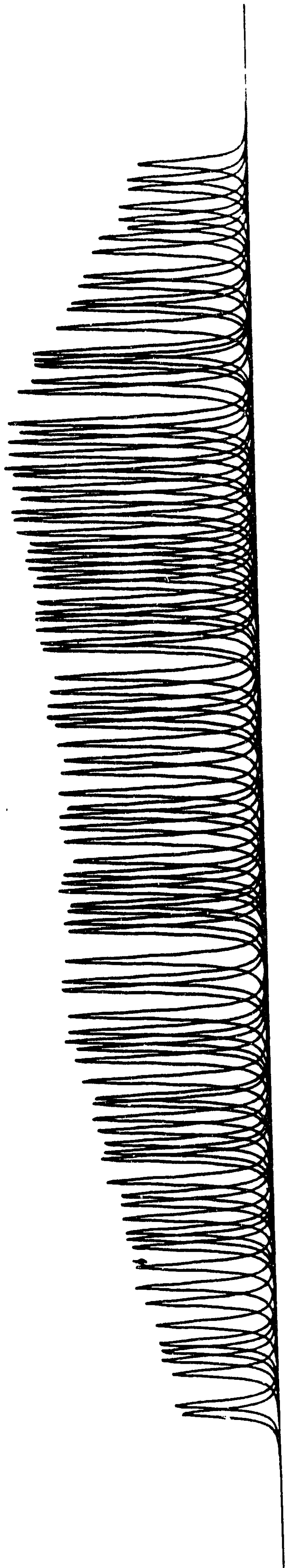
	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14262.32	175.920	100.000	0.833[illegible]E+08	13.42
*	2	11889.61	146.654	25.764	0.2147E+08	2.84
*	3	11338.60	139.857	0.414	0.3446E+06	0.88
*	4	11337.80	139.848	0.437	0.3644E+06	0.88
*	5	11334.80	139.811	0.441	0.3675E+06	0.88
*	6	11333.49	139.794	0.486	0.4050E+06	0.88
*	7	11332.64	139.784	0.496	0.4136E+06	0.88
*	8	11331.91	139.775	0.510	0.4254E+06	0.88
*	9	11330.18	139.754	0.508	0.4235E+06	0.88
*	10	11328.11	139.728	0.544	0.4534E+06	0.88
*	11	11326.62	139.710	0.586	0.4887E+06	0.88
*	12	11324.75	139.687	0.580	0.4833E+06	0.88
*	13	11322.86	139.663	0.603	0.5023E+06	0.88
*	14	11322.08	139.654	0.613	0.5112E+06	0.88
*	15	11321.42	139.646	0.629	0.5243E+06	0.88
*	16	11320.13	139.630	0.635	0.5294E+06	0.88
*	17	11318.80	139.613	0.639	0.5328E+06	0.88
*	18	11317.99	139.603	0.652	0.5433E+06	0.88
*	19	11316.68	139.587	0.706	0.5881E+06	0.88
*	20	11314.55	139.561	0.719	0.5991E+06	0.88
*	21	11313.92	139.553	0.707	0.5890E+06	0.88
*	22	11313.09	139.543	0.712	0.5938E+06	0.88
*	23	11311.90	139.528	0.738	0.6152E+06	0.88
*	24	11310.75	139.514	0.761	0.6342E+06	0.88
*	25	11309.35	139.497	0.745	0.6206E+06	0.88
*	26	11308.83	139.490	0.743	0.6194E+06	0.88
*	27	11307.20	139.470	0.797	0.6639E+06	0.88
*	28	11305.24	139.446	0.832	0.6935E+06	0.88
*	29	11304.12	139.432	0.813	0.6773E+06	0.88
*	30	11303.41	139.423	0.864	0.7203E+06	0.88
*	31	11302.52	139.412	0.848	0.7064E+06	0.88
*	32	11301.04	139.394	0.846	0.7047E+06	0.88
*	33	11298.58	139.364	0.888	0.7400E+06	0.88
*	34	11297.77	139.354	0.869	0.7240E+06	0.88
*	35	11295.88	139.331	0.853	0.7107E+06	0.88
*	36	11293.04	139.296	0.838	0.6984E+06	0.88
*	37	11292.23	139.286	0.862	0.7186E+06	0.88
*	38	11291.14	139.272	0.847	0.7059E+06	0.88
*	39	11290.59	139.265	0.847	0.7060E+06	0.88
*	40	11289.23	139.248	0.878	0.7320E+06	0.88
*	41	11288.48	139.239	0.866	0.7221E+06	0.88
*	42	11287.71	139.230	0.853	0.7113E+06	0.88
*	43	11286.45	139.214	0.824	0.6869E+06	0.88
*	44	11284.56	139.191	0.849	0.7073E+06	0.88

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	45	11283.30	139.175	0.869	0.7242E+06	0.88
*	46	11282.17	139.161	0.871	0.7259E+06	0.88
*	47	11281.41	139.152	0.846	0.7051E+06	0.88
*	48	11280.04	139.135	0.875	0.7292E+06	0.88
*	49	11278.07	139.111	0.852	0.7103E+06	0.88
*	50	11276.90	139.096	0.839	0.6992E+06	0.88
*	51	11275.35	139.077	0.869	0.7243E+06	0.88
*	52	11273.54	139.055	0.893	0.7445E+06	0.88
*	53	11272.80	139.046	0.926	0.7714E+06	0.88
*	54	11271.71	139.032	0.905	0.7540E+06	0.88
*	55	11270.42	139.016	0.904	0.7535E+06	0.88
*	56	11269.09	139.000	0.882	0.7352E+06	0.88
*	57	11266.40	138.967	0.928	0.7734E+06	0.88
*	58	11265.82	138.960	0.934	0.7783E+06	0.88
*	59	11264.53	138.944	0.954	0.7948E+06	0.88
*	60	11263.49	138.931	0.957	0.7977E+06	0.88
*	61	11262.91	138.924	0.950	0.7919E+06	0.88
*	62	11261.98	138.912	0.956	0.7967E+06	0.88
*	63	11260.42	138.893	0.955	0.7959E+06	0.88
*	64	11259.65	138.884	0.942	0.7849E+06	0.88
*	65	11258.83	138.873	0.976	0.8134E+06	0.88
*	66	11258.04	138.864	0.985	0.8210E+06	0.88
*	67	11257.16	138.853	0.975	0.8126E+06	0.88
*	68	11256.50	138.845	0.974	0.8117E+06	0.88
*	69	11255.45	138.832	1.021	0.8506E+06	0.88
*	70	11254.16	138.816	1.037	0.8643E+06	0.88
*	71	11253.45	138.807	1.037	0.8646E+06	0.88
*	72	11252.24	138.792	1.006	0.8383E+06	0.88
*	73	11251.29	138.780	1.035	0.8623E+06	0.88
*	74	11249.99	138.764	1.049	0.8740E+06	0.88
*	75	11249.35	138.757	1.065	0.8874E+06	0.88
*	76	11248.05	138.741	1.051	0.8762E+06	0.88
*	77	11246.82	138.725	1.043	0.8691E+06	0.88
*	78	11245.93	138.714	0.994	0.8288E+06	0.88
*	79	11245.04	138.703	1.043	0.8690E+06	0.88
*	80	11242.08	138.667	0.999	0.8326E+06	0.88
*	81	11241.10	138.655	0.962	0.8021E+06	0.88
*	82	11239.61	138.636	0.936	0.7797E+06	0.88
*	83	11239.11	138.630	0.926	0.7718E+06	0.88
*	84	11238.46	138.622	0.936	0.7801E+06	0.88
*	85	11236.13	138.593	0.829	0.6907E+06	0.88
*	86	11234.34	138.571	0.782	0.6521E+06	0.88
*	87	11233.73	138.564	0.758	0.6318E+06	0.88
*	88	11232.17	138.545	0.731	0.6096E+06	0.88
*	89	11231.28	138.534	0.707	0.5892E+06	0.88
*	90	11228.99	138.505	0.666	0.5551E+06	0.88
*	91	11227.64	138.489	0.644	0.5371E+06	0.88
*	92	11226.74	138.478	0.525	0.4377E+06	0.88
*	93	11225.92	138.468	0.543	0.4523E+06	0.88
*	94	11224.76	138.453	0.543	0.4524E+06	0.88
*	95	11223.06	138.432	0.504	0.4200E+06	0.88
*	96	11222.20	138.422	0.502	0.4188E+06	0.88
*	97	11220.79	138.404	0.471	0.3923E+06	0.88
*	98	11219.18	138.384	0.459	0.3824E+06	0.88
*	99	11218.12	138.371	0.415	0.3457E+06	0.88
*	100	11217.42	138.363	0.424	0.3537E+06	0.88
*	101	11215.86	138.343	0.448	0.3730E+06	0.88
*	102	11215.27	138.336	0.425	0.3542E+06	0.88
*	103	10775.41	132.911	11.921	0.9936E+07	2.64
*	104	10689.09	131.846	0.224	0.1866E+06	21.18

*	1	175.920	100.000	0.5929E+10	14268.83	14255.41
*	2	146.654	5.448	0.3230E+09	11891.02	11888.18
*	3	139.857	0.027	0.1603E+07	11338.95	11338.07
*	4	139.848	0.029	0.1695E+07	11338.21	11337.33
*	5	139.811	0.029	0.1709E+07	11335.24	11334.37
*	6	139.794	0.032	0.1884E+07	11333.91	11333.03
*	7	139.784	0.032	0.1924E+07	11333.02	11332.14
*	8	139.775	0.033	0.1979E+07	11332.28	11331.40
*	9	139.754	0.033	0.1970E+07	11330.65	11329.77
*	10	139.728	0.036	0.2109E+07	11328.58	11327.70
*	11	139.710	0.038	0.2273E+07	11327.09	11326.22
*	12	139.687	0.038	0.2248E+07	11325.17	11324.29
*	13	139.663	0.039	0.2336E+07	11323.24	11322.37
*	14	139.654	0.040	0.2378E+07	11322.50	11321.63
*	15	139.646	0.041	0.2439E+07	11321.76	11320.88
*	16	139.630	0.042	0.2463E+07	11320.58	11319.70
*	17	139.613	0.042	0.2478E+07	11319.24	11318.37
*	18	139.603	0.043	0.2527E+07	11318.35	11317.48
*	19	139.587	0.046	0.2736E+07	11317.02	11316.14
*	20	139.561	0.047	0.2787E+07	11314.95	11314.07
*	21	139.553	0.046	0.2740E+07	11314.35	11313.48
*	22	139.543	0.047	0.2762E+07	11313.47	11312.59
*	23	139.528	0.048	0.2862E+07	11312.28	11311.40
*	24	139.514	0.050	0.2950E+07	11311.10	11310.22
*	25	139.497	0.049	0.2887E+07	11309.76	11308.88
*	26	139.490	0.049	0.2881E+07	11309.17	11308.29
*	27	139.470	0.052	0.3088E+07	11307.54	11306.66
*	28	139.446	0.054	0.3226E+07	11305.61	11304.74
*	29	139.432	0.053	0.3150E+07	11304.58	11303.70
*	30	139.423	0.057	0.3351E+07	11303.84	11302.96
*	31	139.412	0.055	0.3286E+07	11302.95	11302.07
*	32	139.394	0.055	0.3278E+07	11301.47	11300.59
*	33	139.364	0.058	0.3442E+07	11298.95	11298.07
*	34	139.354	0.057	0.3367E+07	11298.21	11297.33
*	35	139.331	0.056	0.3306E+07	11296.28	11295.40
*	36	139.296	0.055	0.3249E+07	11293.47	11292.59
*	37	139.286	0.056	0.3342E+07	11292.58	11291.70
*	38	139.272	0.055	0.3284E+07	11291.54	11290.66
*	39	139.265	0.055	0.3284E+07	11290.95	11290.07
*	40	139.248	0.057	0.3405E+07	11289.62	11288.74
*	41	139.239	0.057	0.3359E+07	11288.87	11288.00
*	42	139.230	0.056	0.3308E+07	11288.13	11287.26
*	43	139.214	0.054	0.3195E+07	11286.80	11285.92
*	44	139.191	0.055	0.3290E+07	11285.02	11284.14
*	45	139.175	0.057	0.3369E+07	11283.69	11282.81
*	46	139.161	0.057	0.3376E+07	11282.65	11281.77
*	47	139.152	0.055	0.3280E+07	11281.76	11280.89
*	48	139.135	0.057	0.3392E+07	11280.43	11279.55
*	49	139.111	0.056	0.3304E+07	11278.50	11277.63
*	50	139.096	0.055	0.3252E+07	11277.32	11276.44
*	51	139.077	0.057	0.3369E+07	11275.69	11274.81
*	52	139.055	0.058	0.3463E+07	11273.91	11273.03
*	53	139.046	0.061	0.3588E+07	11273.17	11272.29
*	54	139.032	0.059	0.3507E+07	11272.13	11271.26
*	55	139.016	0.059	0.3505E+07	11270.80	11269.92
*	56	139.000	0.058	0.3420E+07	11269.47	11268.59
*	57	138.967	0.061	0.3597E+07	11266.80	11265.92
*	58	138.960	0.061	0.3620E+07	11266.21	11265.33
*	59	138.944	0.062	0.3697E+07	11264.88	11264.00
*	60	138.931	0.063	0.3710E+07	11263.84	11262.96
*	61	138.924	0.062	0.3683E+07	11263.25	11262.37
*	62	138.912	0.062	0.3706E+07	11262.36	11261.48
*	63	138.893	0.062	0.3702E+07	11260.88	11260.00
*	64	138.884	0.062	0.3651E+07	11259.99	11259.11
*	65	138.873	0.064	0.3783E+07	11259.25	11258.37

*	66	138.864	0.064	0.3819E+07	11258.50	11257.63
*	67	138.853	0.064	0.3780E+07	11257.62	11256.74
*	68	138.845	0.064	0.3776E+07	11256.88	11256.00
*	69	138.832	0.067	0.3956E+07	11255.84	11254.96
*	70	138.816	0.068	0.4020E+07	11254.50	11253.63
*	71	138.807	0.068	0.4021E+07	11253.91	11253.04
*	72	138.792	0.066	0.3899E+07	11252.58	11251.70
*	73	138.780	0.068	0.4011E+07	11251.69	11250.81
*	74	138.764	0.069	0.4065E+07	11250.36	11249.48
*	75	138.757	0.070	0.4128E+07	11249.76	11248.89
*	76	138.741	0.069	0.4076E+07	11248.43	11247.55
*	77	138.725	0.068	0.4043E+07	11247.25	11246.37
*	78	138.714	0.065	0.3855E+07	11246.36	11245.48
*	79	138.703	0.068	0.4042E+07	11245.47	11244.59
*	80	138.667	0.065	0.3873E+07	11242.50	11241.63
*	81	138.655	0.063	0.3731E+07	11241.47	11240.59
*	82	138.636	0.061	0.3627E+07	11239.99	11239.11
*	83	138.630	0.061	0.3590E+07	11239.54	11238.67
*	84	138.622	0.061	0.3629E+07	11238.80	11237.92
*	85	138.593	0.054	0.3213E+07	11236.58	11235.70
*	86	138.571	0.051	0.3033E+07	11234.80	11233.92
*	87	138.564	0.050	0.2939E+07	11234.21	11233.33
*	88	138.545	0.048	0.2836E+07	11232.58	11231.70
*	89	138.534	0.046	0.2741E+07	11231.69	11230.81
*	90	138.505	0.044	0.2582E+07	11229.47	11228.59
*	91	138.489	0.042	0.2498E+07	11227.99	11227.11
*	92	138.478	0.034	0.2036E+07	11227.10	11226.22
*	93	138.468	0.035	0.2104E+07	11226.36	11225.48
*	94	138.453	0.035	0.2104E+07	11225.17	11224.29
*	95	138.432	0.033	0.1954E+07	11223.39	11222.52
*	96	138.422	0.033	0.1948E+07	11222.65	11221.78
*	97	138.404	0.031	0.1825E+07	11221.17	11220.29
*	98	138.384	0.030	0.1779E+07	11219.54	11218.67
*	99	138.371	0.027	0.1608E+07	11218.51	11217.63
*	100	138.363	0.028	0.1645E+07	11217.77	11216.89
*	101	138.343	0.029	0.1735E+07	11216.28	11215.41
*	102	138.336	0.028	0.1647E+07	11215.69	11214.81
*	103	132.911	2.346	0.1391E+09	10776.73	10774.09
*	104	131.846	0.353	0.2095E+08	10699.64	10678.46

(*) Peaks 1 to 104 are fitted to Lorentzian



USERNAME: tmohan

NMR1
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Filename = TCS9
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 2322.80

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14262.41	175.922	100.000	0.7391E+08	13.60
*	2	11887.03	146.622	20.583	0.1521E+08	2.73
*	3	11328.05	139.727	0.132	0.9786E+05	60.37
*	4	11364.73	140.180	0.041	0.3043E+05	0.92
*	5	11313.13	139.543	0.065	0.4825E+05	11.09
*	6	11306.48	139.461	0.008	6080.	35.64
*	7	11309.61	139.500	0.063	0.4643E+05	28.15
*	8	11305.75	139.452	0.073	0.5422E+05	4.33
*	9	11303.00	139.418	0.055	0.4080E+05	2.86
*	10	11298.87	139.367	0.152	0.1124E+06	6.03
*	11	11296.08	139.333	0.024	0.1745E+05	0.48
*	12	11292.79	139.292	0.153	0.1129E+06	5.80
*	13	11287.00	139.221	0.149	0.1105E+06	6.49
*	14	11283.38	139.176	0.116	0.8550E+05	1.47
*	15	11279.15	139.124	0.185	0.1365E+06	10.28
*	16	11273.87	139.059	0.138	0.1020E+06	6.19
*	17	11269.94	139.011	0.182	0.1347E+06	2.97
*	18	11267.38	138.979	0.119	0.8761E+05	1.37
*	19	11264.68	138.946	0.192	0.1418E+06	3.72
*	20	11262.25	138.916	0.172	0.1274E+06	2.12
*	21	11260.10	138.889	0.110	0.8167E+05	2.84
*	22	11257.34	138.855	0.250	0.1848E+06	3.14
*	23	11254.97	138.826	0.109	0.8058E+05	2.76
*	24	11252.89	138.800	0.150	0.1110E+06	4.96
*	25	11249.71	138.761	0.221	0.1632E+06	3.46
*	26	11247.21	138.730	0.136	0.1004E+06	2.94
*	27	11243.36	138.683	0.253	0.1871E+06	6.68
*	28	11238.32	138.621	0.164	0.1211E+06	7.13
*	29	11233.98	138.567	0.019	0.1396E+05	0.54
*	30	11231.83	138.541	0.110	0.8107E+05	3.40
*	31	11223.02	138.432	0.082	0.6092E+05	0.87
*	32	11252.39	138.794	0.120	0.8898E+05	197.62
*	33	11224.96	138.456	0.140	0.1035E+06	28.63
*	34	10773.45	132.887	9.006	0.6656E+07	2.66
*	35	10690.46	131.863	0.175	0.1292E+06	12.00

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.922	100.000	0.1332E+10	14268.77	14255.17
*	2	146.622	4.134	0.5506E+08	11888.30	11885.57

*	3	139.727	0.588	0.7831E+07	11358.32	11297.95
*	4	140.180	0.003	0.3691E+05	11365.33	11364.42
*	5	139.543	0.053	0.7091E+06	11318.27	11307.18
*	6	139.461	0.022	0.2872E+06	11324.03	11288.39
*	7	139.500	0.130	0.1733E+07	11323.25	11295.09
*	8	139.452	0.023	0.3109E+06	11307.78	11303.45
*	9	139.418	0.012	0.1544E+06	11304.08	11301.23
*	10	139.367	0.067	0.8984E+06	11301.52	11295.49
*	11	139.333	0.001	0.1102E+05	11296.37	11295.90
*	12	139.292	0.065	0.8675E+06	11295.48	11289.68
*	13	139.221	0.071	0.9497E+06	11289.90	11283.41
*	14	139.176	0.012	0.1661E+06	11283.83	11282.37
*	15	139.124	0.140	0.1861E+07	11284.09	11273.81
*	16	139.059	0.063	0.8369E+06	11276.71	11270.52
*	17	139.011	0.040	0.5310E+06	11271.55	11268.58
*	18	138.979	0.012	0.1589E+06	11267.78	11266.42
*	19	138.946	0.052	0.6992E+06	11266.59	11262.87
*	20	138.916	0.027	0.3579E+06	11263.42	11261.30
*	21	138.889	0.023	0.3073E+06	11261.41	11258.57
*	22	138.855	0.058	0.7682E+06	11258.59	11255.46
*	23	138.826	0.022	0.2945E+06	11256.04	11253.28
*	24	138.800	0.055	0.7299E+06	11255.36	11250.40
*	25	138.761	0.056	0.7487E+06	11251.05	11247.59
*	26	138.730	0.029	0.3907E+06	11248.42	11245.48
*	27	138.683	0.124	0.1657E+07	11246.74	11240.06
*	28	138.621	0.086	0.1144E+07	11241.63	11234.50
*	29	138.567	0.001	9994.	11234.19	11233.65
*	30	138.541	0.027	0.3649E+06	11233.24	11229.85
*	31	138.432	0.005	0.7034E+05	11223.09	11222.22
*	32	138.794	1.750	0.2331E+08	11351.09	11153.48
*	33	138.456	0.295	0.3928E+07	11239.34	11210.71
*	34	132.887	1.762	0.2346E+08	10774.82	10772.16
*	35	131.863	0.154	0.2056E+07	10696.53	10684.52

(*) Peaks 1 to 35 are fitted to Lorentzian

NMR1
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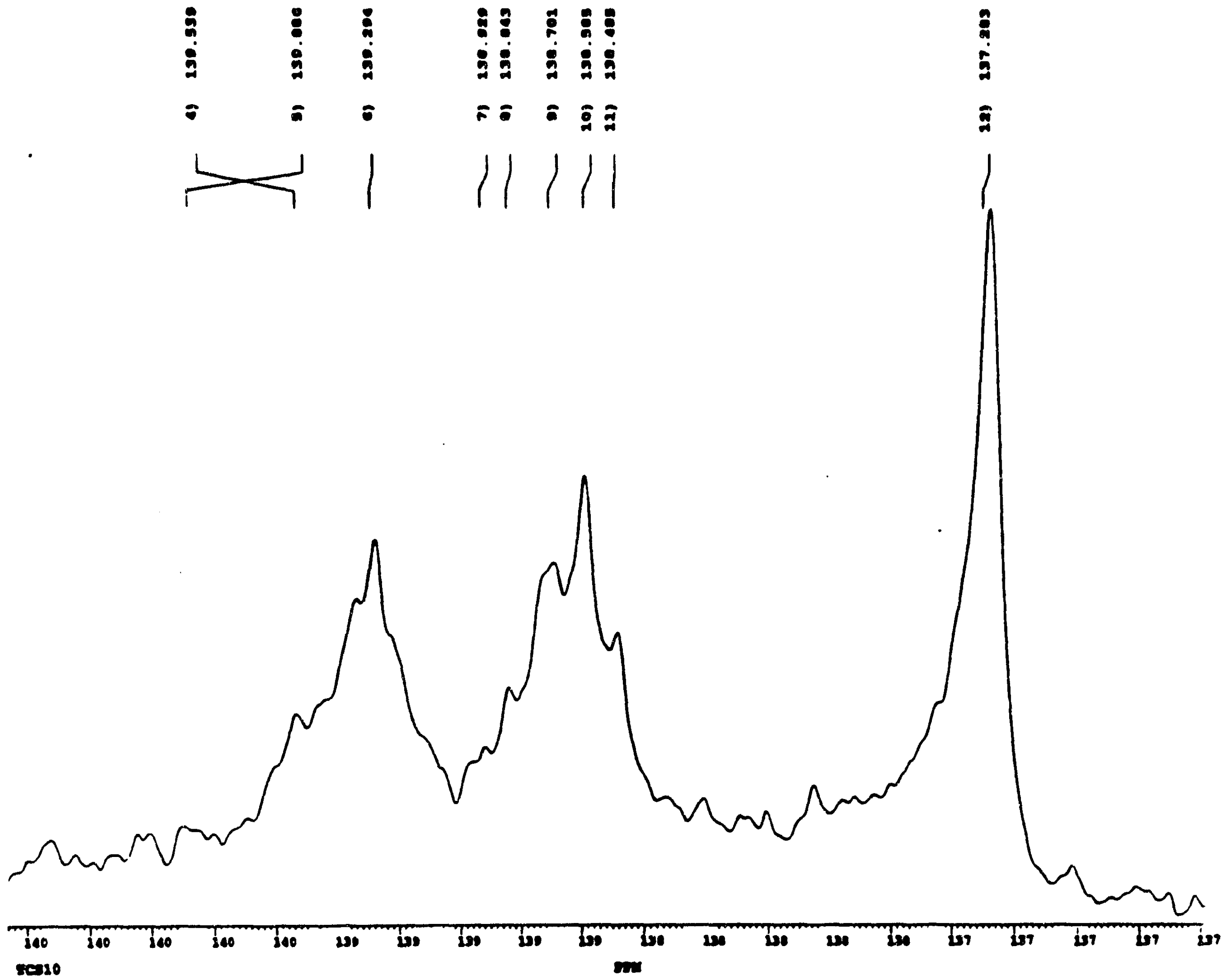
Filename = TCS10
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 1314.04

Peak Analysis

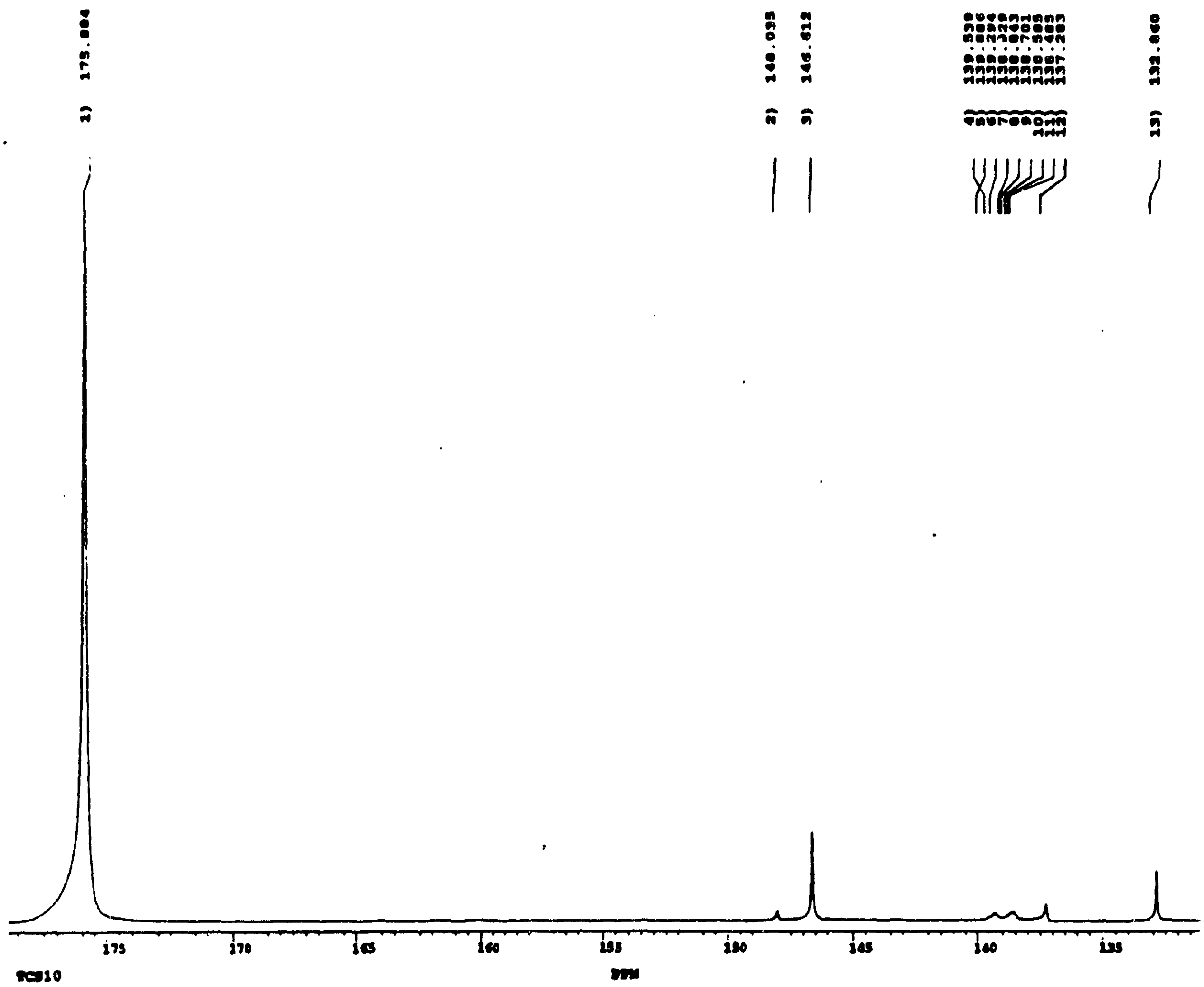
	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14259.33	175.884	100.000	0.5009E+08	14.90
*	2	12001.57	148.035	1.412	0.7071E+06	8.21
*	3	11886.23	146.612	12.314	0.6168E+07	6.24
*	4	11312.78	139.539	0.297	0.1486E+06	13.21
*	5	11340.89	139.886	0.082	0.4126E+05	4.36
*	6	11292.88	139.294	1.083	0.5423E+06	21.26
*	7	11263.31	138.929	0.132	0.6595E+05	6.01
*	8	11256.33	138.843	0.237	0.1187E+06	3.58
*	9	11244.85	138.701	0.986	0.4937E+06	15.47
*	10	11235.42	138.585	0.890	0.4458E+06	5.20
*	11	11227.37	138.485	0.561	0.2809E+06	11.47
*	12	11129.86	137.283	2.341	0.1173E+07	9.77
*	13	10771.32	132.860	7.043	0.3528E+07	5.42

	Peak #	PPM	Relative integral	Absolute integral	Integral start(hz)	Integral end(hz)
*	1	175.884	100.000	0.1979E+10	14266.43	14251.53
*	2	148.035	0.778	0.1538E+08	12005.67	11997.47
*	3	146.612	5.158	0.1021E+09	11889.14	11882.90
*	4	139.539	0.263	0.5207E+07	11319.31	11306.10
*	5	139.886	0.024	0.4769E+06	11343.03	11338.67
*	6	139.294	1.544	0.3056E+08	11303.48	11282.22
*	7	138.929	0.053	0.1050E+07	11266.23	11260.22
*	8	138.843	0.057	0.1127E+07	11257.90	11254.32
*	9	138.701	1.023	0.2025E+08	11252.59	11237.12
*	10	138.585	0.310	0.6140E+07	11237.97	11232.77
*	11	138.485	0.432	0.8539E+07	11233.10	11221.64
*	12	137.283	1.534	0.3036E+08	11134.78	11125.01
*	13	132.860	2.562	0.5069E+08	10774.10	10768.68

(*) Peaks 1 to 13 are fitted to Lorentzian



4) 139.530
5) 139.086
6) 139.204
7) 138.929
8) 138.843
9) 138.701
10) 138.585
11) 138.488
12) 137.283
140 140 140 140 140 139 139 139 139 139 138 138 138 138 138 137 137 137 137 137
TCB10
PPM


1) 175.884
2) 148.035
3) 146.612
13) 132.860
175
170
165
160
155
150
145
140
135
PPM

NMR1
****

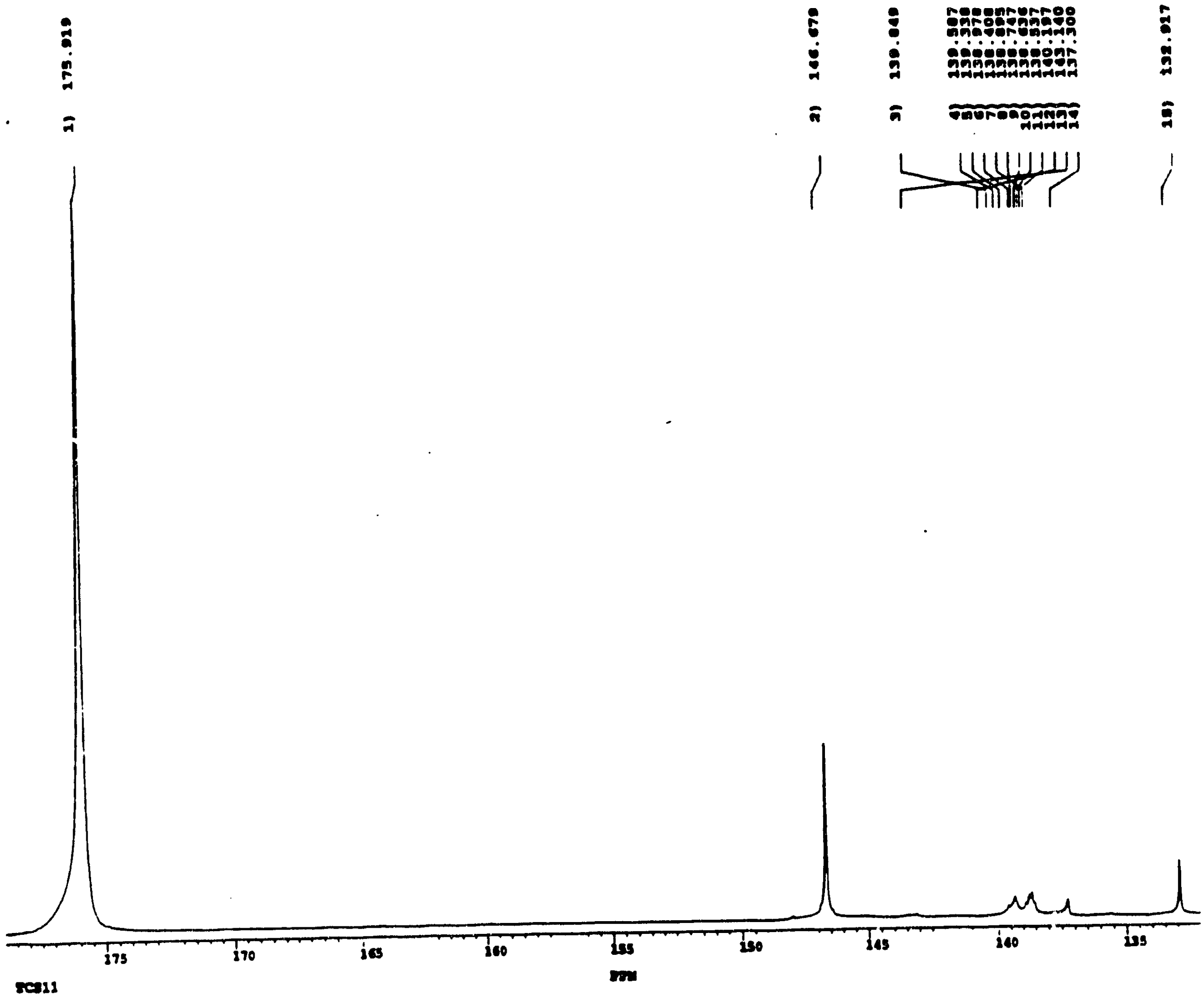
Filename = TCS11
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 2086.35

Peak Analysis

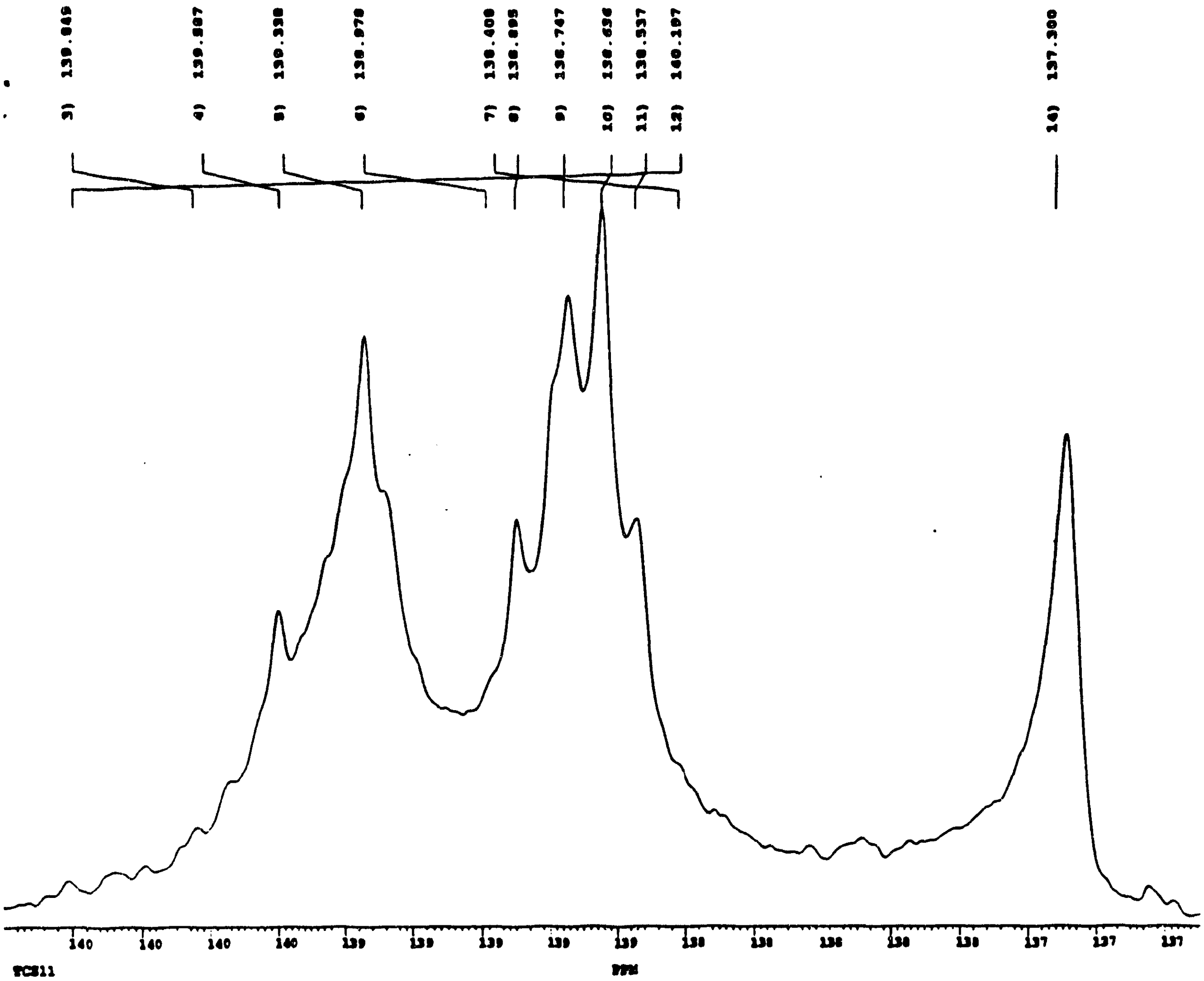
	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14262.21	175.919	100.000	0.5827E+08	15.12
*	2	11891.63	146.679	23.961	0.1396E+08	6.22
*	3	11337.91	139.849	0.080	0.4674E+05	4.42
*	4	11316.69	139.587	0.876	0.5102E+06	21.12
*	5	11296.49	139.338	2.272	0.1324E+07	18.73
*	6	11267.32	138.978	0.455	0.2649E+06	30.69
*	7	11221.08	138.408	0.347	0.2020E+06	55.82
*	8	11260.56	138.895	0.745	0.4341E+06	4.26
*	9	11248.55	138.747	2.368	0.1380E+07	13.14
*	10	11239.59	138.636	2.175	0.1267E+07	5.53
*	11	11231.55	138.537	1.064	0.6202E+06	6.33
*	12	11366.09	140.197	0.714	0.4160E+06	5.45
*	13	11604.73	143.140	0.764	0.4451E+06	72.39
*	14	11131.22	137.300	2.198	0.1281E+07	11.29
*	15	10775.93	132.917	7.382	0.4301E+07	5.65

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.919	100.000	0.2336E+10	14269.64	14254.52
*	2	146.679	9.849	0.2301E+09	11894.59	11888.38
*	3	139.849	0.023	0.5476E+06	11339.94	11335.52
*	4	139.587	1.223	0.2856E+08	11327.25	11306.13
*	5	139.338	2.814	0.6573E+08	11305.91	11287.18
*	6	138.978	0.923	0.2155E+08	11282.55	11251.86
*	7	138.408	1.280	0.2989E+08	11248.90	11193.08
*	8	138.895	0.210	0.4907E+07	11262.53	11258.26
*	9	138.747	2.057	0.4804E+08	11255.11	11241.97
*	10	138.636	0.794	0.1856E+08	11242.42	11236.89
*	11	138.537	0.446	0.1041E+08	11234.52	11228.19
*	12	140.197	0.257	0.6008E+07	11368.60	11363.15
*	13	143.140	3.657	0.8542E+08	11640.88	11568.48
*	14	137.300	1.641	0.3833E+08	11136.86	11125.57
*	15	132.917	2.760	0.6447E+08	10778.79	10773.14

(*) Peaks 1 to 15 are fitted to Lorentzian



1) 175.919
2) 146.679
3) 139.849
15) 132.917
175
170
165
160
155
150
145
140
135
PPM
TCS11



NMR1
****

Filename = TCS12
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 2638.23

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14262.21	175.919	100.000	0.8486E+08	12.65
*	2	11885.00	146.597	19.386	0.1645E+08	2.98
*	3	11359.63	140.117	0.585	0.4968E+06	0.81
*	4	11356.00	140.072	0.572	0.4857E+06	0.81
*	5	11354.27	140.051	0.620	0.5257E+06	0.81
*	6	11352.95	140.034	0.622	0.5278E+06	0.81
*	7	11351.72	140.019	0.629	0.5336E+06	0.81
*	8	11350.61	140.006	0.659	0.5588E+06	0.81
*	9	11348.68	139.982	0.673	0.5715E+06	0.81
*	10	11347.07	139.962	0.730	0.6195E+06	0.81
*	11	11345.67	139.945	0.716	0.6076E+06	0.81
*	12	11343.97	139.924	0.753	0.6393E+06	0.81
*	13	11343.35	139.916	0.747	0.6341E+06	0.81
*	14	11342.36	139.904	0.772	0.6554E+06	0.81
*	15	11341.40	139.892	0.761	0.6456E+06	0.81
*	16	11339.74	139.871	0.833	0.7068E+06	0.81
*	17	11337.79	139.847	0.840	0.7126E+06	0.81
*	18	11337.05	139.838	0.835	0.7083E+06	0.81
*	19	11334.62	139.808	0.929	0.7886E+06	0.81
*	20	11333.87	139.799	0.907	0.7698E+06	0.81
*	21	11333.06	139.789	0.890	0.7555E+06	0.81
*	22	11332.41	139.781	0.899	0.7632E+06	0.81
*	23	11331.66	139.772	0.896	0.7603E+06	0.81
*	24	11330.17	139.753	0.987	0.8372E+06	0.81
*	25	11328.17	139.729	1.034	0.8774E+06	0.81
*	26	11327.37	139.719	1.037	0.8804E+06	0.81
*	27	11326.36	139.707	1.074	0.9113E+06	0.81
*	28	11324.28	139.681	1.105	0.9375E+06	0.81
*	29	11323.30	139.669	1.079	0.9156E+06	0.81
*	30	11321.17	139.642	1.148	0.9738E+06	0.81
*	31	11320.31	139.632	1.202	0.1020E+07	0.81
*	32	11318.92	139.615	1.258	0.1066E+07	0.81
*	33	11318.08	139.604	1.224	0.1039E+07	0.81
*	34	11317.09	139.592	1.258	0.1068E+07	0.81
*	35	11316.06	139.579	1.269	0.1077E+07	0.81
*	36	11314.40	139.559	1.321	0.1121E+07	0.81
*	37	11313.12	139.543	1.383	0.1173E+07	0.81
*	38	11312.50	139.536	1.369	0.1162E+07	0.81
*	39	11311.52	139.523	1.409	0.1196E+07	0.81
*	40	11310.94	139.516	1.419	0.1204E+07	0.81
*	41	11309.97	139.504	1.400	0.1188E+07	0.81
*	42	11308.78	139.490	1.512	0.1283E+07	0.81
*	43	11307.30	139.471	1.486	0.1261E+07	0.81
*	44	11306.07	139.456	1.493	0.1267E+07	0.81

*	45	11304.76	139.440	1.505	0.1277E+07	0.81
*	46	11303.91	139.430	1.519	0.1289E+07	0.81
*	47	11303.18	139.421	1.573	0.1335E+07	0.81
*	48	11302.09	139.407	1.624	0.1378E+07	0.81
*	49	11299.99	139.381	1.669	0.1416E+07	0.81
*	50	11299.36	139.373	1.698	0.1441E+07	0.81
*	51	11298.12	139.358	1.703	0.1445E+07	0.81
*	52	11297.53	139.351	1.693	0.1436E+07	0.81
*	53	11296.79	139.342	1.688	0.1432E+07	0.81
*	54	11295.25	139.323	1.686	0.1430E+07	0.81
*	55	11293.59	139.302	1.722	0.1461E+07	0.81
*	56	11292.69	139.291	1.740	0.1476E+07	0.81
*	57	11291.76	139.280	1.735	0.1472E+07	0.81
*	58	11291.05	139.271	1.746	0.1482E+07	0.81
*	59	11289.42	139.251	1.761	0.1495E+07	0.81
*	60	11288.53	139.240	1.701	0.1443E+07	0.81
*	61	11286.74	139.218	1.740	0.1477E+07	0.81
*	62	11285.23	139.199	1.808	0.1535E+07	0.81
*	63	11284.14	139.186	1.814	0.1540E+07	0.81
*	64	11283.65	139.180	1.814	0.1540E+07	0.81
*	65	11281.60	139.154	1.827	0.1551E+07	0.81
*	66	11280.62	139.142	1.858	0.1577E+07	0.81
*	67	11280.01	139.135	1.857	0.1576E+07	0.81
*	68	11278.59	139.117	1.888	0.1602E+07	0.81
*	69	11277.50	139.104	1.911	0.1622E+07	0.81
*	70	11275.62	139.081	1.946	0.1651E+07	0.81
*	71	11274.87	139.071	1.938	0.1644E+07	0.81
*	72	11272.13	139.038	2.013	0.1708E+07	0.81
*	73	11270.48	139.017	2.045	0.1736E+07	0.81
*	74	11267.35	138.979	2.127	0.1805E+07	0.81
*	75	11264.89	138.948	2.155	0.1828E+07	0.81
*	76	11263.15	138.927	2.192	0.1860E+07	0.81
*	77	11261.85	138.911	2.193	0.1861E+07	0.81
*	78	11260.62	138.896	2.174	0.1845E+07	0.81
*	79	11259.39	138.880	2.234	0.1895E+07	0.81
*	80	11258.97	138.875	2.236	0.1897E+07	0.81
*	81	11258.21	138.866	2.270	0.1926E+07	0.81
*	82	11257.68	138.859	2.257	0.1915E+07	0.81
*	83	11256.85	138.849	2.280	0.1935E+07	0.81
*	84	11255.30	138.830	2.267	0.1924E+07	0.81
*	85	11253.92	138.813	2.331	0.1978E+07	0.81
*	86	11252.80	138.799	2.365	0.2007E+07	0.81
*	87	11252.03	138.790	2.398	0.2035E+07	0.81
*	88	11251.33	138.781	2.395	0.2032E+07	0.81
*	89	11250.13	138.766	2.405	0.2041E+07	0.81
*	90	11248.00	138.740	2.479	0.2103E+07	0.81
*	91	11246.51	138.722	2.491	0.2114E+07	0.81
*	92	11245.68	138.711	2.465	0.2091E+07	0.81
*	93	11243.91	138.689	2.384	0.2023E+07	0.81
*	94	11242.44	138.671	2.339	0.1985E+07	0.81
*	95	11241.19	138.656	2.280	0.1934E+07	0.81
*	96	11240.04	138.642	2.264	0.1921E+07	0.81
*	97	11239.39	138.634	2.223	0.1886E+07	0.81
*	98	11236.81	138.602	2.075	0.1761E+07	0.81
*	99	11235.40	138.585	2.036	0.1728E+07	0.81
*	100	11234.05	138.568	1.961	0.1664E+07	0.81
*	101	11231.48	138.536	1.817	0.1541E+07	0.81
*	102	11229.25	138.509	1.677	0.1423E+07	0.81
*	103	11228.66	138.501	1.656	0.1405E+07	0.81
*	104	11227.96	138.493	1.649	0.1399E+07	0.81
*	105	11227.26	138.484	1.645	0.1396E+07	0.81
*	106	11225.17	138.458	1.487	0.1262E+07	0.81
*	107	11223.75	138.441	1.409	0.1196E+07	0.81
*	108	11222.73	138.428	1.395	0.1183E+07	0.81
*	109	11221.27	138.410	1.335	0.1133E+07	0.81
*	110	11220.21	138.397	1.309	0.1111E+07	0.81

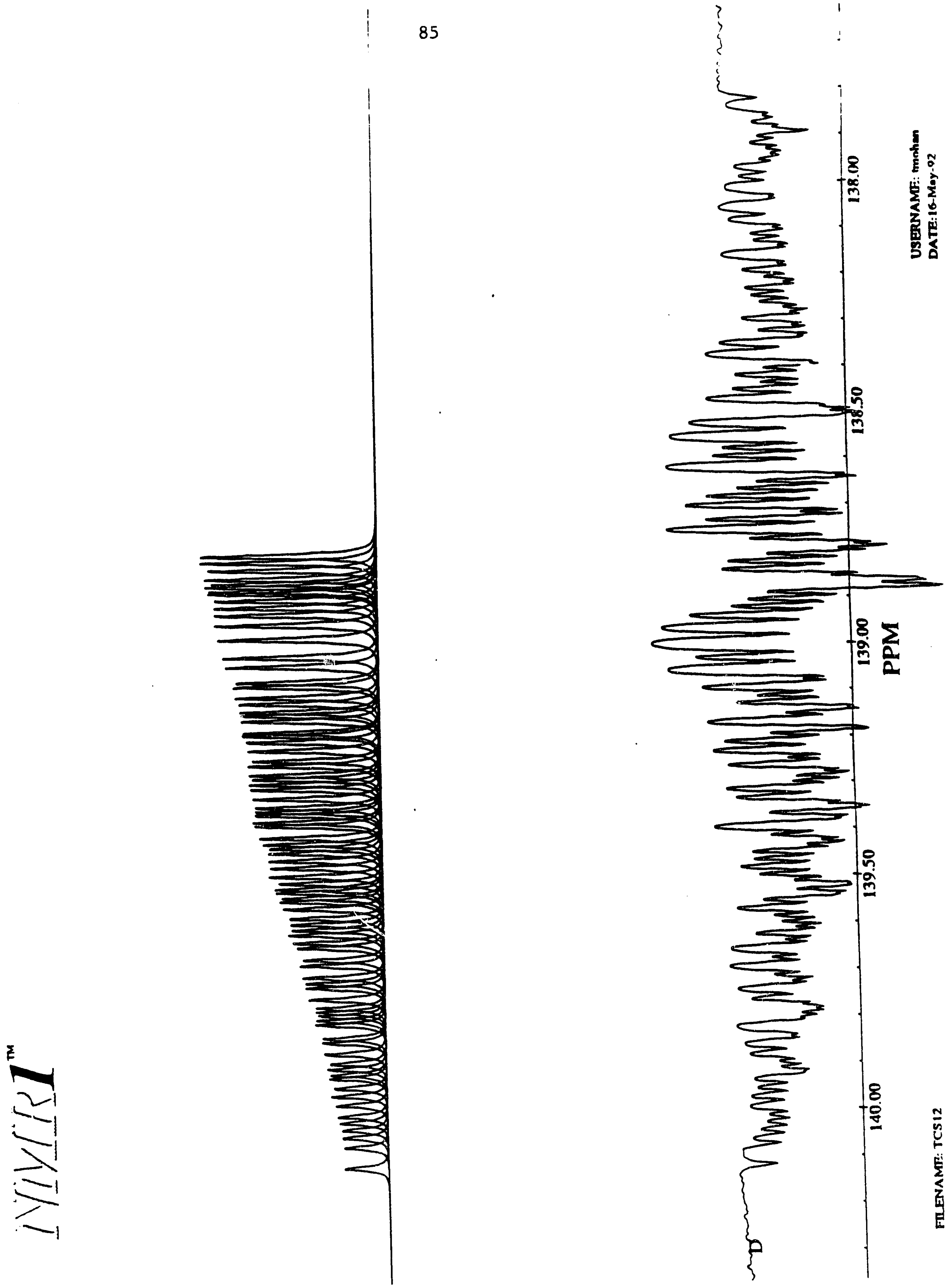
*	111	11219.59	138.390	1.310	0.1111E+07	0.81
*	112	11217.21	138.360	1.237	0.1050E+07	0.81
*	113	11215.37	138.337	1.155	0.9800E-06	0.81
*	114	11214.70	138.329	1.151	0.9765E+06	0.81
*	115	11213.53	138.315	1.105	0.9375E+06	0.81
*	116	11212.82	138.306	1.096	0.9304E+06	0.81
*	117	11211.25	138.287	1.026	0.8709E+06	0.81
*	118	11210.50	138.277	1.050	0.8911E+06	0.81
*	119	11209.67	138.267	1.019	0.8650E+06	0.81
*	120	11208.54	138.253	0.974	0.8264E+06	0.81
*	121	11207.33	138.238	0.958	0.8132E+06	0.81
*	122	11205.97	138.221	0.947	0.8033E+06	0.81
*	123	11205.22	138.212	0.936	0.7943E+06	0.81
*	124	11204.21	138.200	0.873	0.7407E+06	0.81
*	125	11202.77	138.182	0.888	0.7533E+06	0.81
*	126	11202.03	138.173	0.876	0.7431E+06	0.81
*	127	11199.61	138.143	0.883	0.7495E+06	0.81
*	128	11198.88	138.134	0.841	0.7133E+06	0.81
*	129	11197.71	138.120	0.816	0.6926E+06	0.81
*	130	11196.51	138.105	0.787	0.6676E+06	0.81
*	131	11195.75	138.096	0.791	0.6711E+06	0.81
*	132	11193.80	138.071	0.780	0.6622E+06	0.81
*	133	11191.11	138.038	0.726	0.6157E+06	0.81
*	134	11190.39	138.029	0.736	0.6245E+06	0.81
*	135	11187.78	137.997	0.697	0.5911E+06	0.81
*	136	11186.38	137.980	0.649	0.5511E+06	0.81
*	137	11184.53	137.957	0.660	0.5599E+06	0.81
*	138	11183.57	137.945	0.669	0.5674E+06	0.81
*	139	11182.75	137.935	0.616	0.5229E+06	0.81
*	140	11181.87	137.924	0.667	0.5660E+06	0.81
*	141	11180.63	137.909	0.652	0.5536E+06	0.81
*	142	11179.44	137.894	0.628	0.5330E+06	0.81
*	143	11179.18	137.891	0.628	0.5331E+06	0.81
*	144	11178.31	137.880	0.617	0.5239E+06	0.81
*	145	11177.06	137.865	0.609	0.5169E+06	0.81
*	146	11176.21	137.854	0.577	0.4898E+06	0.81
*	147	11173.52	137.821	0.584	0.4953E+06	0.81
*	148	10773.02	132.881	15.614	0.1325E+08	2.80
*	149	10691.71	131.878	0.391	0.3314E+06	30.66
*	150	10682.06	131.759	0.355	0.3011E+06	1.91

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.919	100.000	0.5693E+10	14268.44	14255.78
*	2	146.597	4.561	0.2596E+09	11886.49	11883.51
*	3	140.117	0.038	0.2137E+07	11359.94	11359.13
*	4	140.072	0.037	0.2089E+07	11356.38	11355.57
*	5	140.051	0.040	0.2262E+07	11354.60	11353.79
*	6	140.034	0.040	0.2271E+07	11353.27	11352.46
*	7	140.019	0.040	0.2295E+07	11352.09	11351.27
*	8	140.006	0.042	0.2404E+07	11351.05	11350.24
*	9	139.982	0.043	0.2458E+07	11348.97	11348.16
*	10	139.962	0.047	0.2665E+07	11347.49	11346.68
*	11	139.945	0.046	0.2614E+07	11346.01	11345.20
*	12	139.924	0.048	0.2750E+07	11344.38	11343.57
*	13	139.916	0.048	0.2728E+07	11343.64	11342.83
*	14	139.904	0.050	0.2820E+07	11342.75	11341.94
*	15	139.892	0.049	0.2777E+07	11341.72	11340.90
*	16	139.871	0.053	0.3041E+07	11340.09	11339.27
*	17	139.847	0.054	0.3066E+07	11338.16	11337.35
*	18	139.838	0.054	0.3047E+07	11337.42	11336.61
*	19	139.808	0.060	0.3392E+07	11335.05	11334.24

*	20	139.799	0.058	0.3312E+07	11334.31	11333.50
*	21	139.789	0.057	0.3250E+07	11333.42	11332.61
*	22	139.781	0.056	0.3283E+07	11332.83	11332.02
*	23	139.772	0.057	0.3271E+07	11332.09	11331.28
*	24	139.753	0.063	0.3602E+07	11330.61	11329.79
*	25	139.729	0.066	0.3775E+07	11328.53	11327.72
*	26	139.719	0.067	0.3787E+07	11327.79	11326.98
*	27	139.707	0.069	0.3920E+07	11326.75	11325.94
*	28	139.681	0.071	0.4033E+07	11324.68	11323.87
*	29	139.669	0.069	0.3939E+07	11323.64	11322.83
*	30	139.642	0.074	0.4189E+07	11321.57	11320.76
*	31	139.632	0.077	0.4387E+07	11320.68	11319.87
*	32	139.615	0.081	0.4593E+07	11319.35	11318.54
*	33	139.604	0.079	0.4469E+07	11318.46	11317.65
*	34	139.592	0.081	0.4592E+07	11317.42	11316.61
*	35	139.579	0.081	0.4633E+07	11316.38	11315.57
*	36	139.559	0.085	0.4821E+07	11314.75	11313.94
*	37	139.543	0.089	0.5048E+07	11313.42	11312.61
*	38	139.536	0.088	0.4999E+07	11312.83	11312.02
*	39	139.523	0.090	0.5143E+07	11311.94	11311.13
*	40	139.516	0.091	0.5178E+07	11311.35	11310.54
*	41	139.504	0.090	0.5112E+07	11310.31	11309.50
*	42	139.490	0.097	0.5518E+07	11309.12	11308.31
*	43	139.471	0.095	0.5426E+07	11307.64	11306.83
*	44	139.456	0.096	0.5452E+07	11306.46	11305.65
*	45	139.440	0.097	0.5495E+07	11305.12	11304.31
*	46	139.430	0.097	0.5544E+07	11304.24	11303.42
*	47	139.421	0.101	0.5742E+07	11303.49	11302.68
*	48	139.407	0.104	0.5929E+07	11302.46	11301.65
*	49	139.381	0.107	0.6091E+07	11300.38	11299.57
*	50	139.373	0.109	0.6198E+07	11299.79	11298.98
*	51	139.358	0.109	0.6216E+07	11298.46	11297.65
*	52	139.351	0.109	0.6178E+07	11297.87	11297.05
*	53	139.342	0.108	0.6161E+07	11297.13	11296.31
*	54	139.323	0.108	0.6154E+07	11295.64	11294.83
*	55	139.302	0.110	0.6287E+07	11294.01	11293.20
*	56	139.291	0.112	0.6352E+07	11293.13	11292.31
*	57	139.280	0.111	0.6332E+07	11292.09	11291.28
*	58	139.271	0.112	0.6374E+07	11291.50	11290.68
*	59	139.251	0.113	0.6430E+07	11289.72	11288.91
*	60	139.240	0.109	0.6209E+07	11288.98	11288.17
*	61	139.218	0.112	0.6353E+07	11287.05	11286.24
*	62	139.199	0.116	0.6602E+07	11285.57	11284.76
*	63	139.186	0.116	0.6623E+07	11284.53	11283.72
*	64	139.180	0.116	0.6624E+07	11284.09	11283.28
*	65	139.154	0.117	0.6671E+07	11282.01	11281.20
*	66	139.142	0.119	0.6784E+07	11280.98	11280.17
*	67	139.135	0.119	0.6778E+07	11280.38	11279.57
*	68	139.117	0.121	0.6893E+07	11278.90	11278.09
*	69	139.104	0.123	0.6977E+07	11277.87	11277.05
*	70	139.081	0.125	0.7103E+07	11275.94	11275.13
*	71	139.071	0.124	0.7073E+07	11275.20	11274.39
*	72	139.038	0.129	0.7349E+07	11272.53	11271.72
*	73	139.017	0.131	0.7466E+07	11270.90	11270.09
*	74	138.979	0.136	0.7763E+07	11267.79	11266.98
*	75	138.948	0.138	0.7866E+07	11265.27	11264.46
*	76	138.927	0.141	0.8002E+07	11263.50	11262.68
*	77	138.911	0.141	0.8005E+07	11262.16	11261.35
*	78	138.896	0.139	0.7938E+07	11260.98	11260.17
*	79	138.880	0.143	0.8154E+07	11259.79	11258.98
*	80	138.875	0.143	0.8163E+07	11259.35	11258.54
*	81	138.866	0.146	0.8287E+07	11258.61	11257.80
*	82	138.859	0.145	0.8238E+07	11258.01	11257.20
*	83	138.849	0.146	0.8324E+07	11257.27	11256.46
*	84	138.830	0.145	0.8276E+07	11255.64	11254.83
*	85	138.813	0.149	0.8509E+07	11254.31	11253.50

*	86	138.799	0.152	0.8632E+07	11253.13	11252.31
*	87	138.790	0.154	0.8753E+07	11252.38	11251.57
*	88	138.781	0.154	0.8741E+07	11251.64	11250.83
*	89	138.766	0.154	0.8781E+07	11250.46	11249.65
*	90	138.740	0.159	0.9048E+07	11248.38	11247.57
*	91	138.722	0.160	0.9094E+07	11246.90	11246.09
*	92	138.711	0.158	0.8997E+07	11246.01	11245.20
*	93	138.689	0.153	0.8704E+07	11244.24	11243.43
*	94	138.671	0.150	0.8540E+07	11242.76	11241.94
*	95	138.656	0.146	0.8322E+07	11241.57	11240.76
*	96	138.642	0.145	0.8264E+07	11240.39	11239.57
*	97	138.634	0.143	0.8115E+07	11239.79	11238.98
*	98	138.602	0.133	0.7575E+07	11237.13	11236.32
*	99	13 585	0.131	0.7432E+07	11235.79	11234.98
*	100	138.568	0.126	0.7159E+07	11234.46	11233.65
*	101	138.536	0.116	0.6632E+07	11231.79	11230.98
*	102	138.509	0.108	0.6121E+07	11229.57	11228.76
*	103	138.501	0.106	0.6046E+07	11228.98	11228.17
*	104	138.493	0.106	0.6019E+07	11228.39	11227.57
*	105	138.484	0.106	0.6006E+07	11227.65	11226.83
*	106	138.458	0.095	0.5429E+07	11225.57	11224.76
*	107	138.441	0.090	0.5144E+07	11224.09	11223.28
*	108	138.428	0.089	0.5091E+07	11223.05	11222.24
*	109	138.410	0.086	0.4875E+07	11221.57	11220.76
*	110	138.397	0.084	0.4779E+07	11220.53	11219.72
*	111	138.390	0.084	0.4782E+07	11219.94	11219.13
*	112	138.360	0.079	0.4517E+07	11217.57	11216.76
*	113	138.337	0.074	0.4216E+07	11215.79	11214.98
*	114	138.329	0.074	0.4201E+07	11215.05	11214.24
*	115	138.315	0.071	0.4033E+07	11213.87	11213.06
*	116	138.306	0.070	0.4003E+07	11213.13	11212.32
*	117	138.287	0.066	0.3747E+07	11211.65	11210.83
*	118	138.277	0.067	0.3833E+07	11210.91	11210.09
*	119	138.267	0.065	0.3721E+07	11210.02	11209.21
*	120	138.253	0.062	0.3555E+07	11208.98	11208.17
*	121	138.238	0.061	0.3498E+07	11207.65	11206.83
*	122	138.221	0.061	0.3456E+07	11206.31	11205.50
*	123	138.212	0.060	0.3417E+07	11205.57	11204.76
*	124	138.200	0.056	0.3186E+07	11204.54	11203.72
*	125	138.182	0.057	0.3241E+07	11203.20	11202.39
*	126	138.173	0.056	0.3197E+07	11202.46	11201.65
*	127	138.143	0.057	0.3224E+07	11199.94	11199.13
*	128	138.134	0.054	0.3069E+07	11199.20	11198.39
*	129	138.120	0.052	0.2980E+07	11198.02	11197.21
*	130	138.105	0.050	0.2872E+07	11196.83	11196.02
*	131	138.096	0.051	0.2887E+07	11196.09	11195.28
*	132	138.071	0.050	0.2849E+07	11194.17	11193.35
*	133	138.038	0.047	0.2649E+07	11191.50	11190.69
*	134	138.029	0.047	0.2687E+07	11190.76	11189.95
*	135	137.997	0.045	0.2543E+07	11188.09	11187.28
*	136	137.980	0.042	0.2371E+07	11186.76	11185.95
*	137	137.957	0.042	0.2409E+07	11184.83	11184.02
*	138	137.945	0.043	0.2441E+07	11183.94	11183.13
*	139	137.935	0.040	0.2250E+07	11183.05	11182.24
*	140	137.924	0.043	0.2435E+07	11182.31	11181.50
*	141	137.909	0.042	0.2382E+07	11180.98	11180.17
*	142	137.894	0.040	0.2293E+07	11179.79	11178.98
*	143	137.891	0.040	0.2293E+07	11179.50	11178.69
*	144	137.880	0.040	0.2254E+07	11178.76	11177.95
*	145	137.865	0.039	0.2224E+07	11177.42	11176.61
*	146	137.854	0.037	0.2107E+07	11176.54	11175.72
*	147	137.821	0.037	0.2131E+07	11173.87	11173.06
*	148	132.881	3.460	0.1970E+09	10774.43	10771.63
*	149	131.878	0.946	0.5388E+08	10707.03	10676.37
*	150	131.759	0.053	0.3044E+07	10683.02	10681.12

(*) Peaks 1 to 150 are fitted to Lorentzian


138.00
138.50
139.00
PPM
139.50
140.00
USERNAME: tmohan
DATE:16-May-92
FILENAME: TCS12

NMR1
****

Filename = TCS13
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 4110.53

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14260.98	175.904	100.000	0.1438E+09	8.70
*	2	11890.08	146.660	15.371	0.2210E+08	1.94
*	3	11317.00	139.591	0.073	0.1047E+06	16.19
*	4	11335.56	139.820	0.183	0.2628E+06	74.33
*	5	11322.33	139.657	0.072	0.1042E+06	25.81
*	6	11312.77	139.539	0.042	0.6038E+05	0.64
*	7	11307.50	139.474	0.172	0.2477E+06	9.41
*	8	11302.28	139.409	0.136	0.1949E+06	3.43
*	9	11299.26	139.372	0.131	0.1887E+06	2.69
*	10	11297.21	139.347	0.103	0.1483E+06	1.85
*	11	11295.24	139.323	0.056	0.8023E+05	2.06
*	12	11292.55	139.289	0.143	0.2060E+06	6.28
*	13	11292.47	139.288	0.078	0.1122E+06	11.39
*	14	11289.36	139.250	0.048	0.6898E+05	1.94
*	15	11285.32	139.200	0.196	0.2815E+06	7.26
*	16	11281.85	139.157	0.080	0.1156E+06	0.44
*	17	11279.67	139.131	0.077	0.1102E+06	2.72
*	18	11283.49	139.178	0.016	0.2352E+05	30.84
*	19	11154.07	137.581	0.040	0.5713E+05	71.02
*	20	11276.16	139.087	0.208	0.2990E+06	10.16
*	21	11267.88	138.985	0.227	0.3265E+06	11.36
*	22	11262.31	138.916	0.112	0.1614E+06	8.98
*	23	11308.21	139.483	0.011	0.1578E+05	22.05
*	24	11258.61	138.871	0.078	0.1119E+06	63.13
*	25	11257.76	138.860	0.156	0.2244E+06	9.60
*	26	11253.91	138.813	0.107	0.1534E+06	5.51
*	27	11251.79	138.787	0.127	0.1831E+06	6.70
*	28	11250.20	138.767	0.101	0.1459E+06	2.49
*	29	11247.74	138.737	0.138	0.1986E+06	2.50
*	30	11244.93	138.702	0.182	0.2619E+06	4.65
*	31	11241.72	138.662	0.105	0.1510E+06	3.90
*	32	11237.97	138.616	0.043	0.6121E+05	0.90
*	33	11237.30	138.608	0.103	0.1478E+06	8.31
*	34	11233.11	138.556	0.067	0.9598E+05	12.47
*	35	11230.02	138.518	0.218	0.3130E+06	49.77
*	36	10775.68	132.914	9.999	0.1438E+08	1.89

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.904	100.000	0.1659E+10	14264.81	14256.10

	2	146.660	3.431	0.5691E+08	11891.13	11889.19
*	3	139.591	0.135	0.2247E+07	11325.23	11309.04
*	4	139.820	1.561	0.2589E+08	11372.67	11298.34
*	5	139.657	0.215	0.3565E+07	11335.38	11309.56
*	6	139.539	0.003	0.5083E+05	11312.71	11312.08
*	7	139.474	0.186	0.3089E+07	11311.77	11302.36
*	8	139.409	0.053	0.8853E+06	11304.04	11300.61
*	9	139.372	0.041	0.6740E+06	11300.71	11298.01
*	10	139.347	0.022	0.3631E+06	11297.91	11296.07
*	11	139.323	0.013	0.2193E+06	11296.24	11294.18
*	12	139.289	0.103	0.1715E+07	11295.39	11289.11
*	13	139.288	0.102	0.1694E+07	11297.94	11286.55
*	14	139.250	0.011	0.1776E+06	11290.26	11288.32
*	15	139.200	0.163	0.2708E+07	11288.77	11281.51
*	16	139.157	0.004	0.6684E+05	11281.80	11281.36
*	17	139.131	0.024	0.3979E+06	11281.17	11278.44
*	18	139.178	0.058	0.9611E+06	11298.78	11267.94
*	19	137.581	0.324	0.5377E+07	11189.69	11118.67
*	20	139.087	0.243	0.4025E+07	11281.33	11271.17
*	21	138.985	0.296	0.4915E+07	11273.63	11262.28
*	22	138.916	0.116	0.1921E+07	11266.52	11257.54
*	23	139.483	0.028	0.4613E+06	11319.27	11297.22
*	24	138.871	0.565	0.9367E+07	11290.04	11226.91
*	25	138.860	0.172	0.2854E+07	11262.68	11253.08
*	26	138.813	0.067	0.1119E+07	11256.48	11250.98
*	27	138.787	0.098	0.1626E+07	11255.30	11248.60
*	28	138.767	0.029	0.4822E+06	11251.42	11248.93
*	29	138.737	0.040	0.6589E+06	11249.06	11246.55
*	30	138.702	0.097	0.1615E+07	11247.17	11242.52
*	31	138.662	0.047	0.7810E+06	11243.24	11239.34
*	32	138.616	0.004	0.7298E+05	11238.18	11237.28
*	33	138.608	0.098	0.1628E+07	11241.30	11232.98
*	34	138.556	0.096	0.1586E+07	11239.22	11226.76
*	35	138.518	1.245	0.2065E+08	11254.91	11205.14
*	36	132.914	2.172	0.3603E+08	10776.47	10774.58

(*) Peaks 1 to 36 are fitted to Lorentzian

NMR1
****

Filename = TCS1.001
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 2629.81

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14252.18	175.795	100.000	0.2138E+09	8.17
*	2	11879.26	146.526	29.436	0.6292E+08	1.38
*	3	11338.98	139.862	0.168	0.3585E+06	58.62
*	4	11382.49	140.399	0.032	0.6831E+05	58.00
*	5	11230.47	138.524	0.457	0.9773E+06	64.85
*	6	11320.71	139.637	0.004	9436.	1.28
*	7	11303.95	139.430	0.005	0.1033E+05	49.55
*	8	11324.97	139.689	0.028	0.5894E+05	4.57
*	9	11234.51	138.574	0.078	0.1674E+06	84.53
*	10	11331.44	139.769	0.049	0.1039E+06	18.53
*	11	11299.93	139.380	0.024	0.5221E+05	17.66
*	12	11448.20	141.209	0.030	0.6472E+05	71.59
*	13	11324.88	139.688	0.050	0.1060E+06	9.40
*	14	11286.68	139.217	0.065	0.1396E+06	5.36
*	15	12148.34	149.845	0.011	0.2444E+05	0.34
*	16	11311.72	139.526	0.305	0.6522E+06	25.58
*	17	11296.05	139.333	0.413	0.8819E+06	18.54
*	18	11584.27	142.888	0.047	0.1002E+06	10.90
*	19	11358.68	140.105	0.058	0.1245E+06	67.22
*	20	11287.01	139.221	0.214	0.4568E+06	14.09
*	21	11281.78	139.157	0.178	0.3801E+06	7.38
*	22	11276.08	139.086	0.344	0.7344E+06	9.37
*	23	11269.98	139.011	0.255	0.5441E+06	7.38
*	24	11267.87	138.985	0.045	0.9604E+05	4.00
*	25	11268.50	138.993	0.053	0.1125E+06	6.77
*	26	11263.93	138.936	0.327	0.7001E+06	5.73
*	27	11259.66	138.884	0.207	0.4424E+06	3.19
*	28	11255.46	138.832	0.362	0.7746E+06	8.60
*	29	11250.68	138.773	0.241	0.5156E+06	7.38
*	30	11246.75	138.724	0.118	0.2517E+06	2.70
*	31	11436.18	141.061	0.029	0.6254E+05	80.33
*	32	11245.30	138.707	0.100	0.2139E+06	5.83
*	33	11240.04	138.642	0.386	0.8248E+06	11.36
*	34	11233.47	138.561	0.184	0.3937E+06	12.02
*	35	11226.99	138.481	0.143	0.3057E+06	16.64
*	36	11124.40	137.215	0.765	0.1636E+07	3.70
*	37	10765.96	132.794	25.492	0.5449E+08	1.32
*	38	10684.06	131.784	1.558	0.3330E+07	2.30
*	39	10673.75	131.657	1.534	0.3279E+07	2.19

Peak	PPM	Relative	Absolute	Integral	Integral

	#		integral	integral	start (hz)	end (hz)
*	1	175.795	100.000	0.2315E+10	14255.71	14247.53
*	2	146.526	4.956	0.1147E+09	11879.64	11878.26
*	3	139.862	1.203	0.2786E+08	11368.43	11309.80
*	4	140.399	0.227	0.5252E+07	11411.38	11353.37
*	5	138.524	3.628	0.8400E+08	11262.51	11197.66
*	6	139.637	0.001	0.1599E+05	11321.39	11320.11
*	7	139.430	0.029	0.6783E+06	11328.34	11278.79
*	8	139.689	0.015	0.3573E+06	11327.18	11322.61
*	9	138.574	0.810	0.1876E+08	11276.49	11191.97
*	10	139.769	0.110	0.2550E+07	11340.68	11322.15
*	11	139.380	0.053	0.1222E+07	11308.84	11291.18
*	12	141.209	0.265	0.6141E+07	11483.95	11412.36
*	13	139.688	0.057	0.1321E+07	11329.60	11320.19
*	14	139.217	0.043	0.9919E+06	11289.06	11283.70
*	15	149.845	0.000	0.1113E+05	12148.75	12148.40
*	16	139.526	0.955	0.2211E+08	11324.65	11299.07
*	17	139.333	0.936	0.2167E+08	11305.13	11286.59
*	18	142.888	0.063	0.1448E+07	11589.89	11578.99
*	19	140.105	0.479	0.1109E+08	11392.28	11325.06
*	20	139.221	0.369	0.8532E+07	11294.02	11279.92
*	21	139.157	0.161	0.3719E+07	11285.33	11277.95
*	22	139.086	0.394	0.9124E+07	11280.40	11271.02
*	23	139.011	0.230	0.5324E+07	11273.48	11266.09
*	24	138.985	0.022	0.5096E+06	11270.01	11266.01
*	25	138.993	0.044	0.1009E+07	11271.99	11265.22
*	26	138.936	0.230	0.5320E+07	11266.73	11260.99
*	27	138.884	0.081	0.1868E+07	11261.30	11258.12
*	28	138.832	0.381	0.8830E+07	11259.86	11251.26
*	29	138.773	0.218	0.5042E+07	11254.51	11247.13
*	30	138.724	0.039	0.901IE+06	11248.03	11245.32
*	31	141.061	0.288	0.6659E+07	11476.47	11396.13
*	32	138.707	0.071	0.1654E+07	11247.81	11241.98
*	33	138.642	0.536	0.1242E+08	11245.84	11234.48
*	34	138.561	0.271	0.6269E+07	11239.05	11227.04
*	35	138.481	0.291	0.6743E+07	11235.44	11218.80
*	36	137.215	0.347	0.8024E+07	11125.86	11122.16
*	37	132.794	4.130	0.9560E+08	10766.76	10765.44
*	38	131.784	0.438	0.1013E+08	10684.88	10682.58
*	39	131.657	0.411	0.9517E+07	10674.75	10672.56

(*) Peaks 1 to 39 are fitted to Lorentzian

NMR1
****

Filename = TCSI5
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 3484.23

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14250.61	175.776	100.000	0.1317E+09	8.23
*	2	11875.10	146.475	25.540	0.3364E+08	2.09
*	3	11335.06	139.814	0.325	0.4282E+06	27.49
*	4	11325.61	139.697	0.045	0.5908E+05	3.60
*	5	11320.26	139.631	0.137	0.1802E+06	8.16
*	6	11310.45	139.510	0.048	0.6342E+05	7.22
*	7	11230.47	138.524	0.294	0.3867E+06	26.50
*	8	11308.80	139.490	0.082	0.1079E+06	26.41
*	9	11322.20	139.655	0.004	4948.	2.30
*	10	11309.98	139.504	0.232	0.3053E+06	20.03
*	11	11367.62	140.215	0.217	0.2854E+06	27.49
*	12	11300.08	139.382	0.320	0.4214E+06	10.95
*	13	11284.89	139.195	0.032	0.4197E+05	10.01
*	14	11296.08	139.333	0.099	0.1299E+06	2.72
*	15	11292.52	139.289	0.302	0.3981E+06	6.10
*	16	11287.86	139.232	0.270	0.3551E+06	5.29
*	17	11283.06	139.172	0.132	0.1738E+06	9.60
*	18	11283.77	139.181	0.148	0.1950E+06	8.00
*	19	11256.80	138.848	0.327	0.4314E+06	4.19
*	20	11280.72	139.144	0.145	0.1908E+06	9.57
*	21	11277.71	139.106	0.199	0.2617E+06	5.66
*	22	11285.33	139.200	0.052	0.6901E+05	0.29
*	23	11314.43	139.559	0.020	0.2636E+05	22.26
*	24	11271.38	139.028	0.518	0.6820E+06	11.39
*	25	11264.33	138.941	0.374	0.4925E+06	7.56
*	26	11290.29	139.262	0.034	0.4541E+05	1.00
*	27	11260.79	138.898	0.200	0.2630E+06	3.40
*	28	11258.99	138.875	0.086	0.1131E+06	1.64
*	29	11253.77	138.811	0.271	0.3566E+06	3.96
*	30	11249.13	138.754	0.410	0.5403E+06	7.87
*	31	11242.03	138.666	0.467	0.6150E+06	9.13
*	32	11237.87	138.615	0.093	0.1226E+06	27.14
*	33	11237.08	138.605	0.195	0.2564E+06	3.57
*	34	11234.15	138.569	0.208	0.2736E+06	3.68
*	35	11230.67	138.526	0.201	0.2646E+06	5.24
*	36	11225.53	138.463	0.176	0.2316E+06	7.09
*	37	11182.57	137.933	0.206	0.2712E+06	16.90
*	38	11221.41	138.412	0.068	0.8904E+05	10.50
*	39	11220.19	138.397	0.060	0.7942E+05	3.27
*	40	11210.08	138.272	0.403	0.5311E+06	27.47
*	41	11165.44	137.722	0.212	0.2791E+06	10.36
*	42	11124.04	137.211	0.667	0.8780E+06	9.39
*	43	10763.35	132.762	18.895	0.2489E+08	2.09

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.776	100.000	0.1436E+10	14253.96	14245.73
*	2	146.475	6.485	0.9314E+08	11875.85	11873.76
*	3	139.814	1.086	0.1560E+08	11348.71	11321.22
*	4	139.697	0.020	0.2821E+06	11327.29	11323.69
*	5	139.631	0.136	0.1950E+07	11324.24	11316.07
*	6	139.510	0.042	0.6069E+06	11313.69	11306.47
*	7	138.524	0.946	0.1358E+08	11243.33	11216.83
*	8	139.490	0.263	0.3776E+07	11322.10	11295.69
*	9	139.655	0.001	0.1506E+05	11323.08	11320.78
*	10	139.504	0.564	0.8105E+07	11320.09	11300.07
*	11	140.215	0.724	0.1040E+08	11381.31	11353.81
*	12	139.382	0.426	0.6113E+07	11305.48	11294.53
*	13	139.195	0.039	0.5569E+06	11289.61	11279.59
*	14	139.333	0.033	0.4676E+06	11297.22	11294.50
*	15	139.289	0.224	0.3221E+07	11295.36	11289.25
*	16	139.232	0.173	0.2491E+07	11290.21	11284.92
*	17	139.172	0.154	0.2212E+07	11287.62	11278.02
*	18	139.181	0.144	0.2068E+07	11287.42	11279.41
*	19	138.848	0.167	0.2393E+07	11258.84	11254.66
*	20	139.144	0.169	0.2421E+07	11285.24	11275.67
*	21	139.106	0.137	0.1962E+07	11280.32	11274.66
*	22	139.200	0.002	0.2628E+05	11285.34	11285.05
*	23	139.559	0.054	0.7778E+06	11325.36	11303.10
*	24	139.028	0.717	0.1030E+08	11276.67	11265.27
*	25	138.941	0.343	0.4933E+07	11268.23	11260.67
*	26	139.262	0.004	0.6004E+05	11290.43	11289.43
*	27	138.898	0.082	0.1184E+07	11262.59	11259.20
*	28	138.875	0.017	0.2460E+06	11259.94	11258.30
*	29	138.811	0.130	0.1871E+07	11255.77	11251.81
*	30	138.754	0.392	0.5636E+07	11252.98	11245.11
*	31	138.666	0.518	0.7442E+07	11246.50	11237.37
*	32	138.615	0.307	0.4409E+07	11251.36	11224.22
*	33	138.605	0.085	0.1214E+07	11238.98	11235.41
*	34	138.569	0.093	0.1333E+07	11236.07	11232.39
*	35	138.526	0.128	0.1838E+07	11233.30	11228.05
*	36	138.463	0.152	0.2176E+07	11228.89	11221.80
*	37	137.933	0.423	0.6074E+07	11191.13	11174.23
*	38	138.412	0.086	0.1239E+07	11226.44	11215.94
*	39	138.397	0.024	0.3437E+06	11221.64	11218.38
*	40	138.272	1.347	0.1934E+08	11223.67	11196.20
*	41	137.722	0.267	0.3834E+07	11170.67	11160.31
*	42	137.211	0.761	0.1093E+08	11128.71	11119.32
*	43	132.762	4.804	0.6899E+08	10764.18	10762.09

(*) Peaks 1 to 43 are fitted to Lorentzian


A
M
X
D
140.00
139.50
139.00
138.50
138.00
PPM
USERNAME:
DATE: 7-May-92
FILENAME: TCS15

^{31}P NMR data of the coal samples, obtained by processing the FID's with a line broadening factor of 2.0 Hz.

NMR1
****

Filename = TCSO1
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 4335.22

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14261.09	175.905	100.000	0.1063E+09	10.29
*	2	11888.33	146.638	10.074	0.1071E+08	3.64
*	3	11419.00	140.849	0.088	0.9363E+05	34.92
*	4	11367.51	140.214	0.259	0.2751E+06	58.28
*	5	11241.38	138.658	0.048	0.5108E+05	3.40
*	6	11349.76	139.995	0.133	0.1418E+06	27.54
*	7	11422.87	140.897	0.272	0.2886E+06	9.24
*	8	11335.33	139.817	0.222	0.2357E+06	22.01
*	9	11327.55	139.721	0.081	0.8574E+05	8.49
*	10	11317.99	139.603	0.373	0.3965E+06	23.13
*	11	11303.29	139.422	0.598	0.6354E+06	24.59
*	12	11292.17	139.285	0.085	0.9078E+05	24.92
*	13	11274.83	139.071	0.019	0.2041E+05	8.19
*	14	11293.02	139.295	0.114	0.1214E+06	15.24
*	15	11284.81	139.194	0.334	0.3546E+06	24.26
*	16	11266.36	138.966	0.696	0.7401E+06	43.49
*	17	11233.91	138.566	0.062	0.6547E+05	6.42
	18	11242.76	138.675	1.140	0.1211E+07	52.05
	19	11254.80	138.824	0.151	0.1606E+06	22.96
	20	11217.39	138.362	0.175	0.1865E+06	56.30
	21	11198.04	138.124	0.082	0.8740E+05	29.66
	22	11273.66	139.056	0.096	0.1017E+06	25.27
	23	11176.32	137.856	0.092	0.9767E+05	32.31
	24	11166.92	137.740	0.067	0.7126E+05	31.78
	25	11247.72	138.736	0.307	0.3259E+06	17.13
	26	10060.62	124.094	0.301	0.3204E+06	26.14
	27	10774.69	132.902	13.424	0.1426E+08	3.41
	28	10693.53	131.901	0.241	0.2558E+06	11.26
	29	10682.84	131.769	0.256	0.2721E+06	5.12

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
1	175.905	100.000	0.5796E+10	14266.05	14255.76
2	146.638	3.563	0.2065E+09	11890.05	11886.42
3	140.849	0.299	0.1733E+08	11436.37	11401.46
4	140.214	1.466	0.8498E+08	11396.65	11338.37
5	138.658	0.016	0.9219E+06	11242.99	11239.59
6	139.995	0.357	0.2070E+08	11363.50	11335.96
7	140.897	0.244	0.1414E+08	11427.39	11418.15
8	139.817	0.475	0.2750E+08	11346.37	11324.36

*	9	139.721	0.067	0.3861E+07	11331.76	11323.26
*	10	139.603	0.839	0.4861E+08	11329.45	11306.32
*	11	139.422	1.429	0.8283E+08	11315.51	11290.92
*	12	139.285	0.207	0.1199E+08	11304.56	11279.65
*	13	139.071	0.015	0.8867E+06	11278.87	11270.67
*	14	139.295	0.169	0.9809E+07	11300.61	11285.38
*	15	139.194	0.787	0.4561E+08	11296.83	11272.57
*	16	138.966	2.945	0.1707E+09	11288.07	11244.58
*	17	138.566	0.038	0.2230E+07	11237.10	11230.67
*	18	138.675	5.768	0.3343E+09	11268.80	11216.75
*	19	138.824	0.337	0.1955E+08	11266.25	11243.29
*	20	138.362	0.960	0.5565E+08	11245.44	11189.14
*	21	138.124	0.237	0.1374E+08	11212.87	11183.20
*	22	139.056	0.235	0.1363E+08	11286.22	11260.95
*	23	137.856	0.289	0.1673E+08	11192.41	11160.10
*	24	137.740	0.207	0.1201E+08	11182.81	11151.03
*	25	138.736	0.511	0.2960E+08	11256.23	11239.10
*	26	124.094	0.766	0.4440E+08	10073.66	10047.52
*	27	132.902	4.446	0.2577E+09	10776.34	10772.94
*	28	131.901	0.264	0.1527E+08	10699.09	10687.83
*	29	131.769	0.128	0.7391E+07	10685.35	10680.23

(*) Peaks 1 to 29 are fitted to Lorentzian

TCS1

NMR1
****

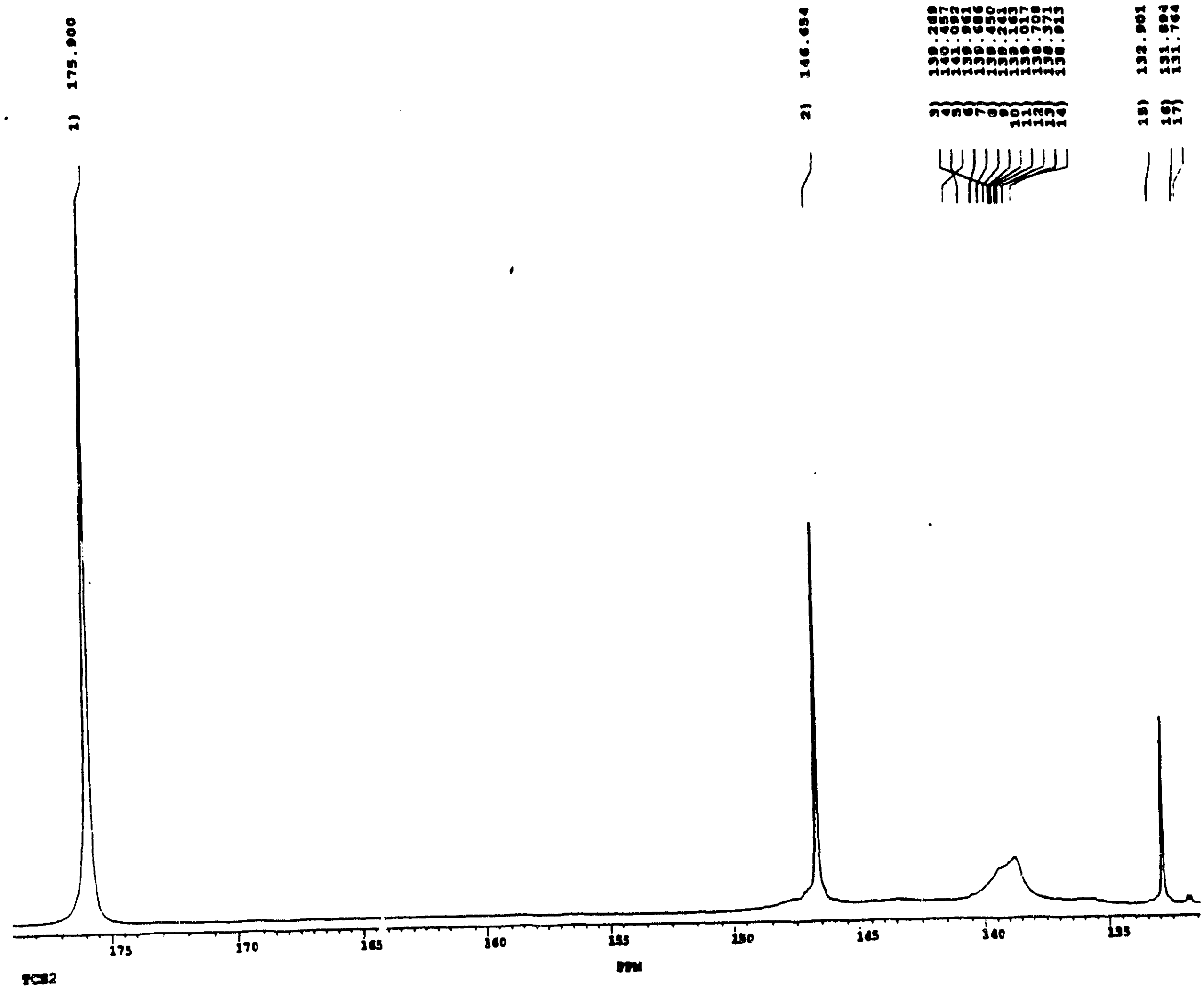
Filename = TCS2
Username = tmohan
Scale factor = 0.0000000E+00

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14260.66	175.900	99.420	0.4281E+08	11.01
*	2	11889.59	146.654	54.957	0.2366E+08	6.74
*	3	11290.91	139.269	0.735	0.3166E+06	26.79
*	4	11387.23	140.457	0.106	0.4575E+05	9.88
*	5	11438.65	141.092	0.520	0.2239E+06	259.93
*	6	11346.96	139.961	0.671	0.2890E+06	76.69
*	7	11324.70	139.686	1.186	0.5105E+06	52.23
*	8	11305.58	139.450	1.177	0.5067E+06	25.96
*	9	11288.59	139.241	0.888	0.3824E+06	76.86
*	10	11282.31	139.163	0.999	0.4302E+06	48.14
*	11	11270.43	139.017	0.514	0.2212E+06	19.62
*	12	11245.39	138.708	4.571	0.1968E+07	45.81
*	13	11218.11	138.371	0.572	0.2461E+06	168.04
*	14	11261.99	138.913	0.655	0.2821E+06	43.69
*	15	10774.64	132.901	26.924	0.1159E+08	5.23
*	16	10692.98	131.894	0.946	0.4074E+06	5.04
*	17	10682.44	131.764	0.957	0.4120E+06	4.76

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.900	100.000	0.1894E+10	14274.29	14246.75
*	2	146.654	33.823	0.6406E+09	11898.05	11881.21
*	3	139.269	1.799	0.3407E+08	11324.62	11257.64
*	4	140.457	0.096	0.1816E+07	11399.77	11375.07
*	5	141.092	12.344	0.2338E+09	11763.60	11113.77
*	6	139.961	4.702	0.8905E+08	11442.99	11251.26
*	7	139.686	5.655	0.1071E+09	11390.19	11259.62
*	8	139.450	2.790	0.5285E+08	11338.10	11273.19
*	9	139.241	6.233	0.1181E+09	11384.83	11192.69
*	10	139.163	4.392	0.8319E+08	11342.71	11222.36
*	11	139.017	0.920	0.1743E+08	11295.21	11246.17
*	12	138.708	19.124	0.3622E+09	11302.76	11188.24
*	13	138.371	8.771	0.1661E+09	11428.29	11008.20
*	14	138.913	2.614	0.4951E+08	11316.70	11207.49
*	15	132.901	12.872	0.2438E+09	10781.24	10768.16
*	16	131.894	0.435	0.8245E+07	10699.52	10686.92
*	17	131.764	0.416	0.7873E+07	10688.50	10676.61

(*) Peaks 1 to 17 are fitted to Lorentzian



1) 175.900
2) 146.654
15) 132.901
16) 131.894
17) 131.764
175
170
165
160
155
150
145
140
135
PPM
TCS2

NMR1
****

Filename = TCS3
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 5597.57

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14261.02	175.904	100.000	0.1066E+09	11.15
*	2	11889.02	146.647	11.448	0.1220E+08	5.23
*	3	11387.45	140.460	0.083	0.8859E+05	117.05
*	4	11343.03	139.912	0.150	0.1596E+06	63.66
*	5	11322.89	139.664	0.118	0.1257E+06	40.07
*	6	11328.30	139.730	0.036	0.3872E+05	5.49
*	7	11320.62	139.636	0.097	0.1031E+06	12.18
*	8	11310.91	[illegible].516	0.166	0.1768E+06	11.29
*	9	11303.39	139.423	0.192	0.2045E+06	9.50
*	10	11293.53	139.302	0.039	0.4173E+05	11.28
*	11	11297.14	139.346	0.091	0.9745E+05	8.92
*	12	11294.73	139.316	0.118	0.1258E+06	10.41
*	13	11290.16	139.260	0.147	0.1563E+06	8.90
*	14	11284.86	139.195	0.164	0.1750E+06	9.05
*	15	11279.43	139.128	0.155	0.1647E+06	11.37
*	16	11273.56	139.055	0.125	0.1334E+06	11.38
*	17	11299.63	139.377	0.032	0.3370E+05	2.98
*	18	11265.47	138.955	0.291	0.3102E+06	21.33
*	19	11980.75	147.778	0.001	1312.	254.14
*	20	11253.25	138.805	0.200	0.2126E+06	17.53
*	21	11242.25	138.669	0.496	0.5286E+06	30.47
*	22	11223.86	138.442	0.191	0.2040E+06	52.91
*	23	11215.00	138.333	0.166	0.1765E+06	224.07
*	24	10774.99	132.906	8.395	0.8948E+07	4.79
*	25	10692.98	131.894	0.270	0.2872E+06	8.36
*	26	10682.40	131.763	0.298	0.3175E+06	4.94

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.904	100.000	0.5507E+10	14288.71	14232.98
*	2	146.647	5.376	0.2960E+09	11901.85	11875.68
*	3	140.460	0.873	0.4806E+08	11680.07	11094.83
*	4	139.912	0.855	0.4709E+08	11502.17	11183.85
*	5	139.664	0.424	0.2335E+08	11423.04	11222.68
*	6	139.730	0.018	0.9852E+06	11341.92	11314.47
*	7	139.636	0.106	0.5820E+07	11350.95	11290.03
*	8	139.516	0.168	0.9249E+07	11338.93	11282.49
*	9	139.423	0.163	0.9003E+07	11327.04	11279.57
*	10	139.302	0.040	0.2181E+07	11321.72	11265.34
*	11	139.346	0.073	0.4030E+07	11319.39	11274.78

*	12	139.316	0.110	0.6074E+07	11320.75	11268.68
*	13	[illegible]	[illegible]	0.6447E+07	11312.21	[illegible]
*	14	[illegible]	0.133	0.7346E+07	11307.57	11262.30
*	15	139.128	0.158	0.8683E+07	11307.73	11250.88
*	16	139.055	0.128	0.7039E+07	11301.83	11244.93
*	17	139.377	0.008	0.4649E+06	11306.89	11292.01
*	18	138.955	0.557	0.3067E+08	11318.70	11212.06
*	19	147.778	0.028	0.1545E+07	12615.97	11345.26
*	20	138.805	0.314	0.1727E+08	11297.05	11209.42
*	21	138.669	1.356	0.7465E+08	11318.44	11166.10
*	22	138.442	0.908	0.5002E+08	11356.16	11091.64
*	23	138.333	3.329	0.1833E+09	11775.18	10654.85
*	24	132.906	3.607	0.1986E+09	10787.00	10763.05
*	25	131.894	0.202	0.1114E+08	10713.86	10672.04
*	26	131.763	0.132	0.7277E+07	10694.65	10669.93

(*) Peaks 1 to 26 are fitted to Lorentzian

NMR1
****

Filename = TCS4
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 3775.67

Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
* 1	14261.06	175.905	100.000	0.9865E+08	11.15
* 2	11886.47	146.615	13.559	0.1338E+08	5.24
* 3	11326.80	139.712	0.112	0.1108E+06	13.41
* 4	11234.79	138.577	0.075	0.7371E+05	17.89
* 5	11353.51	140.041	0.242	0.2391E+06	24.46
* 6	11333.05	139.789	0.294	0.2904E+06	25.29
* 7	11321.82	139.651	0.138	0.1358E+06	6.53
* 8	11317.90	139.602	0.154	0.1515E+06	5.11
* 9	11314.27	139.557	0.246	0.2431E+06	5.28
* 10	11311.30	139.521	0.144	0.1424E+06	2.90
* 11	11309.45	139.498	0.143	0.1407E+06	2.67
* 12	11307.33	139.472	0.161	0.1590E+06	2.90
* 13	11304.66	139.439	0.302	0.2982E+06	6.01
* 14	11301.22	139.396	0.185	0.1820E+06	4.84
* 15	11297.87	139.355	0.280	0.2764E+06	6.77
* 16	11292.80	139.293	0.367	0.3622E+06	7.32
* 17	11290.35	139.262	0.072	0.7134E+05	1.90
* 18	11288.72	139.242	0.141	0.1387E+06	2.65
* 19	11285.98	139.208	0.302	0.2980E+06	5.20
* 20	11281.88	139.158	0.323	0.3190E+06	5.75
* 21	11278.33	139.114	0.225	0.2219E+06	4.36
* 22	11275.51	139.079	0.256	0.2526E+06	4.25
* 23	11272.63	139.044	0.271	0.2671E+06	4.02
* 24	11270.62	139.019	0.138	0.1364E+06	2.46
25	11269.06	139.000	0.161	0.1589E+06	2.48
26	11267.29	138.978	0.144	0.1417E+06	2.52
27	11264.58	138.944	0.297	0.2926E+06	6.28
28	11259.26	138.879	0.310	0.3057E+06	7.90
29	11253.43	138.807	0.248	0.2445E+06	7.62
30	11248.47	138.746	0.092	0.9074E+05	5.12
31	10900.86	134.458	0.870	0.8583E+06	16.45
32	11243.62	138.686	0.463	0.4563E+06	18.81
33	11233.44	138.560	0.090	0.8916E+05	26.53
34	11223.31	138.435	0.239	0.2362E+06	26.59
35	10774.00	132.893	7.085	0.6990E+07	4.84
36	10692.64	131.890	0.407	0.4013E+06	5.14
37	10682.50	131.765	0.402	0.3969E+06	3.52

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)

*	1	175.905	100.000	0.5832E+10	14266.46	14255.31
*	2	146.615	6.375	0.3718E+09	11889.07	11883.82
*	3	139.712	0.135	0.7876E+07	11333.46	11320.05
*	4	138.577	0.120	0.6989E+07	11243.70	11225.82
*	5	140.041	0.532	0.3101E+08	11365.65	11341.19
*	6	139.789	0.668	0.3894E+08	11345.63	11320.33
*	7	139.651	0.081	0.4701E+07	11324.99	11318.46
*	8	139.602	0.070	0.4101E+07	11320.42	11315.32
*	9	139.557	0.117	0.6804E+07	11316.80	11311.53
*	10	139.521	0.037	0.2187E+07	11312.65	11309.75
*	11	139.498	0.034	0.1989E+07	11310.76	11308.09
*	12	139.472	0.042	0.2441E+07	11308.80	11305.90
*	13	139.439	0.163	0.9496E+07	11307.69	11301.68
*	14	139.396	0.080	0.4671E+07	11303.55	11298.71
*	15	139.355	0.170	0.9915E+07	11301.25	11294.49
*	16	139.293	0.241	0.1406E+08	11296.49	11289.17
*	17	139.262	0.012	0.7203E+06	11291.27	11289.36
*	18	139.242	0.033	0.1948E+07	11290.01	11287.36
*	19	139.208	0.141	0.8214E+07	11288.62	11283.42
*	20	139.158	0.167	0.9727E+07	11284.75	11278.99
*	21	139.114	0.088	0.5132E+07	11280.50	11276.13
*	22	139.079	0.098	0.5692E+07	11277.63	11273.38
*	23	139.044	0.098	0.5690E+07	11274.55	11270.53
*	24	139.019	0.030	0.1776E+07	11271.84	11269.38
*	25	139.000	0.036	0.2089E+07	11270.22	11267.74
*	26	138.978	0.032	0.1891E+07	11268.46	11265.95
*	27	138.944	0.167	0.9741E+07	11267.68	11261.40
*	28	138.879	0.219	0.1279E+08	11263.15	11255.26
*	29	138.807	0.169	0.9882E+07	11257.24	11249.61
*	30	138.746	0.042	0.2461E+07	11250.95	11245.83
*	31	134.458	1.283	0.7484E+08	10909.07	10892.62
*	32	138.686	0.780	0.4550E+08	11253.05	11234.25
*	33	138.560	0.215	0.1254E+08	11246.69	11220.16
*	34	138.435	0.571	0.3329E+08	11236.65	11210.06
*	35	132.893	3.076	0.1794E+09	10776.45	10771.61
*	36	131.890	0.187	0.1093E+08	10695.12	10689.99
*	37	131.765	0.127	0.7415E+07	10684.24	10680.72

***) Peaks 1 to 37 are fitted to Lorentzian**

NMR1
****

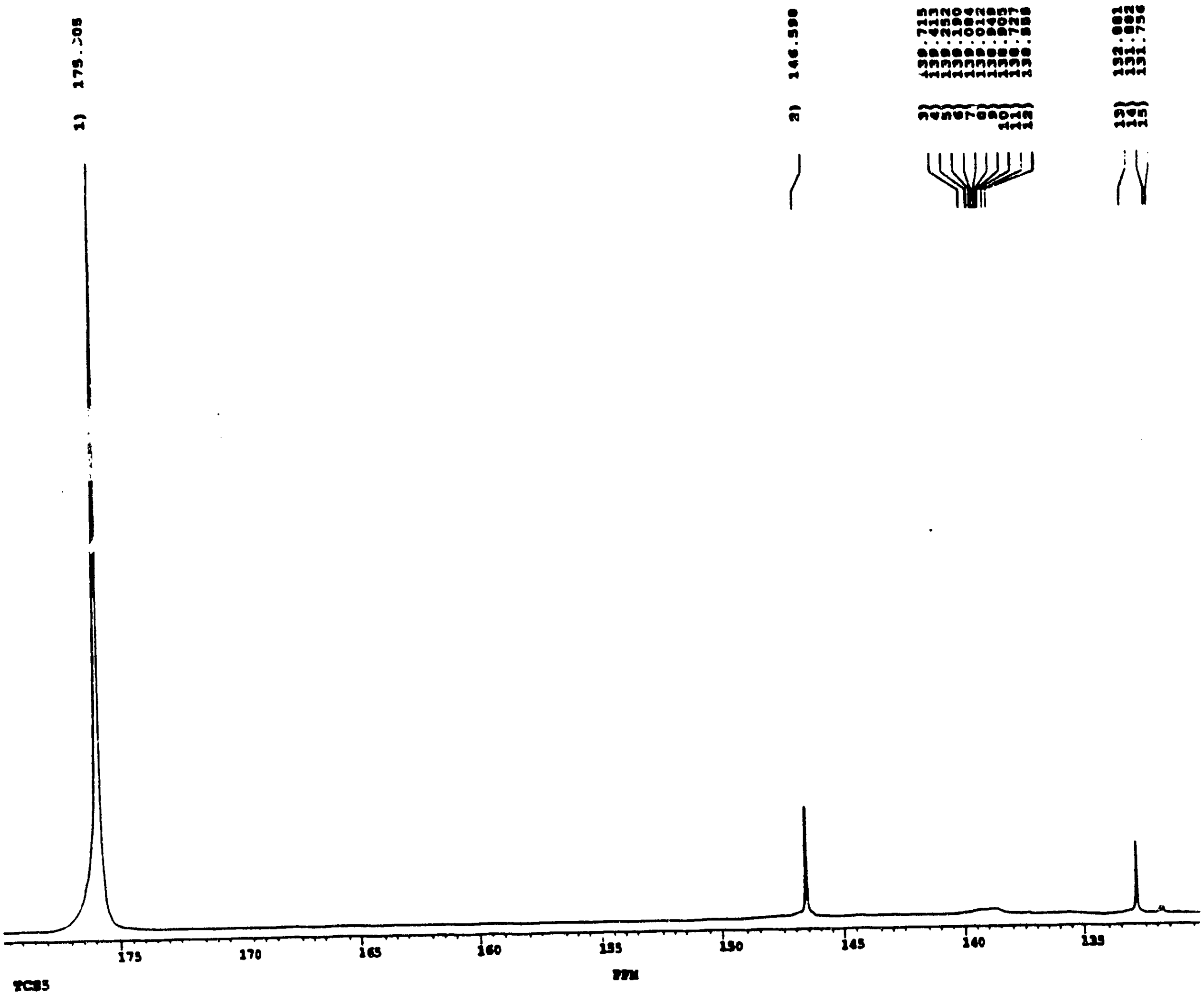
Filename = TCS5
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 3884.83

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14261.09	175.905	100.000	0.8435E+08	11.20
*	2	11885.05	146.598	15.613	0.1317E+08	4.53
*	3	11327.05	139.715	0.334	0.2821E+06	42.72
*	4	11302.56	139.413	0.308	0.2595E+06	41.00
*	5	11289.48	139.252	0.272	0.2298E+06	34.13
*	6	11284.45	139.190	0.038	0.3236E+05	10.73
*	7	11275.93	139.084	0.116	0.9783E+05	10.93
*	8	11270.06	139.012	0.044	0.3735E+05	6.50
*	9	11264.96	138.949	0.061	0.5174E+05	5.99
*	10	11261.36	138.905	0.210	0.1772E+06	43.24
*	11	11246.99	138.727	0.567	0.4782E+06	42.12
*	12	11233.02	138.555	0.254	0.2140E+06	23.70
*	13	10772.97	132.881	10.286	0.8677E+07	4.13
*	14	10692.00	131.882	0.824	0.6948E+06	5.44
*	15	10681.83	131.756	0.792	0.6677E+06	4.50

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.905	100.000	0.2504E+10	14266.42	14255.22
*	2	146.598	6.313	0.1581E+09	11887.16	11882.63
*	3	139.715	1.276	0.3195E+08	11348.34	11305.62
*	4	139.413	1.126	0.2820E+08	11322.89	11281.89
*	5	139.252	0.830	0.2079E+08	11306.42	11272.29
*	6	139.190	0.037	0.9209E+06	11289.68	11278.95
*	7	139.084	0.113	0.2834E+07	11281.19	11270.26
*	8	139.012	0.026	0.6432E+06	11273.34	11266.85
*	9	138.949	0.033	0.8218E+06	11267.76	11261.77
*	10	138.905	0.811	0.2031E+08	11282.83	11239.58
*	11	138.727	2.132	0.5339E+08	11268.04	11225.92
*	12	138.555	0.537	0.1344E+08	11244.91	11221.21
*	13	132.881	3.795	0.9503E+08	10774.99	10770.86
*	14	131.882	0.400	0.1002E+08	10694.76	10689.32
*	15	131.756	0.318	0.7965E+07	10683.92	10679.42

(*) Peaks 1 to 15 are fitted to Lorentzian


1) 175.308
2) 146.590
175
170
165
160
155
150
145
140
135
PPM
TC85

NMR1
****

Filename = TCS6
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 1401.93

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14261.06	175.905	100.000	0.5979E+08	11.68
*	2	11885.70	146.606	42.843	0.2562E+08	7.10
*	3	11375.84	140.317	0.148	0.8860E+05	15.04
*	4	11464.23	141.407	0.369	0.2208E+06	84.30
*	5	11392.98	140.528	0.111	0.6630E+05	3.87
*	6	11352.08	140.024	0.061	0.3657E+05	2.80
*	7	10313.91	127.218	0.016	9646.	7.21
*	8	11333.65	139.796	0.264	0.1576E+06	333.25
*	9	11323.33	139.669	2.370	0.1417E+07	86.97
*	10	11298.78	139.366	0.490	0.2929E+06	16.38
*	11	11304.25	139.434	1.416	0.8466E+06	38.12
*	12	11288.73	139.242	0.653	0.3905E+06	16.93
*	13	11278.82	139.120	1.018	0.6088E+06	22.67
*	14	11266.25	138.965	1.064	0.6362E+06	26.16
*	15	11247.47	138.733	3.035	0.1815E+07	66.39
*	16	11245.36	138.707	2.564	0.1533E+07	37.41
*	17	11167.58	137.748	0.280	0.1676E+06	128.81
*	18	10773.19	132.883	24.648	0.1474E+08	6.14
*	19	10692.56	131.889	0.599	0.3582E+06	5.89
*	20	10682.61	131.766	0.512	0.3058E+06	4.66

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.905	100.000	0.1852E+10	14266.61	14254.93
*	2	146.606	26.052	0.4824E+09	11889.28	11882.18
*	3	140.317	0.191	0.3533E+07	11383.34	11368.30
*	4	141.407	2.665	0.4934E+08	11506.26	11421.96
*	5	140.528	0.037	0.6798E+06	11394.94	11391.07
*	6	140.024	0.015	0.2714E+06	11353.52	11350.72
*	7	127.218	0.010	0.1845E+06	10317.53	10310.32
*	8	139.796	7.521	0.1393E+09	11500.08	11166.82
*	9	139.669	17.642	0.3267E+09	11366.86	11279.89
*	10	139.366	0.687	0.1272E+08	11306.97	11290.59
*	11	139.434	4.620	0.8555E+08	11323.18	11285.06
*	12	139.242	0.946	0.1752E+08	11297.17	11280.25
*	13	139.120	1.976	0.3658E+08	11289.97	11267.30
*	14	138.965	2.382	0.4413E+08	11279.27	11253.11
*	15	138.733	17.251	0.3194E+09	11280.72	11214.33
*	16	138.707	8.212	0.152[illegible]E+09	11263.86	11226.45
*	17	137.748	3.091	0.5723E+08	11231.94	11103.12

*	18	132.883	12.958	0.2399E+09	10776.24	10770.10
*	19	131.889	0.302	0.5596E+07	10695.53	10689.63
*	20	131.766	0.204	0.3779E+07	10684.84	10680.18

(*) Peaks 1 to 20 are fitted to Lorentzian

NMR1
****

Filename = TCS7
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 4875.42

Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
* 1	14262.15	175.918	100.000	0.8514E+08	14.41
* 2	11887.28	146.625	9.743	0.8295E+07	6.40
* 3	11331.21	139.766	0.311	0.2648E+06	42.80
* 4	11360.10	140.123	0.118	0.1003E+06	27.23
* 5	11318.91	139.615	0.159	0.1353E+06	17.72
* 6	11310.13	139.506	0.285	0.2423E+06	12.74
* 7	11304.02	139.431	0.198	0.1685E+06	6.81
* 8	11299.79	139.379	0.181	0.1543E+06	7.99
* 9	11293.98	139 307	0.370	0.3146E+06	11.59
* 10	11290.01	139.258	0.088	0.7511E+05	4.81
* 11	11286.37	139.213	0.244	0.2081E+06	6.89
* 12	11281.99	139.159	0.186	0.1587E+06	6.86
* 13	11278.11	139.111	0.184	0.1569E+06	8.05
* 14	11272.98	139.048	0.259	0.2202E+06	10.39
* 15	11268.81	138.997	0.093	0.7877E+05	9.45
* 16	11264.25	138.940	0.151	0.1284E+06	9.94
* 17	11123.71	137.207	0.673	0.5732E+06	27.48
* 18	11258.11	138.865	0.275	0.2340E+06	23.47
* 19	11248.59	138.747	0.104	0.8869E+05	14.62
* 20	11241.48	138.659	0.831	0.7074E+06	42.78
* 21	10773.92	132.892	5.635	0.4798E+07	5.78
* 22	10691.65	131.878	0.177	0.1506E+06	5.17
* 23	10681.67	131.754	0.162	0.1377E+06	3.05

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
* 1	175.918	100.000	0.5689E+10	14297.85	14225.77
* 2	146.625	4.325	0.2460E+09	11903.06	11871.07
* 3	139.766	0.923	0.5253E+08	11438.23	11224.23
* 4	140.123	0.223	0.1266E+08	11428.05	11291.89
* 5	139.615	0.195	0.1111E+08	11363.08	11274.49
* 6	139.506	0.252	0.1431E+08	11342.06	11278.33
* 7	139.431	0.094	0.5319E+07	11321.00	11286.95
* 8	139.379	0.100	0.5713E+07	11319.80	11279.85
* 9	139.307	0.297	0.1691E+08	11322.88	11264.92
* 10	139.258	0.029	0.1673E+07	11302.06	11278.03
* 11	139.213	0.117	0.6650E+07	11303.43	11268.96
* 12	139.159	0.089	0.5049E+07	11299.21	11264.89
* 13	139.111	0.103	0.5855E+07	11298.03	11257.77
* 14	139.048	0.187	0.1061E+08	11298.84	11246.88

*	15	138.997	0.061	0.3451E+07	11292.35	11245.08
*	16	138.940	0.204	0.5918E+07	11289.13	11239.42
*	17	137.207	1.283	0.7301E+08	11192.23	11054.83
*	18	138.865	0.448	0.2547E+08	11316.74	11199.36
*	19	138.747	0.106	0.6011E+07	11285.12	11212.01
*	20	138.659	2.466	0.1403E+09	11348.42	11134.50
*	21	132.892	2.261	0.1286E+09	10788.37	10759.46
*	22	131.878	0.063	0.3612E+07	10704.48	10678.62
*	23	131.754	0.034	0.1944E+07	10689.38	10674.16

(*) Peaks 1 to 23 are fitted to Lorentzian

NMR1
****

Filename = TCS8
Username = tmohan
Scale factor = ⌣.0000000E+00
Signal/Noise = 3532.10

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14262.63	175.924	100.000	0.7270E+08	15.87
*	2	11889.84	146.657	16.495	0.1199E+08	6.39
*	3	11351.80	140.020	0.214	0.1559E+06	55.54
*	4	11336.63	139.833	0.063	0.4552E+05	21.88
*	5	11324.51	139.684	0.262	0.1908E+06	29.06
*	6	11311.48	139.523	0.369	0.2684E+06	21.85
*	7	11303.83	139.429	0.197	0.1433E+06	9.61
*	8	11297.70	139.353	0.281	0.2041E+06	10.43
*	9	11289.68	139.254	0.372	0.2707E+06	12.75
*	10	11283.63	139.179	0.131	0.9493E+05	6.63
*	11	11280.72	139.144	0.098	0.7091E+05	7.35
*	12	11273.16	139.050	0.253	0.1839E+06	11.09
*	13	11264.54	138.944	0.155	0.1126E+06	12.34
*	14	11278.62	139.118	0.080	0.5842E+05	8.24
*	15	11248.32	138.744	1.053	0.7656E+06	48.24
*	16	10775.60	132.913	7.820	0.5685E+07	5.78
*	17	10693.24	131.897	0.267	0.1939E+06	7.10
*	18	10683.10	131.772	0.286	0.2079E+06	4.17

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.924	100.000	0.3058E+10	14270.26	14254.39
*	2	146.657	6.639	0.2030E+09	11892.85	11886.47
*	3	140.020	0.751	0.2295E+08	11379.37	11323.83
*	4	139.833	0.086	0.2641E+07	11347.43	11325.55
*	5	139.684	0.481	0.1470E+08	11338.87	11309.81
*	6	139.523	0.508	0.1554E+08	11322.23	11300.38
*	7	139.429	0.119	0.3651E+07	11308.71	11299.09
*	8	139.353	0.185	0.5641E+07	11302.89	11292.46
*	9	139.254	0.299	0.9147E+07	11296.05	11283.30
*	10	139.179	0.055	0.1669E+07	11286.77	11280.14
*	11	139.144	0.045	0.1381E+07	11284.46	11277.12
*	12	139.050	0.177	0.5408E+07	11278.63	11267.54
*	13	138.944	0.120	0.3681E+07	11270.66	11258.32
*	14	139.118	0.042	0.1276E+07	11282.54	11274.30
*	15	138.744	3.202	0.9790E+08	11272.32	11224.08
*	16	132.913	2.848	0.8707E+08	10778.51	10772.73
*	17	131.897	0.119	0.3650E+07	10696.80	10689.70
*	18	131.772	0.075	0.2297E+07	10685.26	10681.09

(*) Peaks 1 to 18 are fitted to Lorentzian

NMR1
****

Filename = TCS9
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 3790.36

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14262.63	175.924	100.000	0.6476E+08	15.00
*	2	11887.21	146.624	12.956	0.8390E+07	6.28
*	3	11329.47	139.745	0.236	0.1530E+06	41.98
*	4	11314.25	139.557	0.117	0.7546E+05	17.93
*	5	11301.21	139.396	0.067	0.4329E+05	16.36
*	6	11310.66	139.513	0.026	0.1667E+05	3.75
*	7	11304.74	139.440	0.145	0.9400E+05	11.89
*	8	11298.20	139.359	0.119	0.7688E+05	8.26
*	9	11292.42	139.288	0.192	0.1242E+06	9.69
*	10	11287.35	139.225	0.113	0.7312E+05	7.36
*	11	11283.00	139.172	0.192	0.1246E+06	8.33
*	12	11276.73	139.094	0.232	0.1503E+06	10.50
*	13	11273.33	139.052	0.062	0.3987E+05	5.03
*	14	11270.21	139.014	0.104	0.6702E+05	4.83
*	15	11267.20	138.977	0.174	0.1129E+06	8.89
*	16	11262.66	138.921	0.172	0.1117E+06	6.43
*	17	11256.47	138.844	0.300	0.1942E+06	9.67
*	18	11249.24	138.755	0.209	0.1351E+06	8.50
*	19	11242.39	138.671	0.323	0.2091E+06	15.33
*	20	11232.92	138.554	0.092	0.5975E+05	13.70
*	21	11230.83	138.528	0.011	7323.	8.91
*	22	11220.82	138.405	0.223	0.1445E+06	41.77
*	23	10773.54	132.888	5.828	0.3774E+07	5.66
*	24	10691.54	131.876	0.201	0.1301E+06	7.32
*	25	10681.12	131.748	0.191	0.1239E+06	3.52

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.924	100.000	0.4502E+10	14299.82	14224.83
*	2	146.624	5.426	0.2442E+09	11902.69	11871.29
*	3	139.745	0.662	0.2978E+08	11434.34	11224.42
*	4	139.557	0.139	0.6272E+07	11359.10	11269.44
*	5	139.396	0.073	0.3284E+07	11342.14	11260.32
*	6	139.513	0.006	0.2901E+06	11320.10	11301.33
*	7	139.440	0.115	0.5181E+07	11334.51	11275.07
*	8	139.359	0.065	0.2943E+07	11318.92	11277.62
*	9	139.288	0.124	0.5577E+07	11316.56	11268.13
*	10	139.225	0.055	0.2495E+07	11305.71	11268.91
*	11	139.172	0.107	0.4814E+07	11303.70	11262.03
*	12	139.094	0.162	0.7314E+07	11302.89	11250.40

*	13	139.052	0.021	0.9295E+06	11285.96	11260.81
*	14	139.014	0.033	0.1500E+07	11282.19	11258.06
*	15	138.977	0.103	0.4651E+07	11289.39	11244.93
*	16	138.921	0.074	0.3330E+07	11278.80	11246.64
*	17	138.844	0.193	0.8704E+07	11280.67	11232.32
*	18	138.755	0.118	0.5323E+07	11270.34	11227.83
*	19	138.671	0.330	0.1486E+08	11280.59	11203.96
*	20	138.554	0.084	0.3793E+07	11267.03	11198.55
*	21	138.528	0.007	0.3026E+06	11253.00	11208.43
*	22	138.405	0.621	0.2798E+08	11325.06	11116.23
*	23	132.888	2.200	0.9904E+08	10787.70	10759.39
*	24	131.876	0.098	0.4411E+07	10709.76	10673.18
*	25	131.748	0.045	0.2022E+07	10689.91	10672.30

(*) Peaks 1 to 25 are fitted to Lorentzian

NMR1
****

Filename = TCS12
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 3446.40

Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
* 1	14262.42	175.922	100.000	0.7341E+08	14.22
* 2	11885.10	146.598	12.932	0.9493E+07	6.35
* 3	11346.22	139.951	0.080	0.5880E+05	40.35
* 4	11312.95	139.541	0.388	0.2848E+06	92.55
* 5	11297.83	139.355	0.610	0.4476E+06	63.52
* 6	11269.40	139.004	0.329	0.2415E+06	26.60
* 7	11287.40	139.226	0.366	0.2687E+06	67.82
* 8	11180.75	137.910	0.197	0.1446E+06	75.25
* 9	11245.95	138.715	1.788	0.1312E+07	46.22
* 10	11652.82	143.733	1.080	0.7931E+06	128.11
* 11	11211.28	138.287	0.134	0.9850E+05	57.22
* 12	11309.90	139.503	0.020	0.1451E+05	91.55
* 13	10773.08	132.882	10.407	0.7640E+07	5.58
* 14	10691.46	131.875	0.432	0.3169E+06	26.89
* 15	10681.75	131.756	0.248	0.1819E+06	2.80

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
* 1	175.922	100.000	0.4839E+10	14297.72	14226.61
* 2	146.598	5.774	0.2794E+09	11900.93	11869.18
* 3	139.951	0.227	0.1100E+08	11446.99	11245.23
* 4	139.541	2.525	0.1222E+09	11544.29	11081.56
* 5	139.355	2.723	0.1318E+09	11456.62	11139.01
* 6	139.004	0.615	0.2978E+08	11335.86	11202.88
* 7	139.226	1.745	0.8446E+08	11457.00	11117.89
* 8	137.910	1.042	0.5044E+08	11368.92	10992.65
* 9	138.715	5.810	0.2811E+09	11361.51	11130.42
* 10	143.733	9.733	0.4710E+09	11973.04	11332.49
* 11	138.287	0.540	0.2612E+08	11354.35	11068.25
* 12	139.503	0.127	0.6159E+07	11538.84	11081.09
* 13	132.882	4.086	0.1977E+09	10787.05	10759.13
* 14	131.875	0.816	0.3951E+08	10758.55	10624.08
* 15	131.756	0.049	0.2360E+07	10688.83	10674.84

(*) Peaks 1 to 15 are fitted to Lorentzian

NMR1
****

Filename = TCS13
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 5483.18

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14261.05	175.905	100.000	0.1203E+09	10.65
*	2	11890.07	146.660	10.035	0.1207E+08	3.82
*	3	11342.13	139.901	0.046	0.5484E+05	15.49
*	4	11291.67	139.279	0.036	0.4341E+05	43.43
*	5	11329.96	139.751	0.108	0.1301E+06	18.76
*	6	11319.99	139.628	0.124	0.1491E+06	16.00
*	7	11307.66	139.476	0.255	0.3073E+06	20.00
*	8	11302.33	139.410	0.031	0.3737E+05	2.13
*	9	11298.73	139.366	0.077	0.9281E+05	7.49
*	10	11294.18	139.310	0.119	0.1430E+06	14.72
*	11	11354.34	140.052	0.146	0.1753E+06	55.91
*	12	11287.19	139.223	0.138	0.1656E+06	16.22
*	13	11277.29	139.101	0.163	0.1959E+06	19.50
*	14	11292.40	139.288	0.014	0.1734E+05	3.45
*	15	11268.70	138.995	0.096	0.1150E+06	24.07
*	16	11266.36	138.966	0.033	0.3917E+05	10.32
*	17	11251.58	138.784	0.295	0.3553E+06	39.18
*	18	11236.17	138.594	0.010	0.1162E+05	2.31
*	19	11244.19	138.693	0.392	0.4720E+06	55.70
*	20	11194.36	138.078	0.036	0.4374E+05	55.96
*	21	10775.67	132.914	6.551	0.7881E+07	3.61

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.905	100.000	0.5941E+10	14287.32	14234.06
*	2	146.660	3.594	0.2135E+09	11899.63	11880.56
*	3	139.901	0.066	0.3938E+07	11380.69	11303.24
*	4	139.279	0.147	0.8738E+07	11400.16	11183.02
*	5	139.751	0.190	0.1131E+08	11376.71	11282.92
*	6	139.628	0.186	0.1106E+08	11360.03	11280.04
*	7	139.476	0.480	0.2849E+08	11357.60	11257.59
*	8	139.410	0.006	0.3688E+06	11307.58	11296.94
*	9	139.366	0.054	0.3221E+07	11317.43	11279.98
*	10	139.310	0.164	0.9758E+07	11330.78	11257.15
*	11	140.052	0.765	0.4543E+08	11494.19	11214.63
*	12	139.223	0.209	0.1245E+08	11327.69	11246.61
*	13	139.101	0.298	0.1770E+08	11326.12	11228.63
*	14	139.288	0.005	0.2776E+06	11300.82	11283.55
*	15	138.995	0.216	0.1283E+08	11328.65	11208.31
*	16	138.966	0.032	0.1875E+07	11292.22	11240.60

17	138.784	1.086	0.6454E+08	11349.56	11153.64
18	138.594	0.002	0.1245E+06	11241.97	11230.41
19	138.693	2.051	0.1219E+09	11383.43	11104.94
20	138.078	0.191	0.1135E+08	11334.32	11054.51
21	132.914	2.222	0.1320E+09	10784.79	10766.72

(*) **Peaks 1 to 21 are fitted to Lorentzian**

NMR1
****

Filename = TCS1.001
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 4088.89

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14260.99	175.904	100.000	0.1766E+09	10.17
*	2	11887.83	146.632	16.447	0.2905E+08	3.20
*	3	11351.96	140.022	0.073	0.1282E+06	35.77
*	4	11326.58	139.709	0.280	0.4944E+06	38.21
*	5	11302.94	139.418	0.506	0.8944E+06	31.55
*	6	11276.85	139.096	0.141	0.2493E+06	28.28
*	7	11289.99	139.258	0.133	0.2348E+06	20.42
*	8	11285.78	139.206	0.089	0.1568E+06	18.95
*	9	11272.89	139.047	0.248	0.4379E+06	29.29
*	10	11256.03	138.839	0.264	0.4670E+06	32.90
*	11	11259.41	138.881	0.201	0.3554E+06	30.96
*	12	11132.06	137.310	0.338	0.5963E+06	1.79
*	13	11723.90	144.610	0.014	0.2411E+05	1.36
*	14	11241.09	138.655	0.783	0.1382E+07	36.95
*	15	11133.85	137.332	0.456	0.8048E+06	3.33
*	16	10774.50	132.899	14.177	0.2504E+08	2.97
*	17	10692.56	131.889	1.072	0.1893E+07	2.99
*	18	10682.35	131.763	1.060	0.1873E+07	2.99

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.904	100.000	0.8326E+10	14286.26	14235.42
*	2	146.632	5.175	0.4309E+09	11895.87	11879.88
*	3	140.022	0.255	0.2125E+08	11441.31	11262.47
*	4	139.709	1.052	0.8757E+08	11421.93	11230.89
*	5	139.418	1.571	0.1308E+09	11381.88	11224.13
*	6	139.096	0.393	0.3269E+08	11347.34	11205.93
*	7	139.258	0.267	0.2222E+08	11341.01	11238.93
*	8	139.206	0.165	0.1377E+08	11333.18	11238.46
*	9	139.047	0.714	0.5945E+08	11346.00	11199.56
*	10	138.839	0.855	0.7123E+08	11338.15	11173.64
*	11	138.881	0.613	0.5101E+08	11336.86	11182.04
*	12	137.310	0.059	0.4952E+07	11136.52	11127.57
*	13	144.610	0.002	0.1518E+06	11727.13	11720.33
*	14	138.655	2.844	0.2368E+09	11333.45	11148.71
*	15	137.332	0.149	0.1241E+08	11142.14	11125.51
*	16	132.899	4.146	0.3452E+09	10781.86	10766.99
*	17	131.889	0.316	0.2627E+08	10700.13	10685.17
*	18	131.763	0.312	0.2595E+08	10689.75	10674.81

(*) Peaks 1 to 18 are fitted to Lorentzian

TCS15

NMR1
****

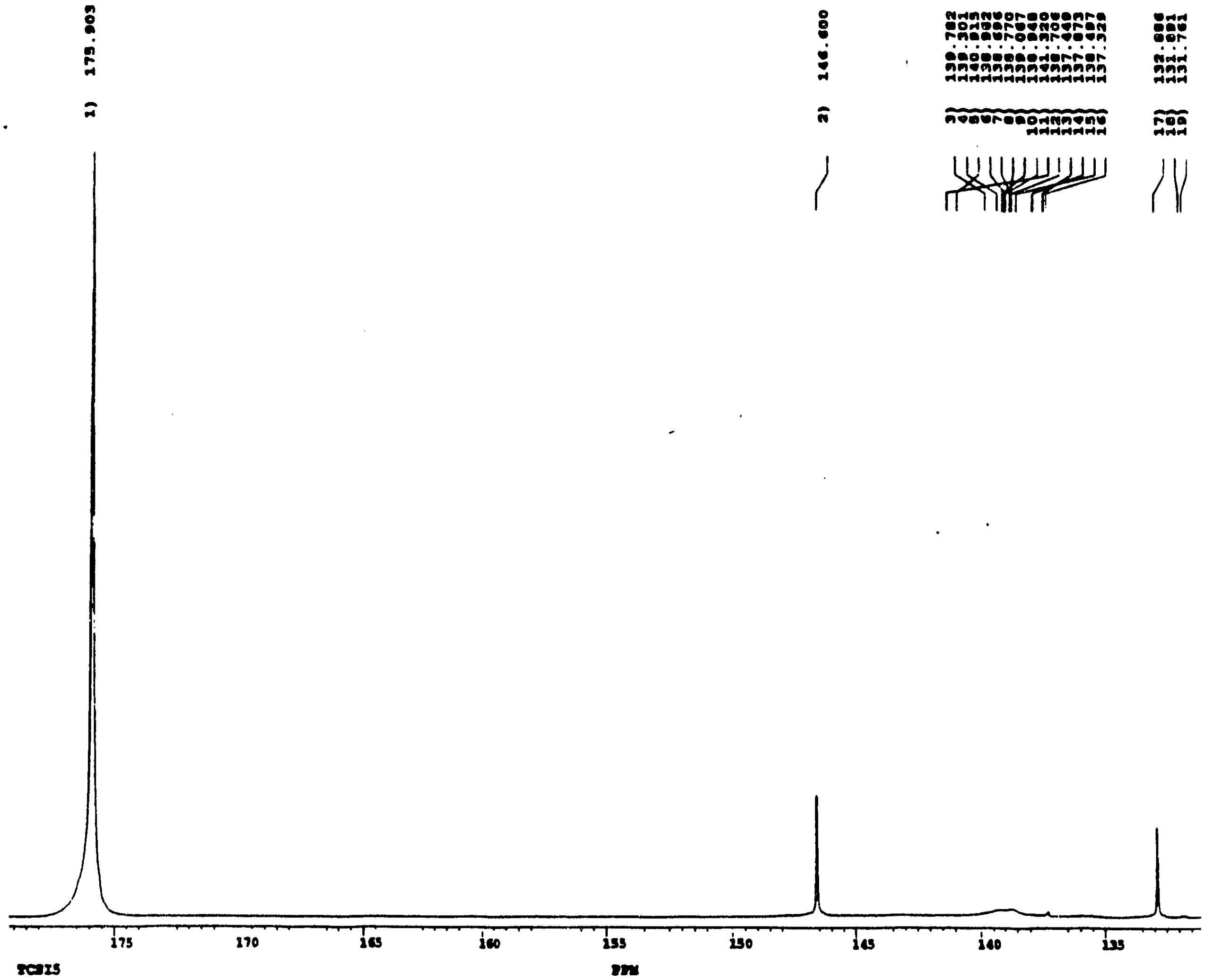
Filename = TCSI5
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 4756.95

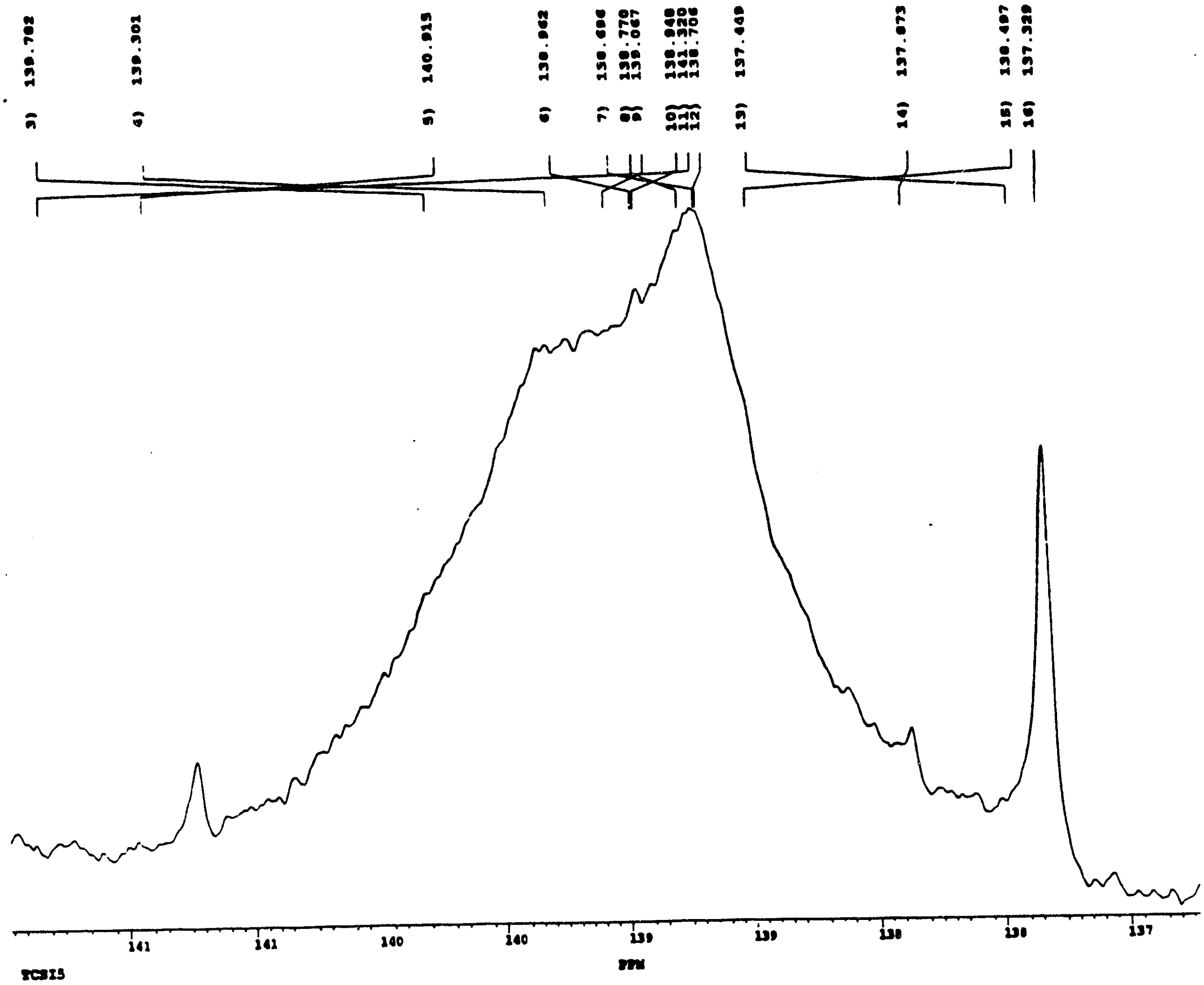
Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
1	14260.94	175.903	100.000	0.1092E+09	10.16
2	11885.21	146.600	17.233	0.1881E+08	4.00
3	11332.49	139.782	0.199	0.2174E+06	80.35
4	11293.47	139.301	0.575	0.6278E+06	62.18
5	11424.37	140.915	0.030	0.3261E+05	65.91
6	11265.96	138.962	0.020	0.2151E+05	8.29
7	11244.48	138.696	0.056	0.6061E+05	91.25
8	11250.42	138.770	0.126	0.1376E+06	79.48
9	11274.52	139.067	0.051	0.5608E+05	14.38
10	11264.90	138.948	0.047	0.5160E+05	4.29
11	11457.19	141.320	0.016	0.1709E+05	348.54
12	11245.21	138.706	0.590	0.6446E+06	38.78
13	11143.33	137.449	0.089	0.9681E+05	19.98
14	11177.70	137.873	0.049	0.5345E+05	29.18
15	11228.28	138.497	0.198	0.2165E+06	120.41
16	11133.58	137.329	0.649	0.7084E+06	5.07
17	10773.44	132.886	13.033	0.1423E+08	3.80
18	10692.71	131.891	0.268	0.2923E+06	9.62
19	10682.21	131.761	0.272	0.2971E+06	5.53

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
1	175.903	100.000	0.5141E+10	14286.00	14235.20
2	146.600	6.784	0.3488E+09	11894.97	11874.97
3	139.782	1.575	0.8098E+08	11533.27	11131.51
4	139.301	3.520	0.1810E+09	11448.74	11137.82
5	140.915	0.194	0.9962E+07	11589.02	11259.46
6	138.962	0.016	0.8269E+06	11286.75	11245.29
7	138.696	0.499	0.2564E+08	11472.52	11016.27
8	138.770	0.986	0.5069E+08	11449.01	11051.63
9	139.067	0.073	0.3737E+07	11310.26	11238.38
10	138.948	0.020	0.1026E+07	11275.56	11254.12
11	141.320	0.537	0.2761E+08	12328.47	10585.79
12	138.706	2.254	0.1159E+09	11342.24	11148.33
13	137.449	0.174	0.8964E+07	11193.30	11093.42
14	137.873	0.141	0.7229E+07	11250.67	11104.79
15	138.497	2.350	0.1208E+09	11529.11	10927.09
16	137.329	0.324	0.1664E+08	11146.25	11120.92
17	132.886	4.873	0.2505E+09	10782.79	10763.80

18	131.891	0.253	0.1303E+08	10716.75	10668.67
19	131.761	0.148	0.7613E+07	10695.86	10668.22





^{31}P NMR spectral data of the coal samples obtained by processing the FID's by the Matched Filter Apodization Parameter Technique.

NMR1
****

Filename = TCSO1
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 5713.11

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14261.31	175.908	100.000	0.6932E+08	16.61
*	2	11888.37	146.639	6.214	0.4308E+07	10.52
*	3	11268.37	138.991	2.866	0.1987E+07	115.62
*	4	10774.80	132.903	8.080	0.5601E+07	9.59

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.908	100.000	0.2669E+10	14302.48	14219.42
*	2	146.639	3.936	0.1051E+09	11914.59	11861.97
*	3	138.991	19.948	0.5324E+09	11557.50	10979.39
*	4	132.903	4.664	0.1245E+09	10798.80	10750.86

(*) Peaks 1 to 4 are fitted to Lorentzian

NMR1
****

Filename = TCS2
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 1125.58

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14252.39	175.798	100.000	0.3092E+08	15.42
*	2	11880.97	146.547	45.537	0.1408E+08	11.99
*	3	11259.77	138.885	8.915	0.2757E+07	118.54
*	4	10765.97	132.794	20.718	0.6406E+07	9.71
*	5	10682.47	131.764	0.855	0.2645E+06	24.24
*	6	10673.23	131.650	0.485	0.1499E+06	5.64

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.798	100.000	0.1105E+10	14290.17	14213.07
*	2	146.547	35.406	0.3912E+09	11910.70	11850.76
*	3	138.885	68.543	0.7573E+09	11556.05	10963.37
*	4	132.794	13.045	0.1441E+09	10790.37	10741.83
*	5	131.764	1.345	0.1486E+08	10743.15	10621.94
*	6	131.650	0.177	0.1960E+07	10687.16	10658.96

(*) Peaks 1 to 6 are fitted to Lorentzian

NMR1
****

Filename = TCS3
Username = tmohan
Scale factor = 0.0000000E+00

Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
* 1	14261.27	175.908	100.000	0.7099E+08	17.44
* 2	11889.10	146.648	8.252	0.5857E+07	12.15
* 3	11270.58	139.018	1.285	0.9122E+06	136.13
* 4	10775.13	132.907	5.981	0.4245E+07	10.37
* 5	10692.38	131.887	0.234	0.1659E+06	15.28
* 6	10682.45	131.764	0.163	0.1160E+06	5.52

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
* 1	175.908	100.000	0.2869E+10	14304.18	14216.99
* 2	146.648	5.749	0.1649E+09	11919.47	11858.73
* 3	139.018	10.032	0.2878E+09	11610.79	10930.12
* 4	132.907	3.555	0.1020E+09	10800.98	10749.15
* 5	131.887	0.205	0.5878E+07	10730.31	10653.89
* 6	131.764	0.052	0.1483E+07	10696.41	10668.83

(*) Peaks 1 to 6 are fitted to Lorentzian

NMR1
****

Filename = TCS4
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 5575.85

Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
* 1	14261.38	175.909	100.000	0.6031E+08	19.48
* 2	11886.18	146.612	9.395	0.5665E+07	13.89
* 3	11274.85	139.071	1.145	0.6902E+06	132.51
* 4	10773.62	132.889	4.898	0.2954E+07	11.79
* 5	10691.97	131.882	0.349	0.2104E+06	12.25
* 6	10681.93	131.758	0.284	0.1710E+06	8.57

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
* 1	175.909	100.000	0.2723E+10	14309.30	14211.89
* 2	146.612	6.696	0.1823E+09	11920.87	11851.44
* 3	139.071	7.785	0.2120E+09	11605.90	10943.33
* 4	132.889	2.964	0.8070E+08	10802.77	10743.83
* 5	131.882	0.219	0.5976E+07	10722.75	10661.48
* 6	131.758	0.125	0.3398E+07	10703.47	10660.61

(*) Peaks 1 to 6 are fitted to Lorentzian

NMR1
****

Filename = TCS5
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 4020.26

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14261.06	175.905	100.000	0.8427E+08	11.20
*	2	11884.98	146.597	15.611	0.1316E+08	4.55
*	3	11295.32	139.324	0.116	0.9740E+05	29.91
*	4	11283.54	139.178	0.088	0.7431E+05	24.26
*	5	11321.82	139.650	0.369	0.3113E+06	83.98
*	6	11307.31	139.472	0.019	0.1642E+05	2[illegible].34
*	7	11241.57	138.661	0.303	0.2551E+06	30.52
*	8	11300.62	139.389	0.120	0.1013E+06	39.99
*	9	11265.08	138.951	0.344	0.2897E+06	49.53
*	10	11238.18	138.619	0.303	0.2555E+06	70.50
*	11	10772.90	132.880	10.275	0.8659E+07	4.15
*	12	10691.92	131.881	0.824	0.6946E+06	5.52
*	13	10681.75	131.755	0.790	0.6660E+06	4.34

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.905	100.000	0.2188E+10	14288.40	14232.40
*	2	146.597	6.338	0.1386E+09	11896.14	11873.40
*	3	139.324	0.309	0.6752E+07	11369.93	11220.39
*	4	139.178	0.191	0.4178E+07	11343.95	11222.66
*	5	139.650	2.770	0.6059E+08	11531.78	11111.87
*	6	139.472	0.048	0.1040E+07	11375.35	11238.67
*	7	138.661	0.825	0.1805E+08	11317.53	11164.94
*	8	139.389	0.429	0.9393E+07	11400.46	11200.52
*	9	138.951	1.520	0.3326E+08	11388.77	11141.10
*	10	138.619	1.909	0.4176E+08	11414.53	11062.01
*	11	132.880	3.810	0.8334E+08	10783.48	10762.72
*	12	131.881	0.407	0.8894E+07	10705.73	10678.11
*	13	131.755	0.306	0.6693E+07	10692.68	10671.00

(*) Peaks 1 to 13 are fitted to Lorentzian

NMR1
****

Filename = TCS6
Username = tmohan
Scale factor = 0.0000000E+00

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14255.67	175.838	100.000	0.4047E+08	17.64
*	2	11879.34	146.527	34.503	0.1400E+08	13.63
*	3	11257.62	138.859	9.993	0.4044E+07	119.10
*	4	10766.55	132.801	19.075	0.7720E+07	12.70

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.838	100.000	0.1654E+10	14299.27	14211.08
*	2	146.527	26.7[illegible]1	0.4421E+09	11913.02	11844.88
*	3	138.859	67.471	0.1116E+10	11555.08	10959.60
*	4	132.801	13.730	0.2272E+09	10798.43	10734.95

(*) Peaks 1 to 4 are fitted to Lorentzian

NMR1
****

Filename = TCS7
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 5635.85

Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
1	14257.96	175.867	100.000	0.6077E+08	20.71
2	11883.30	146.576	7.123	0.4329E+07	14.15
3	11267.22	138.977	1.381	0.8395E+06	113.88
4	10769.99	132.844	4.027	0.2447E+07	12.42
5	10686.53	131.814	0.121	0.7379E+05	5.55
6	10677.95	131.709	0.078	0.4743E+05	3.42

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
1	175.867	100.000	0.2917E+10	14309.32	14205.77
2	146.576	4.866	0.1419E+09	11918.47	11847.73
3	138.977	7.597	0.2216E+09	11551.53	10982.12
4	132.844	2.414	0.7042E+08	10800.69	10738.61
5	131.814	0.033	0.9493E+06	10700.57	10672.81
6	131.709	0.013	0.3764E+06	10686.36	10669.24

*) Peaks 1 to 6 are fitted to Lorentzian

NMR1
****

Filename = TCS8
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 4207.80

Peak Analysis

Peak #		Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14262.69	175.925	100.000	0.7058E+08	16.45
*	2	11889.98	146.659	15.474	0.1092E+08	7.28
*	3	11299.28	139.372	0.305	0.2155E+06	53.56
*	4	11306.29	139.459	0.559	0.3943E+06	103.31
*	5	11376.80	140.329	0.032	0.2253E+05	14.92
*	6	11260.87	138.899	0.174	0.1230E+06	37.63
*	7	11271.67	139.032	0.139	0.9839E+05	37.47
*	8	11245.31	138.707	0.671	0.4737E+06	37.73
*	9	11446.76	141.192	0.083	0.5879E+05	16.22
*	10	10775.71	132.914	7.325	0.5170E+07	6.48
*	11	10693.21	131.897	0.255	0.1802E+06	6.58
*	12	10683.19	131.773	0.268	0.1890E+06	3.87

Peak #		PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.925	100.000	0.2691E+10	14303.09	14220.82
*	2	146.659	6.849	0.1843E+09	11908.08	11871.67
*	3	139.372	0.994	0.2675E+08	11432.98	11165.18
*	4	139.459	3.508	0.9442E+08	11564.47	11047.91
*	5	140.329	0.029	0.7790E+06	11414.00	11339.41
*	6	138.899	0.398	0.1072E+08	11354.63	11166.50
*	7	139.032	0.317	0.8545E+07	11365.50	11178.14
*	8	138.707	1.539	0.4142E+08	11339.47	11150.84
*	9	141.192	0.082	0.2211E+07	11487.19	11406.08
*	10	132.914	2.883	0.7761E+08	10792.03	10759.65
*	11	131.897	0.102	0.2750E+07	10709.34	10676.42
*	12	131.773	0.063	0.1696E+07	10693.08	10673.72

(*) Peaks 1 to 12 are fitted to Lorentzian

NMR1
****

Filename = TCS9
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 4676.15

Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
* 1	14263.01	175.929	100.000	0.4867E+08	22.29
* 2	11888.09	146.635	8.925	0.4344E+07	14.59
* 3	11326.32	139.706	0.218	0.1062E+06	99.37
* 4	11297.25	139.347	0.320	0.1558E+06	54.47
* 5	11269.74	139.008	0.201	0.9779E+05	44.89
* 6	11245.70	138.712	0.478	0.2325E+06	42.93
* 7	10774.53	132.900	3.901	0.1899E+07	12.73
* 8	10683.35	131.775	0.072	0.3520E+05	3.93
* 9	10691.30	131.873	0.121	0.5906E+05	5.41

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
1	175.929	100.000	0.2514E+10	14318.03	14206.58
2	146.635	5.842	0.1469E+09	11924.33	11851.39
3	139.706	0.973	0.2447E+08	11574.53	11077.66
4	139.347	0.782	0.1967E+08	11433.24	11160.88
5	139.008	0.405	0.1017E+08	11382.03	11157.58
6	138.712	0.920	0.2313E+08	11352.84	11138.18
7	132.900	2.229	0.5605E+08	10806.25	10742.58
8	131.775	0.013	0.3209E+06	10692.99	10673.32
9	131.873	0.029	0.7402E+06	10704.97	10677.93

*) Peaks 1 to 9 are fitted to Lorentzian

NMR1
****

Filename = TCS10
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 2124.10

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14260.59	175.899	100.000	0.3661E+08	22.40
*	2	12001.65	148.036	1.117	0.4089E+06	16.68
*	3	11886.83	146.620	8.767	0.3210E+07	13.91
*	4	11293.63	139.303	1.257	0.4602E+06	36.51
*	5	11240.16	138.643	1.494	0.5469E+06	36.48
*	6	11131.39	137.302	2.069	0.7576E+06	16.19
*	7	10771.75	132.866	4.848	0.1775E+07	11.90

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.899	100.000	0.1901E+10	14315.82	14203.83
*	2	148.036	0.831	0.1580E+08	12043.22	11959.84
*	3	146.620	5.445	0.1035E+09	11921.34	11851.79
*	4	139.303	2.049	0.3894E+08	11384.66	11202.14
*	5	138.643	2.432	0.4623E+08	11331.26	11148.88
*	6	137.302	1.496	0.2843E+08	11171.52	11090.55
*	7	132.866	2.577	0.4898E+08	10801.70	10742.17

(*) Peaks 1 to 7 are fitted to Lorentzian

NMR1
****

Filename = TCS11
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 2227.59

Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
1	14258.57	175.874	100.000	0.4465E+08	20.96
2	11887.98	146.634	17.848	0.7970E+07	13.11
3	11296.07	139.333	2.580	0.1152E+07	38.91
4	11242.58	138.673	2.761	0.1233E+07	30.38
5	11234.05	138.568	0.931	0.4155E+06	15.85
6	11315.57	139.573	0.049	0.2205E+05	118.10
7	11128.36	137.264	1.911	0.8535E+06	15.74
8	10772.28	132.872	5.352	0.2390E+07	11.78

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
1	175.874	100.000	0.2169E+10	14310.53	14205.75
2	146.634	11.168	0.2422E+09	11920.62	11855.06
3	139.333	4.789	0.1039E+09	11393.12	11198.59
4	138.673	4.003	0.8682E+08	11318.48	11166.58
5	138.568	0.704	0.1526E+08	11273.26	11194.02
6	139.573	0.278	0.6035E+07	11610.66	11020.17
7	137.264	1.436	0.3114E+08	11167.51	11088.81
8	132.872	3.008	0.6523E+08	10801.47	10742.58

*) Peaks 1 to 8 are fitted to Lorentzian

NMR1
****

Filename = TCS12
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 3689.62

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14262.89	175.927	100.000	0.5011E+08	23.37
*	2	11885.51	146.603	8.577	0.4299E+07	17.94
*	3	11267.25	138.977	3.220	0.1614E+07	115.80
*	4	10773.31	132.885	6.785	0.3400E+07	15.60

	Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
*	1	175.927	100.000	0.2715E+10	14320.66	14203.80
*	2	146.603	6.582	0.1787E+09	11930.25	11840.57
*	3	138.977	15.956	0.4332E+09	11556.87	10977.85
*	4	132.885	4.528	0.1229E+09	10812.15	10734.15

(*) Peaks 1 to 4 are fitted to Lorentzian

NMR1
****

Filename = TCS13
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 7020.59

Peak Analysis

	Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
*	1	14261.19	175.907	100.000	0.8723E+08	15.34
*	2	11890.11	146.660	6.768	0.5904E+07	8.69
*	3	11272.85	139.046	0.985	0.8595E+06	113.83
*	4	10775.76	132.915	4.424	0.3859E+07	7.71
*	5	10693.18	131.896	0.100	0.8752E+05	5.42
*	6	10683.16	131.773	0.100	0.8733E+05	3.93

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
1	175.907	100.000	0.3102E+10	14299.19	14222.49
2	146.660	3.836	0.1190E+09	11911.68	11868.21
3	139.046	7.311	0.2267E+09	11557.05	10987.92
4	132.915	2.224	0.6898E+08	10795.19	10756.63
5	131.896	0.035	0.1098E+07	10706.48	10679.41
6	131.773	0.026	0.7952E+06	10692.69	10673.05

*) Peaks 1 to 6 are fitted to Lorentzian

NMR1
****

Filename = TCS1.001
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 4322.52

Peak Analysis

Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
* 1	14261.17	175.906	100.000	0.1202E+09	15.73
* 2	11887.62	146.629	9.942	0.1195E+08	9.46
* 3	11268.81	138.997	1.870	0.2248E+07	111.44
* 4	11136.46	137.364	0.535	0.6434E+06	27.70
* 5	10774.27	132.897	8.562	0.1029E+08	8.13
* 6	10692.26	131.885	0.780	0.9371E+06	11.14
* 7	10681.81	131.756	0.744	0.8948E+06	8.42

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
* 1	175.906	100.000	0.4382E+10	14300.02	14221.37
* 2	146.629	5.979	0.2621E+09	11911.09	11863.79
* 3	138.997	13.250	0.5807E+09	11547.39	10990.19
* 4	137.364	0.942	0.4130E+08	11205.29	11066.81
* 5	132.897	4.424	0.1939E+09	10794.31	10753.67
* 6	131.885	0.552	0.2418E+08	10720.05	10664.38
* 7	131.756	0.398	0.1746E+08	10702.59	10660.50

(*) Peaks 1 to 7 are fitted to Lorentzian

NMR1
****

Filename = TCSI5
Username = tmohan
Scale factor = 0.0000000E+00
Signal/Noise = 5744.53

Peak Analysis

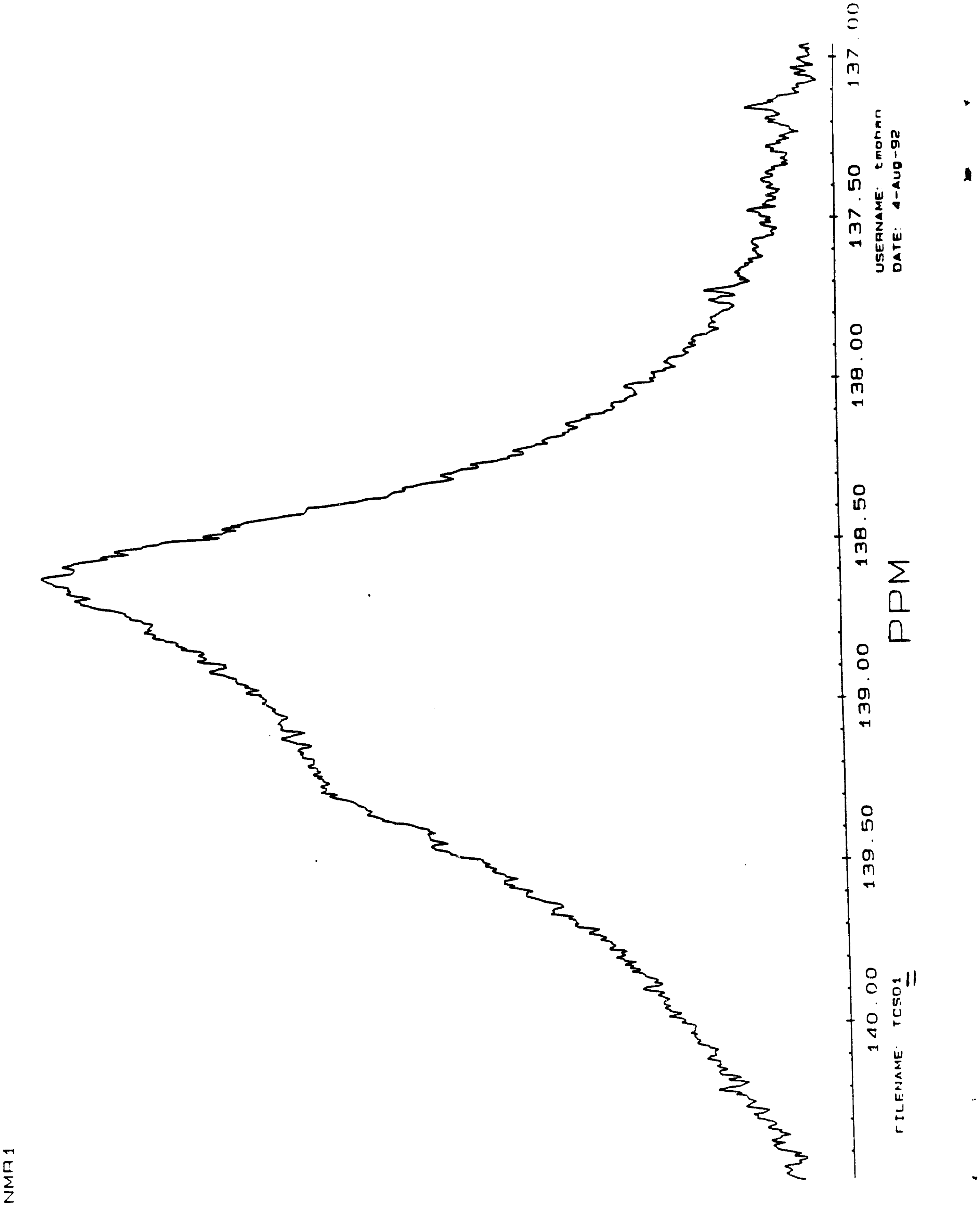
Peak #	Hz	PPM	Relative Intensity	Absolute Intensity	Linewidth (Hz)
* 1	14261.06	175.905	100.000	0.9394E+08	12.03
* 2	11885.18	146.599	14.230	0.1337E+08	5.91
* 3	11379.34	140.360	0.127	0.1190E+06	198.61
* 4	11084.16	136.719	0.040	0.3771E+05	8.16
* 5	11291.41	139.275	0.934	0.8777E+06	102.33
* 6	11177.75	137.873	0.129	0.1215E+06	87.20
* 7	11243.95	138.690	0.768	0.7216E+06	46.04
* 8	11133.94	137.333	0.599	0.5624E+06	7.10
* 9	10773.42	132.886	10.743	0.1009E+08	5.52
* 10	10691.22	131.872	0.233	0.2193E+06	22.11
* 11	10682.11	131.760	0.177	0.1664E+06	3.66

Peak #	PPM	Relative integral	Absolute integral	Integral start (hz)	Integral end (hz)
* 1	175.905	100.000	0.2619E+10	14290.58	14230.44
* 2	146.599	6.995	0.1832E+09	11899.67	11870.10
* 3	140.360	2.092	0.5479E+08	11875.95	10882.89
* 4	136.719	0.027	0.7131E+06	11104.71	11063.92
* 5	139.275	7.949	0.2082E+09	11546.95	11035.29
* 6	137.873	0.937	0.2455E+08	11395.36	10959.34
* 7	138.690	2.940	0.7699E+08	11358.81	11128.63
* 8	137.333	0.353	0.9257E+07	11151.85	11116.34
* 9	132.886	4.927	0.1290E+09	10787.01	10759.42
* 10	131.872	0.429	0.1124E+08	10746.70	10636.17
* 11	131.760	0.054	0.1413E+07	10691.11	10672.80

(*) Peaks 1 to 11 are fitted to Lorentzian

Appendix C: ^{31}P NMR Spectra of the Phenol Region of Samples 1-15

The spectra are grouped according to spectral appearance as given in Table V.



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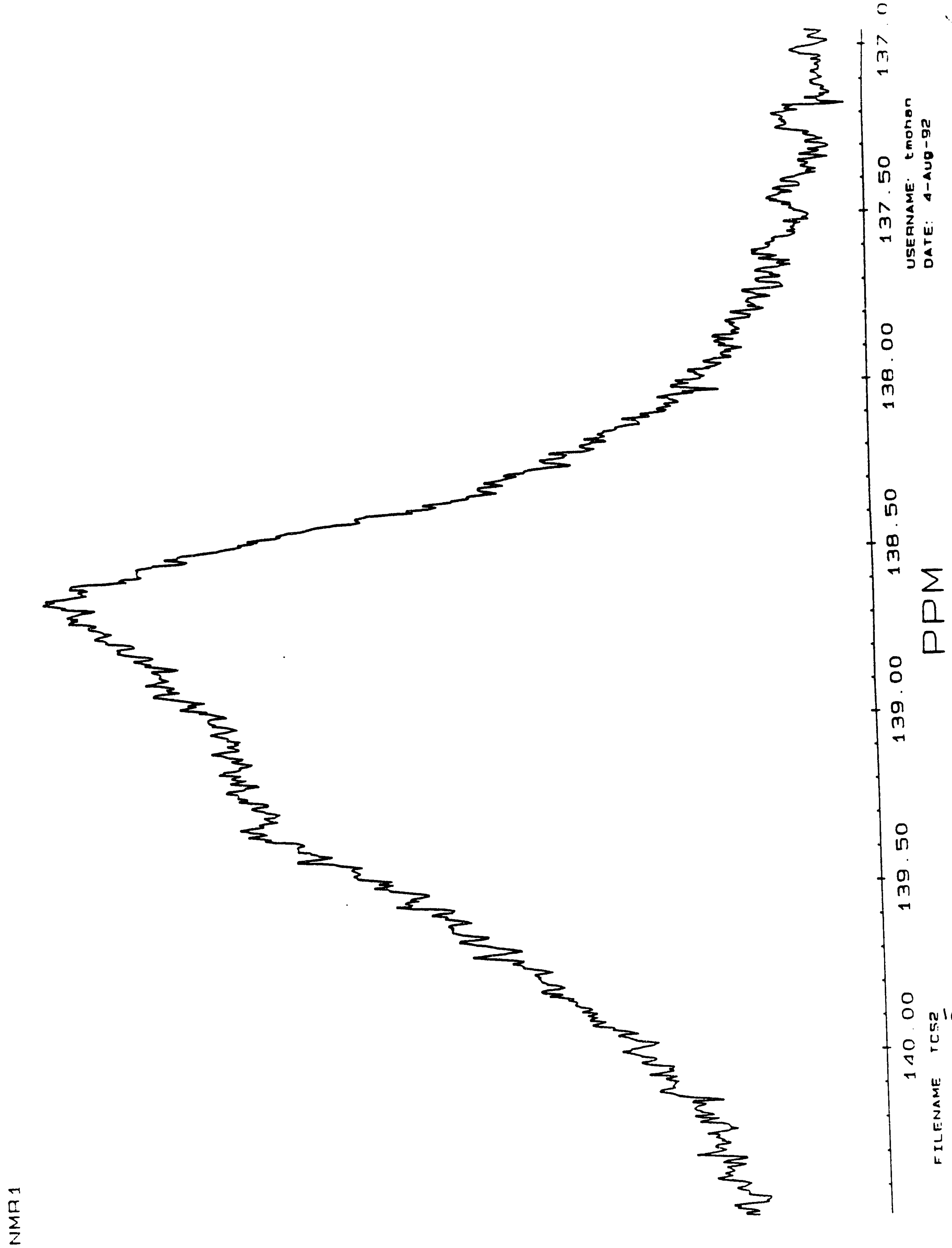
NMR1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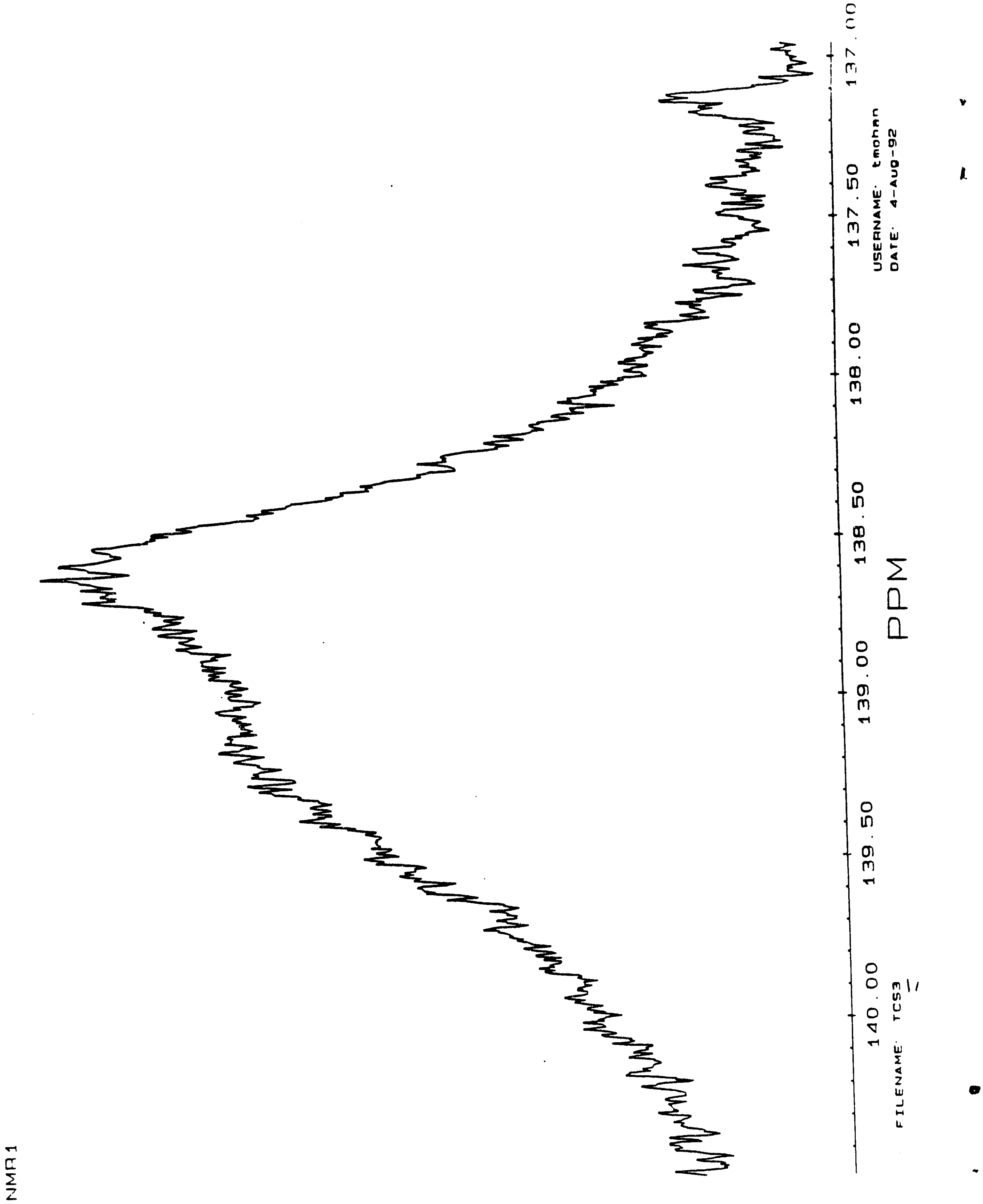

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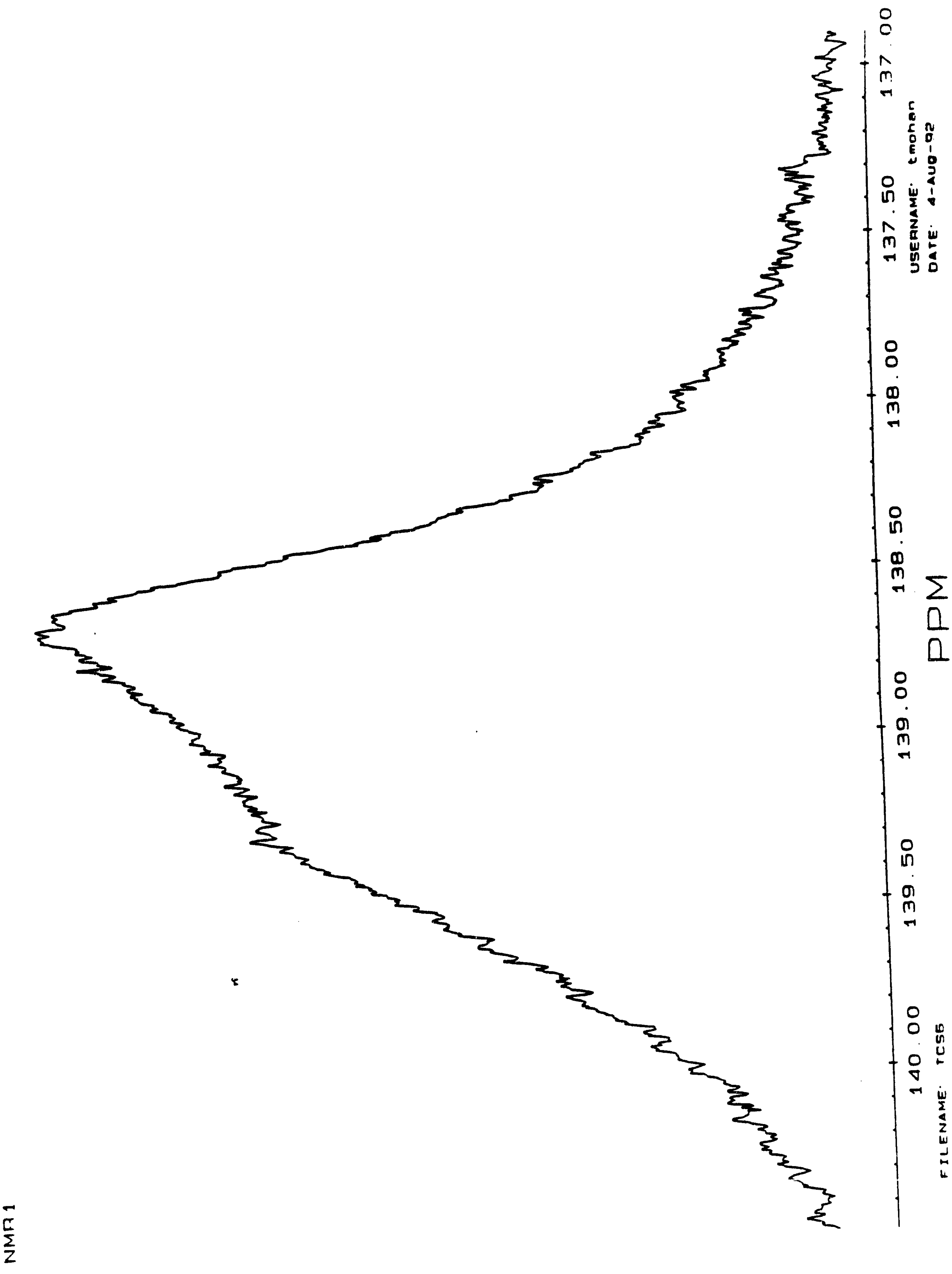

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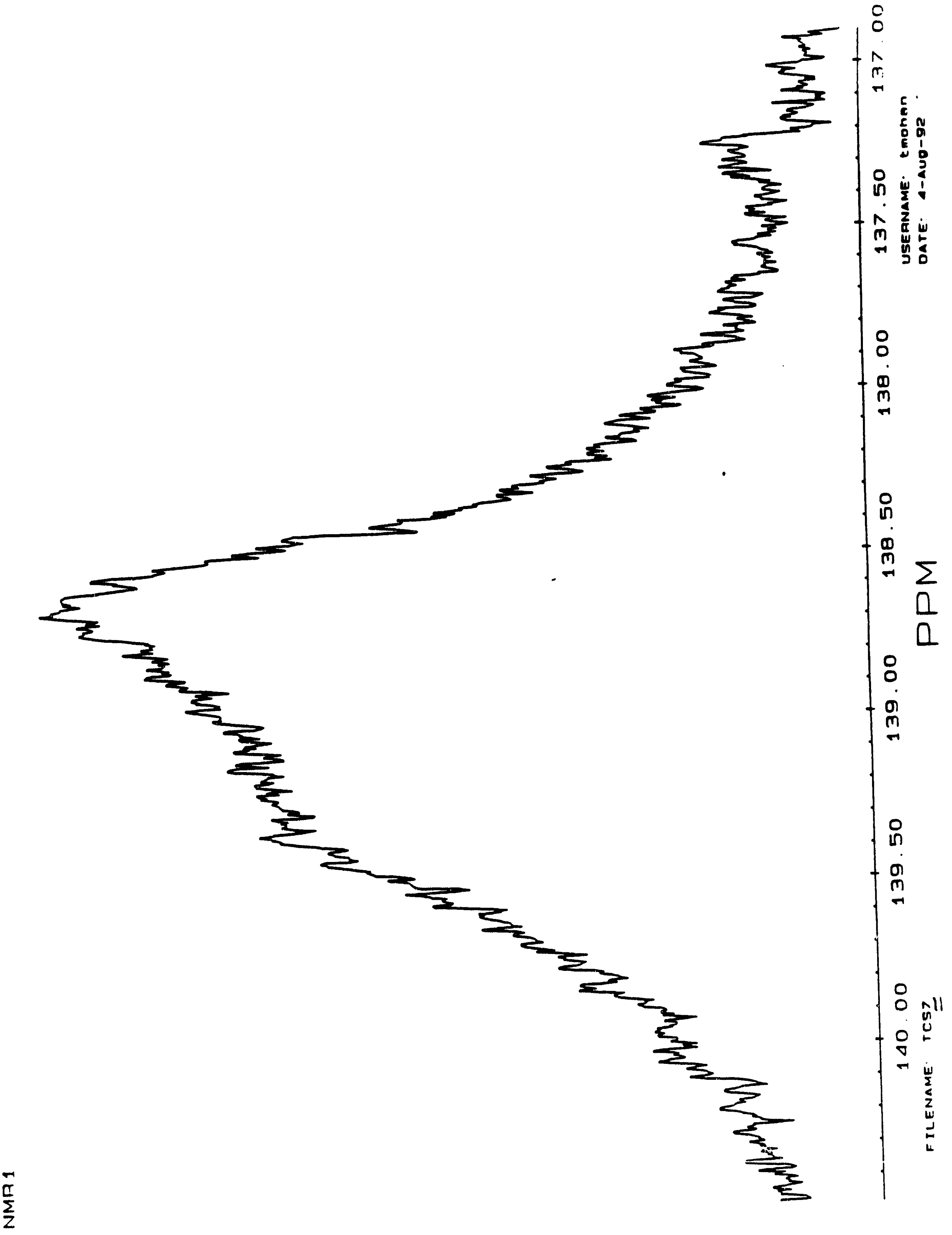
DATE: 4-AUG-92
FILENAME: TCS6
NMR1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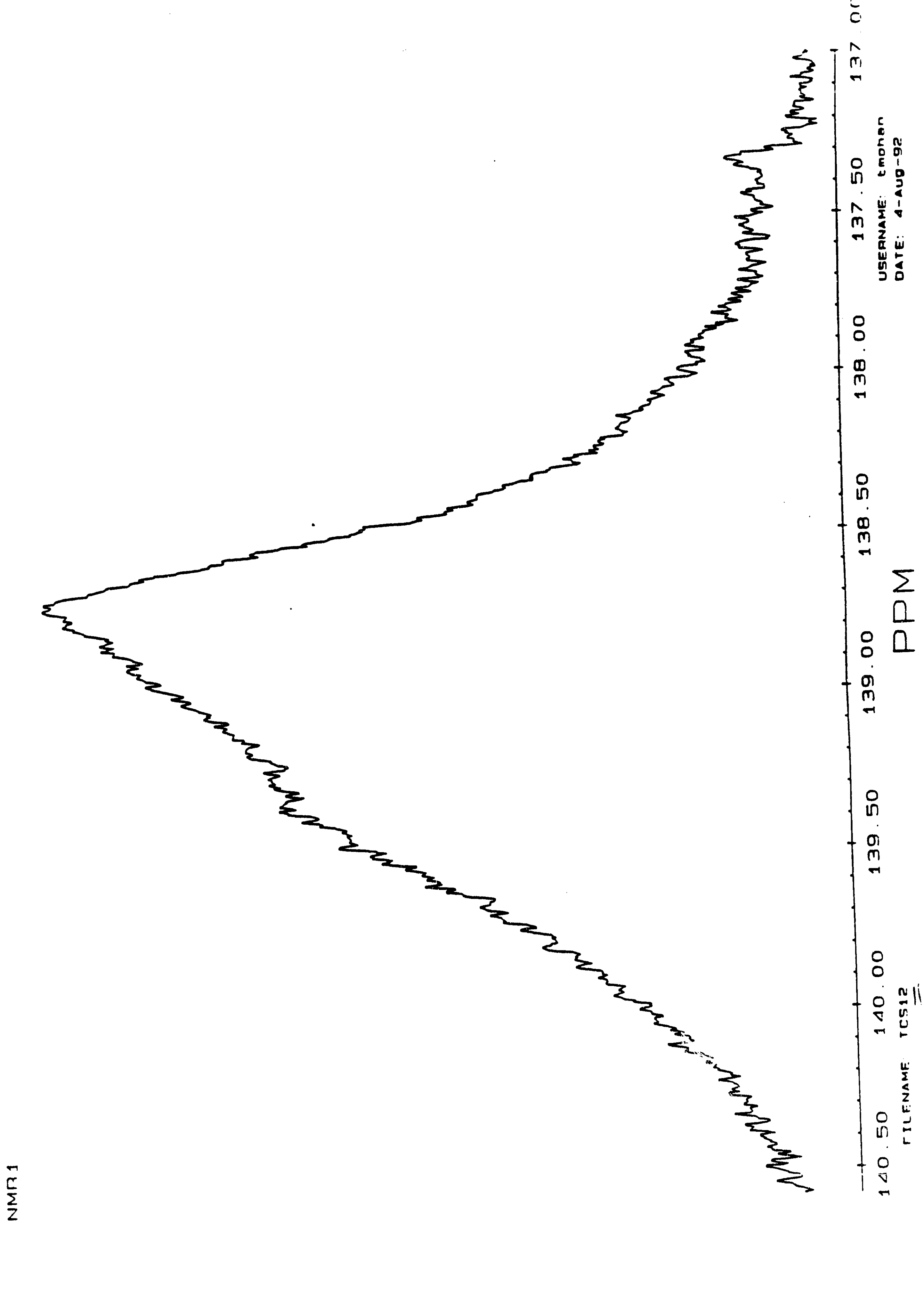
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FILENAME TCS12
PPM
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139.00
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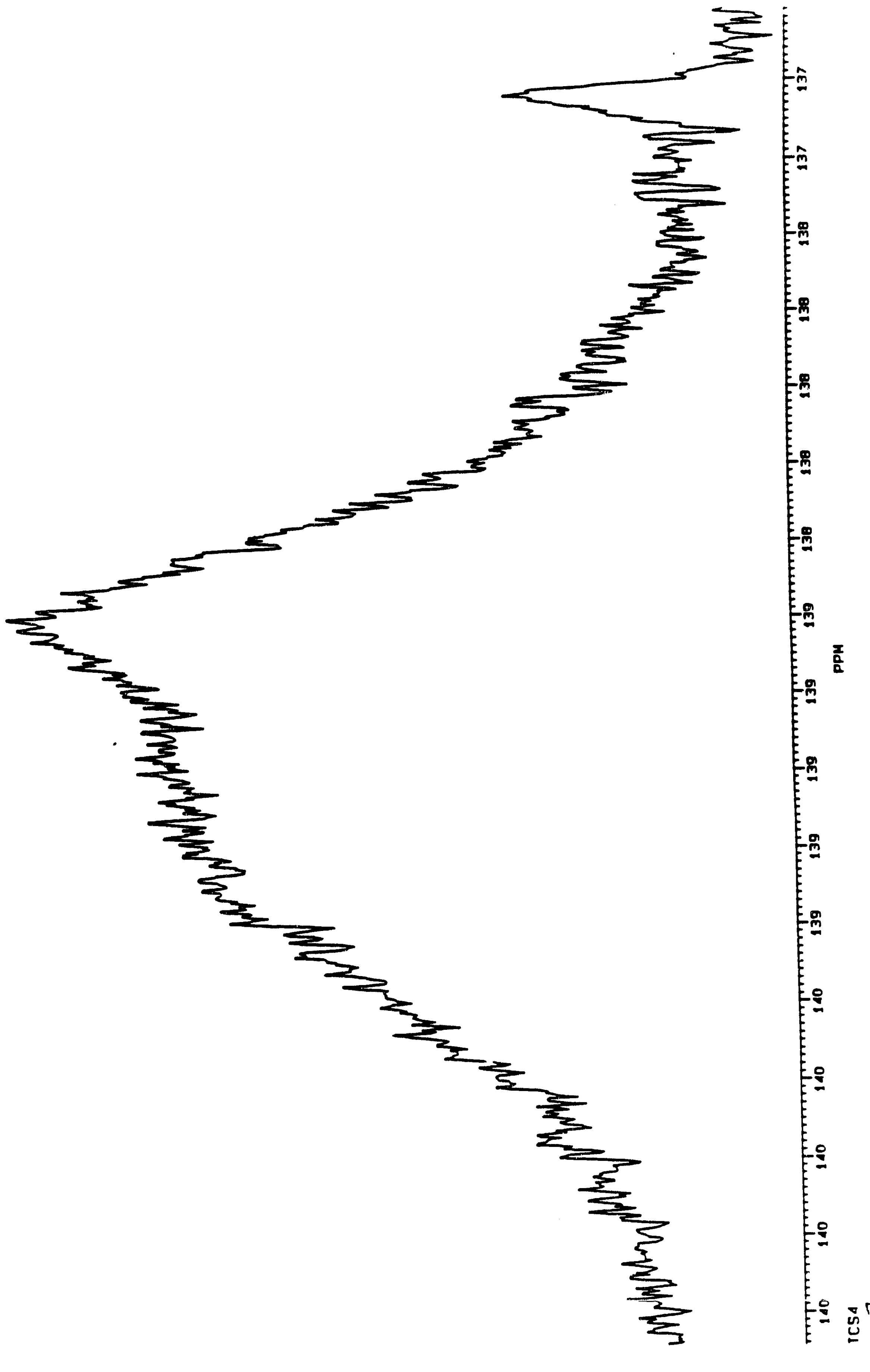
137.50
137.00



137
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138
138
138
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PPM
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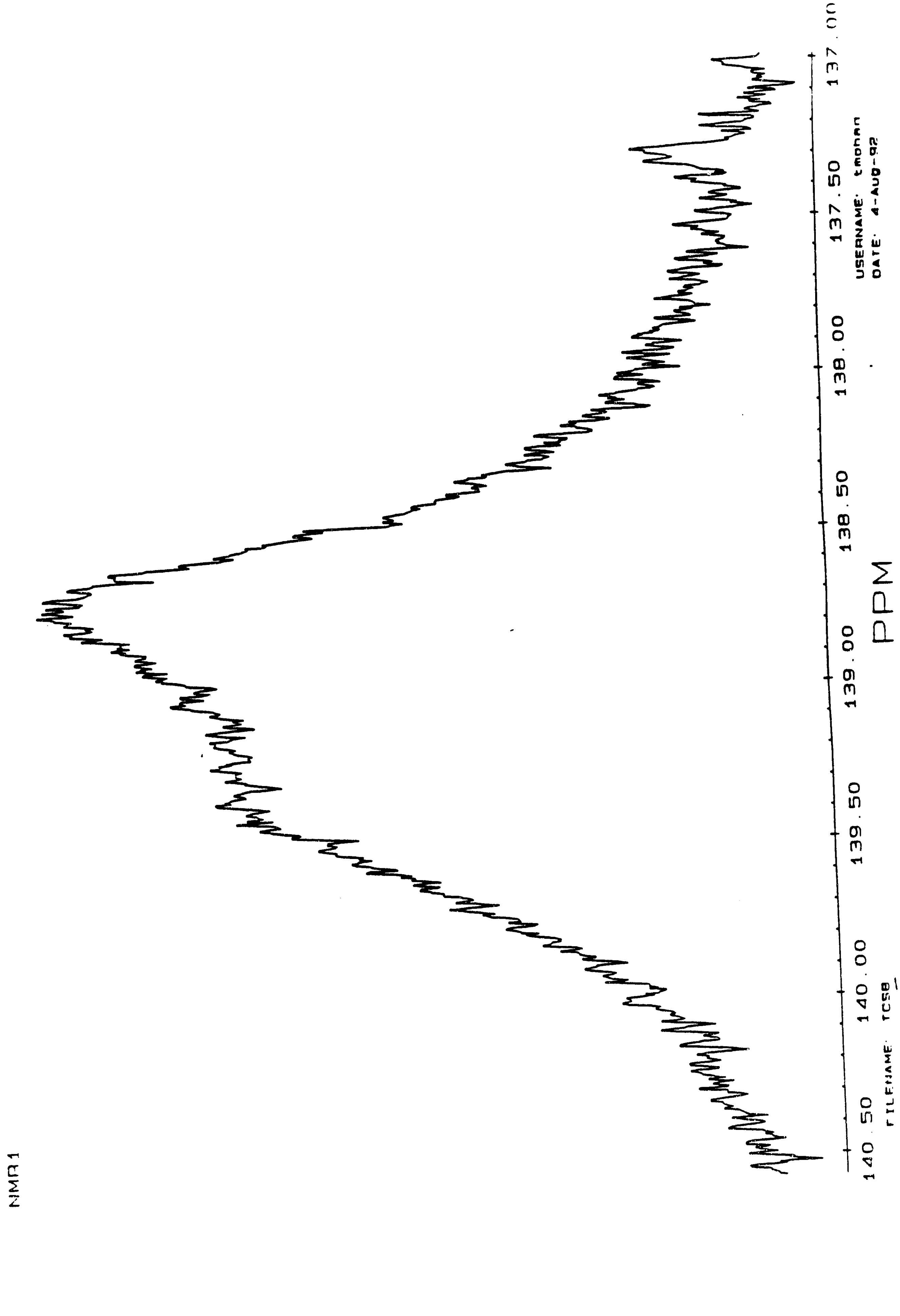
140
140
140
140
TC54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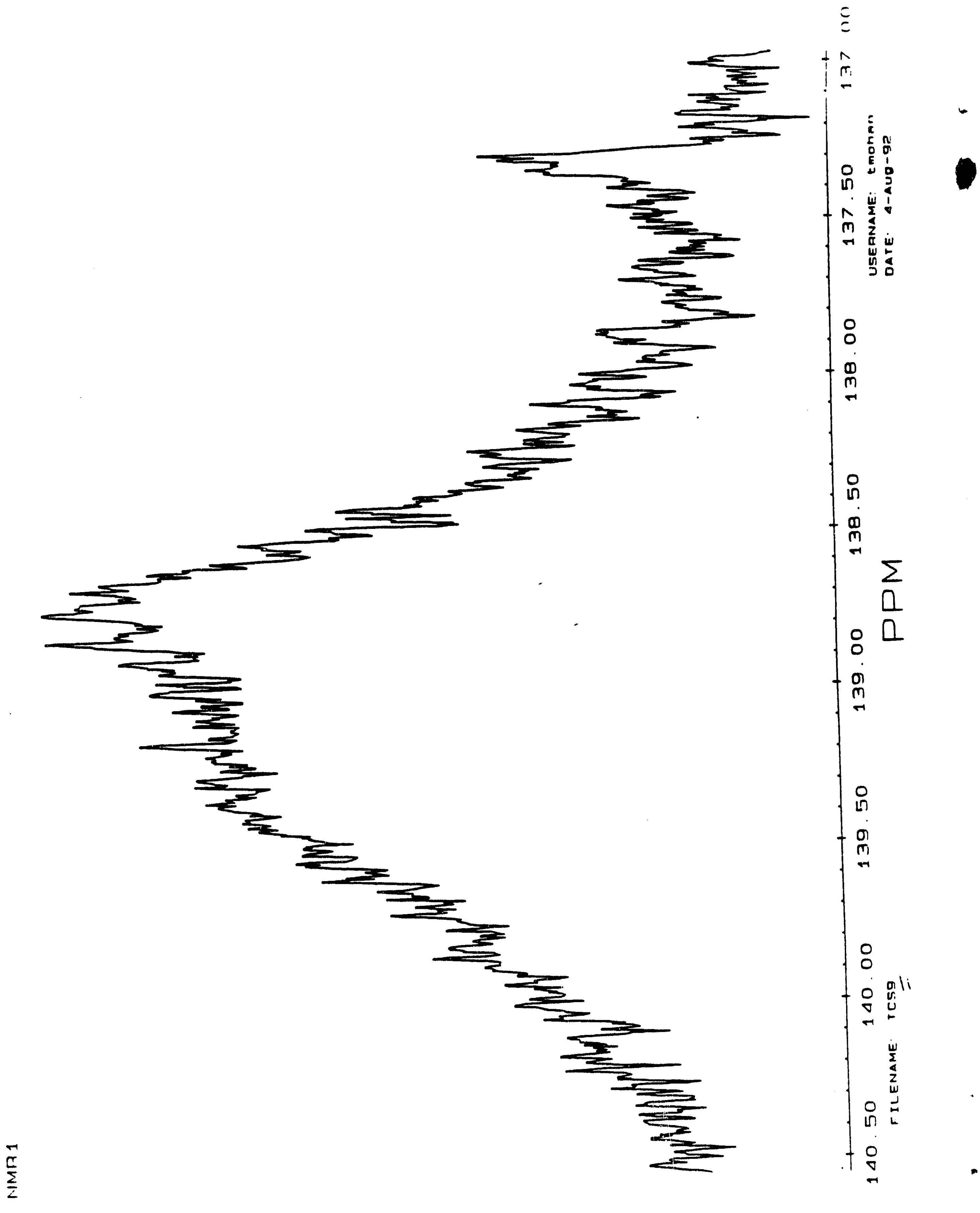
FILENAME: TCSB
NMR1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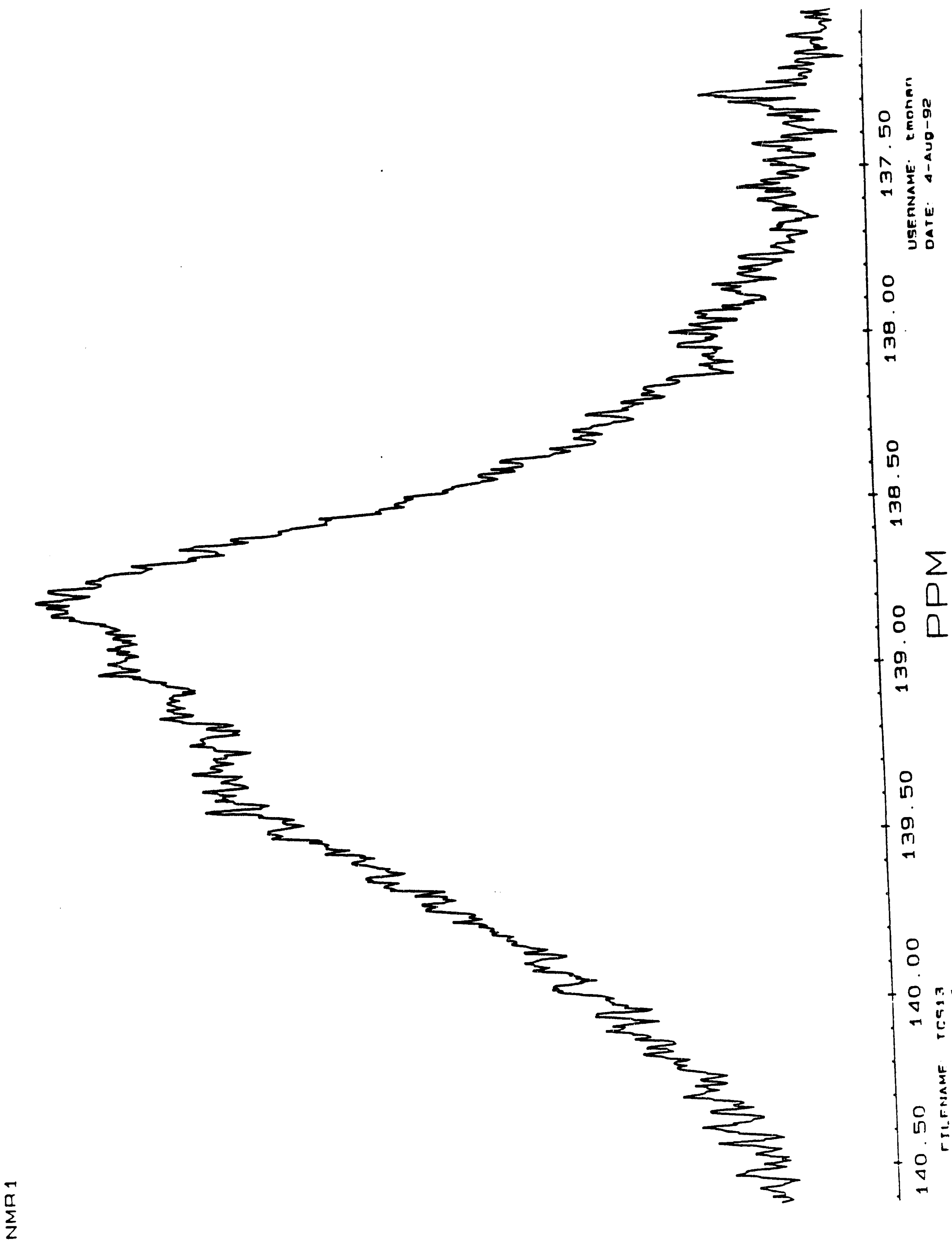
DATE: 4-AUG-92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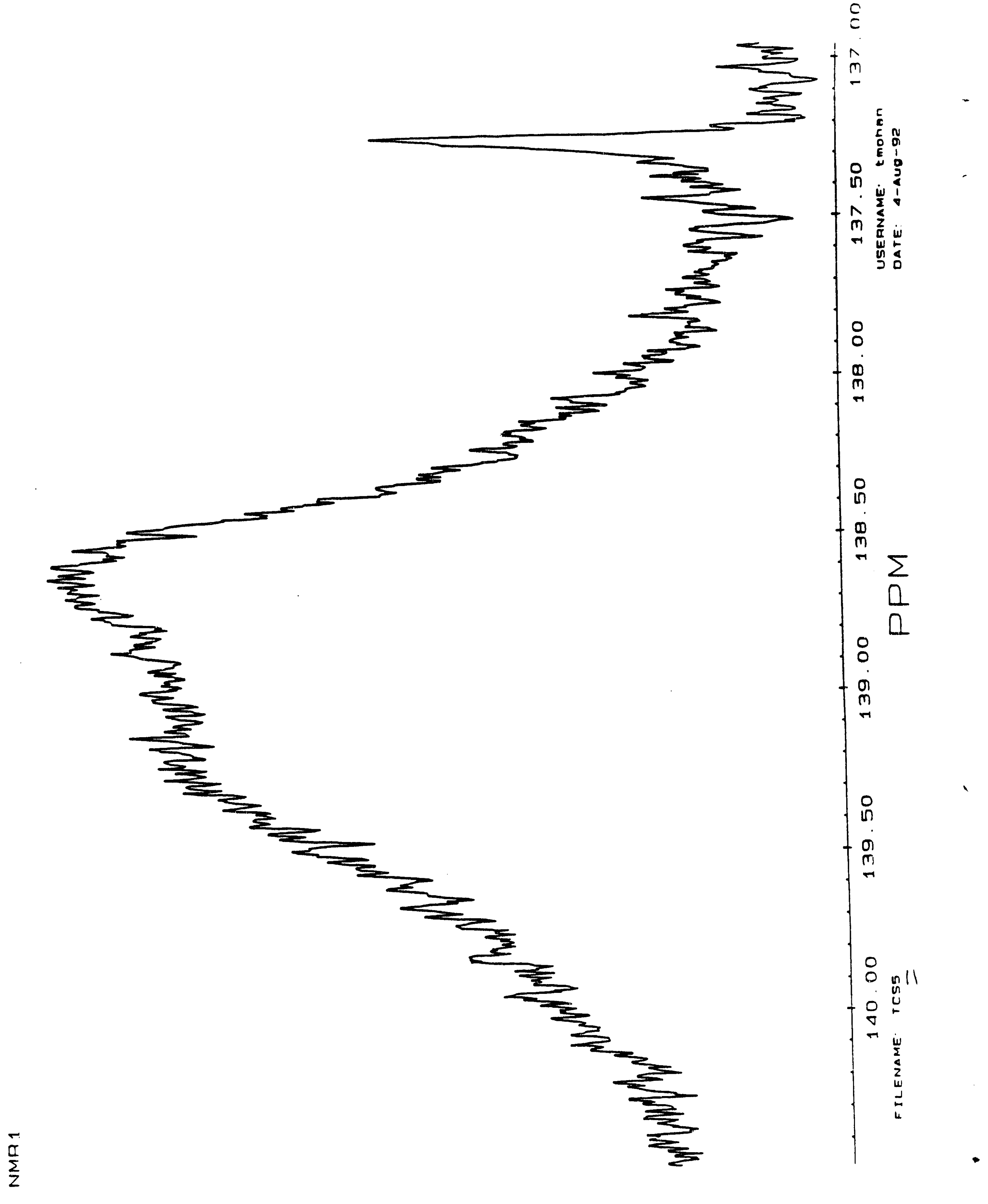
DATE: 4-Aug-92
FILENAME:
NMR1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139.00
139.50
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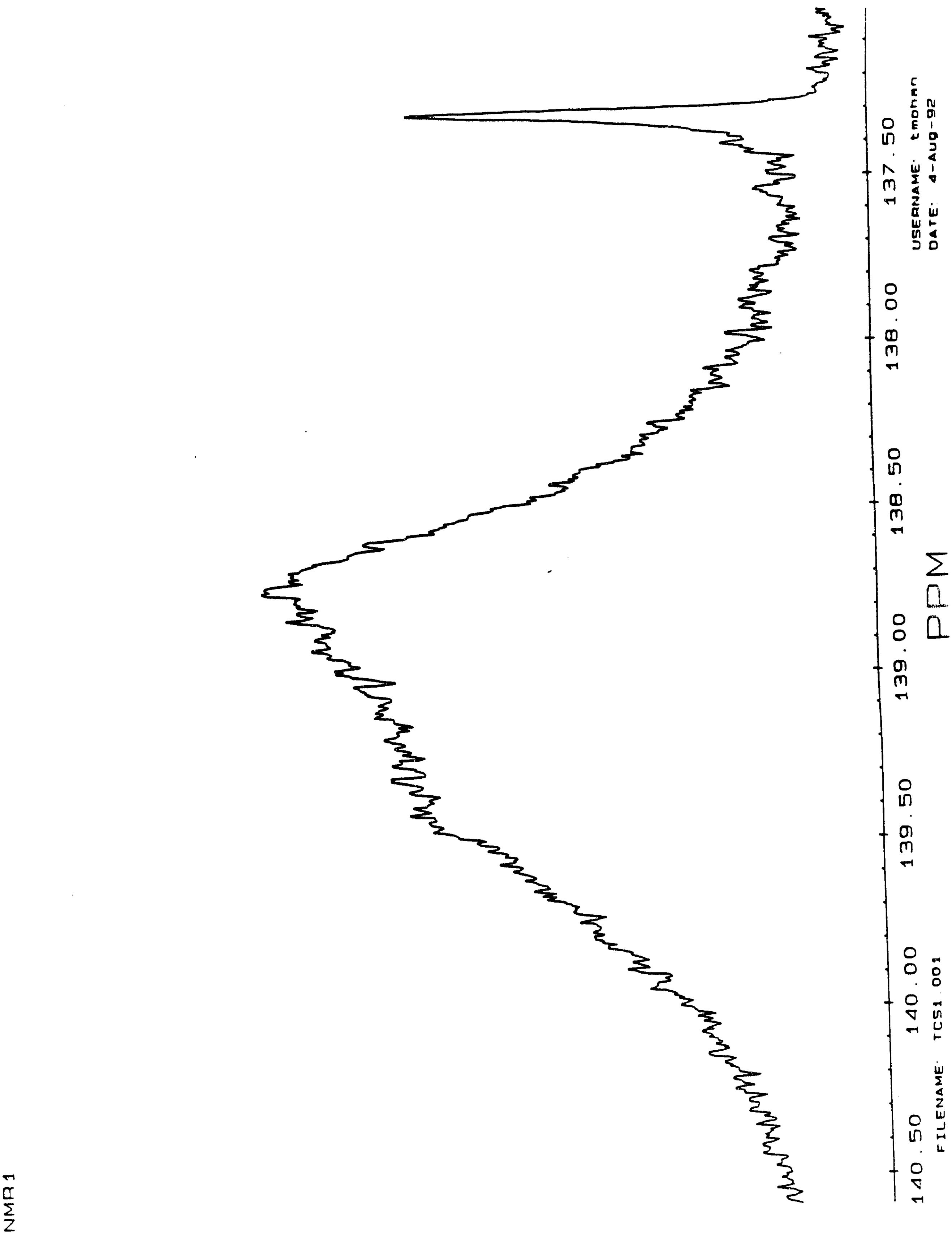
DATE: 4-Aug-92
FILENAME: TCS5
NMR1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PPM
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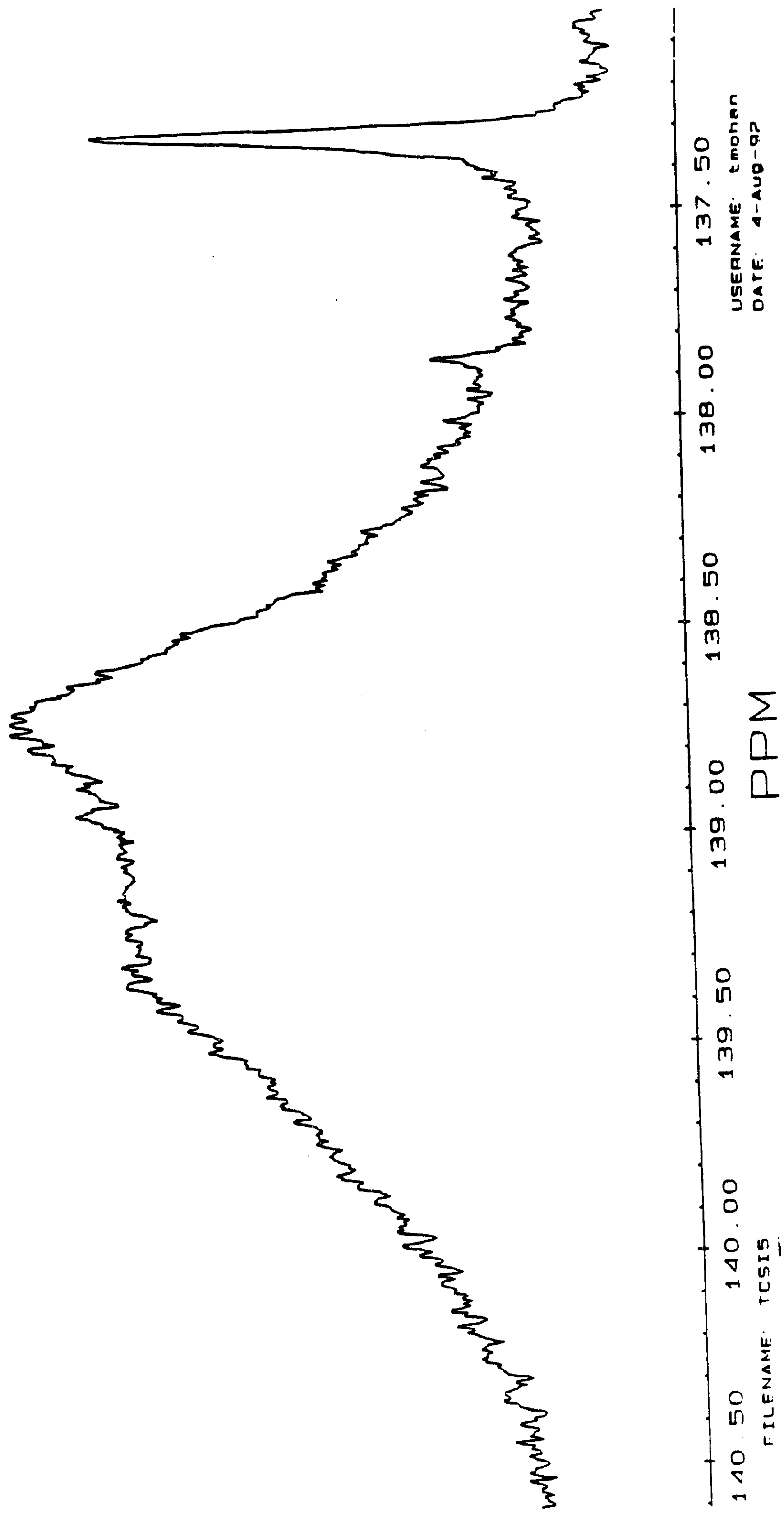
DATE: 4-AUG-92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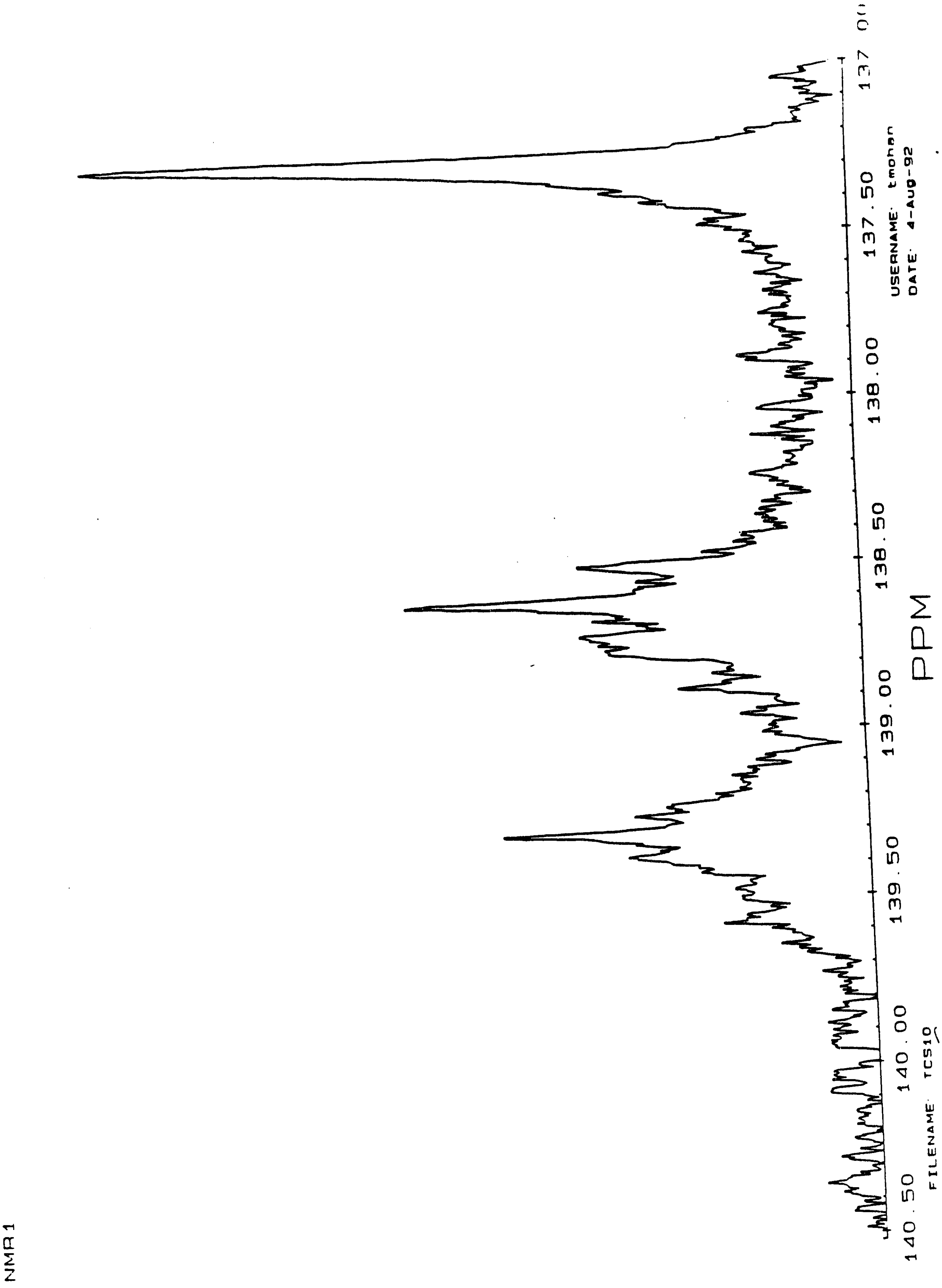
DATE: 4-Aug-97
FILENAME: TCSIS

NMR1



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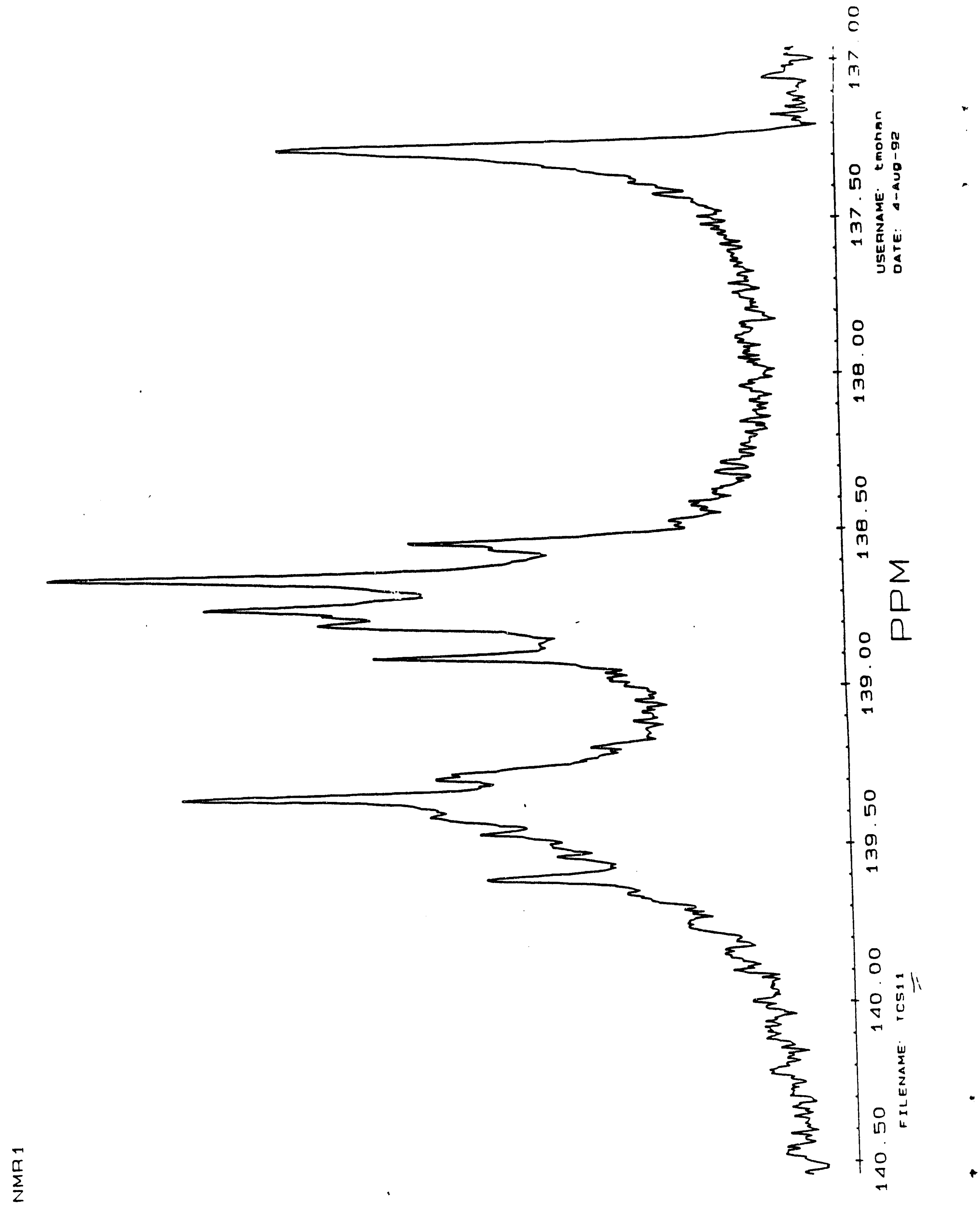
137.50
137.00
PPM


NMR1
PPM
140.50
140.00
139.50
139.00
138.50
138.00
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137.00
FILENAME: TCS11
USERNAME: tmohan
DATE: 4-AUG-92

END

DATE FILMED

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