Chemical Shift Ranges in Carbon-13 NMR Spectroscopy

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of Reference Material

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Preface

Nearly three years have passed since the initial publication of *Carbon-13 NMR Spectral Data.* This work is now in its 3rd edition and comprises 30 000 spectra of 23 450 compounds. The novel approach of presenting data and indexes on microfiche has been well accepted. The introduction of spherical substructure codes (HOSE) for the first time allows one to search for structural units without using a computer, thus permitting fast access to the desired spectral parameters. Of particular interest in this context is the correlation of chemical shifts with structures. A file listing expectation ranges of chemical shifts as functions of partial structures provides a means of predicting the positions of the ^{13}C NMR signals of almost any given structure. This tool proved to be the most frequently used component of the BASF CNMR Information System.

In the light of this we felt that a printed version of this file should be made available so that fellow spectroscopists should be able to gain from our experience. For the sake of handiness it was decided to publish the data on paper rather than in microform. With some experience the reader will soon realize the usefulness of these tables for the evaluation of chemical shift data and for the interpretation of ^{13}C NMR spectra. Comparison of adjacent entries will show subtle differences between similar substructures and provide an intuitive understanding of the influence of structural changes on chemical shifts. Numerous misassignments in the literature could have been avoided had authors been in a position to consult these tables.

Users of this book should feel free to notify the authors, if they happen to detect errors in the data or their presentation. In this way they would help improve the quality of the data bank for future editions.

Ludwigshafen, in January 1982

W. Bremser
B. Franke
H. Wagner

Introduction

1 General Remarks

More than three years have passed since the initial publication of *Carbon-13 NMR Spectral Data*. This work is now in its 3rd edition [1] and comprises 30 000 spectra of 23 450 compounds. As the 34 000 pages of computer printout contained in this collection can no longer be accomodated by conventional printing, the novel approach of presenting data and indexes on microfiche had to be used and has been well received. The introduction of spherical substructure codes (HOSE) for the first time allowed one to search for structural units without using a computer, thus permitting fast access to the desired spectral parameters.

Of particular interest in this connection is the correlation of chemical shift data with structures. A file listing expectation ranges of chemical shifts as functions of partial structures provides a means of predicting the positions of the signals in the ^{13}C NMR spectrum of almost any given structure [2]. This tool proved to be the most frequently used component of the BASF CNMR Information System [3, 4]. In the light of this we felt that a printed version of this file should be made available so that our colleagues in other laboratories may gain from our experience. For convenience it was decided to publish the correlation tables in bookform rather than on microfiche, as this will facilitate their use on the laboratory desk or at the spectrometer where a microfiche reader may not always be available or convenient. It is strongly recommended that the original reference data on microfiche be consulted in critical cases, a procedure necessitating simultaneous use of microfilm projection and scanning of the present tables.

After some experience, and with the necessary knowledge of the priority rules, the reader will soon realize the usefulness of these tables for the evaluation of chemical shift data and for the interpretation of ^{13}C NMR spectra. Comparison of adjacent entries will show subtle differences between similar substructures and provide an intuitive understanding of the influence of structural changes on chemical shifts. If authors had been in a position to consult these tables previously we believe that numerous misassignments in the literature might have been avoided.

As the tables form an integral part of the collection of *Carbon-13 NMR Spectral Data,* however, erroneous spectra, structures, or misassignments in the primary material will occur also in the index listing. If the conscious user of this book detects errors in the data or their presentation, he should feel free to notify the authors. In this way he would help to improve the quality of the data bank in future editions.

The introduction to the microfiche collection is reprinted as an Appendix to these tables.

2 How to Use this Book

The tables in this book list the expectation ranges of Carbon-13 chemical shifts for carbon atoms with defined environment. The material has been prepared from about 240 000 chemical shifts corresponding to 100 000 different substructure codes, thus giving a fairly representative and complete picture for typical organic molecules. It can serve either to predict (or better to estimate) the chemical shifts of a compound on the basis of its structure, a procedure necessary to verify a trial structure postulated from an experimental spectrum in the process of structure elucidation [4]. The user will gain an idea of the sensitivity of chemical shifts to steric or electronic interactions from a comparison of adjacent entries in the tables. Unexpected deviations in this hierarchical presentation can reveal hitherto unobserved structural effects in the molecule.

The first entry in the table is the substructure HOSE code ("**H**ierarchically **O**rdered **S**pherical Description of **E**nvironment"). All chemical shift values are arranged in decreasing numerical value of the code. Thus the reader must be acquainted with this novel structure

representation before consulting the tables. The practical hints in Section 7 "How to generate a HOSE code" (p. XIV) and in Chapter 4 of the Appendix (p. 859 ff.) should be studied carefully. After some practice the user will be able to generate his own codes for various structural elements with the help of the fold-out table at the end of the book, and thus be able to scan the tables observing the priority rules of the different alphanumeric characters. He will then find the desired average chemical shift and standard deviation together with the number of entries and maximum/minimum values observed (see following sections for further details). Allthough all chemical shifts are reported relative to TMS, some have been converted from the original reference using standard procedures as described in Chapter 5.9 of the Appendix.

If the desired entry is not found the structural element may not be contained in the data collection. In this case comparison with neighbouring HOSE codes and the corresponding shift ranges will help to locate the most suitable reference value. It will, at the same time, allow an estimate of the accuracy of this interpolation. Initially it is recommended that these related substructures corresponding to the selected codes be drawn out. It is also possible that the assigned HOSE code may be incomplete or not hierarchical. This again can be best tested by consulting the adjacent entries or the HOSE code index on microfiches 231–242 [1]. As usual the beginner should start with easy examples where he is sure to find an entry, and then progress on to real problems.

3 Why Two Substructure Indexes?

The alert reader will realize that the tables in this book actually represent a substructure index comparable to the HOSE-index on comfiches 231 to 242 in the data collection. The only change is that spectrum and atom number in that section (cf. Fig. 17 in the Appendix) have been replaced by the corresponding shift values. For multiple entries average values and standard deviations have been calculated. However, there are some minor differences which should be specifically stated:

The material presented in the tables of this book is based on the entries in the 3rd edition of the microfiche collection with an additional 2 100 spectra of over 2 000 compounds from unpublished internal BASF references not yet described in the literature. The latter were omitted in the HOSE code index, but contribute to the expectation ranges of chemical shifts in this book. The HOSE code index also contains entries for carbon atoms for which chemical shifts were not reported in the literature. These are marked in the printout of the spectral parameters in the reference section by "N.R." ("Not reported"). Apart from these exceptions the substructure codes entered in both indexes should be congruent. Thus the user should consult the microfiche indexes when a desired HOSE code cannot be located, or when a surprising deviation from the regularity of shift ranges is encountered. This may help detect errors in code generation or in the material of the original data collection.

Both indexes are arranged according to the numerical value of the HOSE code, as described in Chapters 4 and 6.10 of the Appendix. As the spectroscopist is not normally interested in the identification of a particular reference compound with the desired substructure, but directly in the spectral parameters associated with the structural element the reference number has been replaced by the corresponding chemical shift value. If daughter references were available, more than one shift had to be considered, thus a mean value and a standard deviation have been calculated. In addition, the number of shifts contributing is listed as well as the total range covered by the individual values.

4 Large Deviations

In some cases the standard errors or deviations between adjacent entries are relatively high. These might result from errors in the data base which we have tried to minimize with the help of the correction routines described in Section 6. However, this spread of the shift values may also arise as a consequence of long range effects and steric interactions not accounted for by the HOSE code, or from the influence of the experimental conditions (solvent, temperature, pH, etc.). Thus it is desirable that the extreme values be eliminated if more than 3 values are available. The following procedure was adopted to give the modified mean and standard deviation values listed in parentheses:

Every sixth line out of N lines ($N \geq 4$) was eliminated. The exact number, NE, was calculated by the equation $NE = (N+2)/6$. Initially, NE/2 lines were suppressed at both high and low field and then, if NE was odd, the line with the largest deviation from the mean was deleted.

5 Why Double Entries?

The topological representation of chemical structures does not accomodate stereochemical features of the molecule, i. e. configuration or conformation (cf. Chapter 4.1 of the Appendix). The index of chemical shift ranges would therefore list only one average value for cis-trans, exo-endo, syn-anti, alpha-beta, erythro-threo, etc. isomers. The influence of steric interactions on chemical shifts, however, is well known and an important tool in structure elucidation. Thus if the standard deviation, SE, is larger than a predefined limit ($SE \geqslant 2$ ppm for 6 to 9 values, $SE \geqslant 1$ ppm for 10 and more values), provision has been made for the possibility of more than one maximum in the Gaussian distribution. The following simplified technique for detecting two maxima was applied:

We assumed that the sum of the standard deviations of the two subgroups must be considerably lower (at least 33 %) than the original standard deviation. We then defined the smallest and the largest chemical shifts as starting values for the mean values and assigned all remaining values to the nearest group. The mean values of these groups were then calculated and used as the starting values for the next cycle in which all chemical shifts were reassigned to the nearest mean value. This procedure was continued until the new mean values did not differ from the preceding ones. If the resulting partial standard deviations SE_1 and SE_2 fulfill the condition

$$1.5\ (SE_1 + SE_2) < SE$$

it can be assumed that the chemical shifts are grouped around two maxima and two separate shift ranges are entered under the same HOSE code. The ratio of the residual and original standard deviation values (SE_1/SE) is listed at the end of each line (expressed as %).

The two methyl groups in a 2-methyl-2-pentene fragment exemplify the application of these double entries. If we search the index for the HOSE code

C(=CC/C,/C)

we find two entries with about 150 values each grouped around the chemical shift values of 25.6 and 17.6 ppm. With some basic spectroscopic knowledge the high field resonance may be assigned to the cisoid and the low field to the transoid methyl group. In doubtful cases the original data in the collection should be consulted.

6 An Ideal Test for Errors

The process of sorting inverted index files provides an ideal opportunity for detecting inconsistencies in the data bank. The deviation of individual values from the mean should not be greater than a certain predefined limit. Likewise, differences between neighbouring entries in the index should be relatively small for those cases in which the only changes occur in outer spheres; this results in them being arranged together in the hierarchical ordering scheme. Finally, the difference between the means of the two subgroups of double entries must not exceed the well known value of 10 ppm associated with steric interactions. Whenever one of these three limits is surpassed, an error message is printed and the corresponding reference compound has to be inspected for possible errors. In most cases these can be corrected by either changing the shift values, the structure or the assignment. From time to time, however, dubious spectral data are encountered which are a result of undefined sources such as printing errors or misinterpretations. In these cases the data were omitted from the index and marked accordingly in the microfiche collection.

7 How to Generate a HOSE code

This section contains some practical hints based on experience gained in routine work with HOSE indexes. They should serve as a guideline for the beginner:

(1) Study the explanations in Chapters 4.3, 4.4 and 6.10 of the Appendix, especially Table 1 (p. 863 and fold-out page at the end of the book) and the two examples discussed there.

(2) Open the fold-out table at the end of the book for direct reference and start with some easy examples first, e.g. long chains, simple rings, many heteroatoms and multiple bonds, preferably with no symmetry.

(3) It is recommended that one chooses a structure that is known to be present in the data base. Try your hand at common substituents, like ethyl, nitro, benzyl, etc.

(4) Initially you should number the substituents sequentially as exemplified in Fig. 9 of the Appendix. Otherwise you will often forget important substituents.

(5) When scanning the index entries remember the hierarchical sequence of alphanumeric characters as defined by the HOSE system:

% = * C O N S P Q F X Y I 'MM' & + − > D , /

Less common elements 'MM' are arranged with decreasing atomic number.

(6) Try to adopt an interactive procedure of coding and finding the code fragment in the index. This will show whether your code is canonical or not. Normally, if you lose your way in the second sphere, there is an error in the hierarchical sequence. Consult the neighbouring structure to detect differences and locate the error.

(7) Interactive correspondence with the index entries will also save you completing the code when no suitable compounds are in the data collection. In these cases you should consult the preceding and/or following entries to make sure that they are similar and that your code was correct.

(8) When you have problems it will often help to look up the adjacent entries in the HOSE index on microfiches 231–242 and the corresponding reference structure in the data section of *Carbon-13 NMR Spectral Data*. Detect the differences in substitution and test whether you have violated the priority rules or forgotten to code a substituent.

(9) Drawing the substructure corresponding to these adjacent codes often gives you additional hints on possible errors; in any case these provide good practice for becoming acquainted with the principle of the coding system and its limitations.

(10) If substituents are undefined you can code them with a "?". Keep in mind that ?=C has a different priority than ?=N or ?=Mn.

8 Literature

[1] W. Bremser, L. Ernst, B. Franke, R. Gerhards and A. Hardt, "Carbon-13 NMR Spectral Data", 3rd Ed., Verlag Chemie, Weinheim (1981)

[2] W. Bremser, Anal. Chim. Acta **103**, 335 (1978)

[3] W. Bremser, Z. Anal. Chem. **286**, 1 (1977)

[4] W. Bremser, Chem. Ztg. **104**, 53 (1980)

It is recommended that the detailed literature in Chapter 8 of the Appendix be consulted for further references (p. 889).

Tables of Substructures and Chemical Shift Ranges

Contents

Introduction

HOSE - CODE	RANGE 1	RANGE 2	NO.	MAX.	MIN.	
%CC'+'(C'+',*C*C/*C*C,*C*C,*C	126.6 # 0. PPM		2 LINES	(126.6 -	126.6 PPM)	
%CC'+'(C,*C*C/*C*C,*C,*C/*C*C,*C	159.1 # 0. PPM		1 LINES	(159.1 -	159.1 PPM)	
%CC'+'(C,*C*C/*CC,*C,*C/*C*C,,	167.5 # 0. PPM		1 LINES	(167.5 -	167.5 PPM)	
%CC'+'(C,/*C*C/*C*C,*C*C)	165.1 # 0. PPM		1 LINES	(165.1 -	165.1 PPM)	
%CC+(C,*C*C/=O&,*C,*C/,*C,*	134.2 # 0. PPM		1 LINES	(134.2 -	134.2 PPM)	
%CC+(C,*C*C/CC&,*C,*C/,,*C,	199.4 # 0. PPM		1 LINES	(199.4 -	199.4 PPM)	
%CC+(C,/=O&/)	130.8 # 0. PPM		1 LINES	(130.8 -	130.8 PPM)	
%CC+(C,/CC&/,)	219.1 # 0. PPM		1 LINES	(219.1 -	219.1 PPM)	
%CC)'W'(C,C,'++)C)C	160.8 # 2.0 PPM		2 LINES	(162.2 -	159.4 PPM)	
%CC)'W'(C,,'++)C)C:	160.4 # 0. PPM		2 LINES	(160.4 -	160.4 PPM)	0 %
	142.6 # 1.4 PPM	(142.0 # 0.4 PPM)	4 LINES	(144.8 -	141.5 PPM)	5 %
%CC)'MO')'MO'(C,,+)C	82.6 # 0. PPM		2 LINES	(82.6 -	82.6 PPM)	
%CC)'MO'(C,,0+)C)C:	172.1 # 3.9 PPM	(173.2 # 3.9 PPM)	4 LINES	(175.5 -	168.7 PPM)	
%CC)'MO'(C,,'++)C)C:	180.3 # 0. PPM		2 LINES	(180.3 -	180.3 PPM)	0 %
	162.1 # 2.0 PPM	(162.7 # 2.0 PPM)	4 LINES	(163.8 -	160.4 PPM)	24 %
%CC(C'+',*C*C/*C*C,*C*C,*C*C/*C,	105.9 # 0. PPM		1 LINES	(105.9 -	105.9 PPM)	
%CC(C'+',*C*C/,*C*C,*C*C/*C,*C,	93.2 # 0. PPM		1 LINES	(93.2 -	93.2 PPM)	
%CC(C'+',*CC/*C*C,*C*C,/*C,*C,	111.1 # 0. PPM		1 LINES	(111.1 -	111.1 PPM)	
%CC(C+,=O&/*C*C,/*C,*C)	56.9 # 0. PPM		1 LINES	(56.9 -	56.9 PPM)	
%CC(C+,=O&/,/)	45.9 # 0. PPM		1 LINES	(45.9 -	45.9 PPM)	
%CC(C+,CC&/*C*C,,/*C,*C)	123.5 # 0. PPM		1 LINES	(123.5 -	123.5 PPM)	
%CC(C+,CC&/,,/)	110.6 # 0. PPM		1 LINES	(110.6 -	110.6 PPM)	
%CC(C)'MO',/,'++)C)C	144.7 # 0. PPM		2 LINES	(144.7 -	144.7 PPM)	
%CC(C,%C/%C,C/C,%C)	62.0 # 0.2 PPM	(61.9 # 0.1 PPM)	6 LINES	(62.2 -	61.8 PPM)	
%CC(C,%C/%C,C/C,=C)	59.1 # 0. PPM		1 LINES	(59.1 -	59.1 PPM)	
%CC(C,%C/%C,C/C,=OC)	59.2 # 0. PPM		1 LINES	(59.2 -	59.2 PPM)	
%CC(C,%C/%C,C/C,CCC)	63.9 # 3.2 PPM	(62.8 # 0.8 PPM)	7 LINES	(71.0 -	62.2 PPM)	
%CC(C,%C/%C,C/C,CO)	60.6 # 0. PPM		1 LINES	(60.6 -	60.6 PPM)	
%CC(C,%C/%C,C/C,O)	61.9 # 1.4 PPM		3 LINES	(62.8 -	60.3 PPM)	
%CC(C,%C/%C,C/C,)	64.1 # 7.1 PPM		3 LINES	(72.3 -	60.0 PPM)	
%CC(C,%C/=C,C/CO,)	77.6 # 1.1 PPM	(77.1 # 0.6 PPM)	4 LINES	(79.0 -	76.4 PPM)	
%CC(C,%C/=C,C/C,%C)	85.9 # 0. PPM		1 LINES	(85.9 -	85.9 PPM)	
%CC(C,%C/=C,C/C,C)	86.7 # 0. PPM		1 LINES	(86.7 -	86.7 PPM)	
%CC(C,%C/=OC,C/,*C*C,CCC)	78.5 # 0. PPM		1 LINES	(78.5 -	78.5 PPM)	
%CC(C,%C/=OC,C/,CCC,%C)	77.0 # 0. PPM		1 LINES	(77.0 -	77.0 PPM)	
%CC(C,%C/=OC,C/,CCC,CCC)	77.3 # 0. PPM		1 LINES	(77.3 -	77.3 PPM)	
%CC(C,%C/=O,C/,O)	78.1 # 0.4 PPM		2 LINES	(78.3 -	77.8 PPM)	
%CC(C,%C/*C*C,C/*C,*C,*C*C)	74.1 # 0.1 PPM	(74.1 # 0.1 PPM)	4 LINES	(74.1 -	74.0 PPM)	
%CC(C,%C/*C*C,C/*C,*C,O)	70.2 # 0. PPM		1 LINES	(70.2 -	70.2 PPM)	
%CC(C,%C/CCC,C/,,,%C)	65.4 # 2.3 PPM	(64.5 # 0.2 PPM)	7 LINES	(70.7 -	64.1 PPM)	
%CC(C,%C/CCC,C/,,,=OC)	63.1 # 0.4 PPM		2 LINES	(63.3 -	62.8 PPM)	
%CC(C,%C/CCC,C/,,,CO)	63.6 # 0.1 PPM		2 LINES	(63.7 -	63.5 PPM)	
%CC(C,%C/CCO,C/CC,,,CCO,)	68.2 # 0. PPM		2 LINES	(68.2 -	68.2 PPM)	
%CC(C,%C/CCO,C/C,C,,CCO,)	68.2 # 0. PPM		2 LINES	(68.2 -	68.2 PPM)	
%CC(C,%C/CCO,C/C,,,CCO,)	68.0 # 0.7 PPM	(67.8 # 0.6 PPM)	6 LINES	(68.9 -	67.6 PPM)	
%CC(C,%C/CCO,C/,,,CCO)	66.2 # 0. PPM		2 LINES	(66.2 -	66.2 PPM)	
%CC(C,%C/CO,C/=C,,CO)	69.3 # 0. PPM		2 LINES	(69.3 -	69.3 PPM)	
%CC(C,%C/CO,C/*C*C,,CCC)	71.7 # 0. PPM		1 LINES	(71.7 -	71.7 PPM)	
%CC(C,%C/CO,C/*C*C,,CO)	69.9 # 0. PPM		2 LINES	(69.9 -	69.9 PPM)	
%CC(C,%C/CO,C/CCC,,%C)	70.7 # 0. PPM		1 LINES	(70.7 -	70.7 PPM)	
%CC(C,%C/CO,C/CCC,,CCC)	70.7 # 0. PPM		1 LINES	(70.7 -	70.7 PPM)	
%CC(C,%C/CO,C/C,,C)	69.9 # 0.1 PPM		2 LINES	(70.0 -	69.9 PPM)	
%CC(C,%C/CO,C/,,CO)	67.8 # 0. PPM		2 LINES	(67.8 -	67.8 PPM)	
%CC(C,%C/CO,C/,,C)	68.9 # 0. PPM		1 LINES	(68.9 -	68.9 PPM)	
%CC(C,%C/C,C/CO,C)	67.8 # 0. PPM		2 LINES	(67.8 -	67.8 PPM)	
%CC(C,%C/C,C/C,=C)	65.3 # 0. PPM		1 LINES	(65.3 -	65.3 PPM)	
%CC(C,%C/C,C/C,CO)	64.6 # 0.1 PPM		3 LINES	(64.7 -	64.5 PPM)	
%CC(C,%C/C,C/C,C)	67.1 # 2.6 PPM	(66.6 # 0.9 PPM)	38 LINES	(77.4 -	65.1 PPM)	
%CC(C,%C/C,C/C,O)	64.7 # 0. PPM		1 LINES	(64.7 -	64.7 PPM)	
%CC(C,%C/C,C/O,C)	66.5 # 0. PPM		2 LINES	(66.5 -	66.5 PPM)	
%CC(C,%C/C,C/,C)	64.9 # 0.6 PPM	(65.0 # 0.6 PPM)	4 LINES	(65.4 -	64.3 PPM)	
%CC(C,%C/O,C/C,%C)	70.8 # 0. PPM		1 LINES	(70.8 -	70.8 PPM)	
%CC(C,%C/O,C/C,=O)	68.8 # 0.4 PPM		2 LINES	(69.0 -	68.5 PPM)	
%CC(C,%C/O,C/C,O)	70.0 # 0.4 PPM	(69.9 # 0.1 PPM)	6 LINES	(70.7 -	69.8 PPM)	
%CC(C,%C/O,C/,%C)	70.4 # 0.4 PPM		2 LINES	(70.7 -	70.1 PPM)	
%CC(C,%C/O,C/,*C*C)	73.5 # 0. PPM		1 LINES	(73.5 -	73.5 PPM)	
%CC(C,%C/O,C/,C)	70.5 # 0. PPM		1 LINES	(70.5 -	70.5 PPM)	
%CC(C,%C/O,C/,O)	69.2 # 0.2 PPM	(69.3 # 0. PPM)	4 LINES	(69.3 -	69.0 PPM)	
%CC(C,%C/O,/)	69.7 # 0. PPM		2 LINES	(69.7 -	69.7 PPM)	
%CC(C,%C/N,C/CC,N)	69.7 # 0. PPM		2 LINES	(69.7 -	69.7 PPM)	
%CC(C,%C/,C/%C)	65.1 # 0.1 PPM		3 LINES	(65.2 -	65.0 PPM)	
%CC(C,%C/,C/=C)	65.0 # 0.4 PPM	(64.8 # 0.3 PPM)	4 LINES	(65.4 -	64.6 PPM)	
%CC(C,%C/,C/)	64.8 # 0. PPM		2 LINES	(64.8 -	64.8 PPM)	
%CC(C,=CC/=CC,CC,CCC/C,,C	95.3 # 2.9 PPM	(94.3 # 1.6 PPM)	6 LINES	(100.3 -	92.2 PPM)	
%CC(C,=CC/=CC,C,CCC/C,,C:	94.1 # 0. PPM		1 LINES	(94.1 -	94.1 PPM)	
%CC(C,=CC/=CC,C,/CC,CCC,=	95.8 # 4.1 PPM	(93.9 # 1.9 PPM)	4 LINES	(101.6 -	92.5 PPM)	
%CC(C,=CC/=CC,C,/CC,CCC,*C	96.8 # 0. PPM		1 LINES	(96.8 -	96.8 PPM)	
%CC(C,=CC/=CC,C,/CC,CCC,;	86.7 # 0. PPM		1 LINES	(86.7 -	86.7 PPM)	
%CC(C,=CC/=CC,C,/C,CCC,=C	92.8 # 0. PPM		1 LINES	(92.8 -	92.8 PPM)	
%CC(C,=CC/,C,/=C)	78.6 # 0. PPM		1 LINES	(78.6 -	78.6 PPM)	
%CC(C,=CS/=CS,C,C/C,C,	86.4 # 0.4 PPM		2 LINES	(86.7 -	86.1 PPM)	
%CC(C,=CS/=C,C,C/,=&,=&	83.6 # 0. PPM		1 LINES	(83.6 -	83.6 PPM)	
%CC(C,=CS/OO,C,C/C,C,	79.0 # 0. PPM		1 LINES	(79.0 -	79.0 PPM)	
%CC(C,=CS/O,C,C/C,=&,*C	80.0 # 0. PPM		1 LINES	(80.0 -	80.0 PPM)	
%CC(C,=CS/,C,C/=&,=&C)	72.9 # 0. PPM		1 LINES	(72.9 -	72.9 PPM)	
%CC(C,=C/%C,CO/C,=C,C)	70.9 # 0.6 PPM		3 LINES	(71.4 -	70.2 PPM)	
%CC(C,=C/%C,CO/C,CO,C)	68.5 # 0. PPM		1 LINES	(68.5 -	68.5 PPM)	
%CC(C,=C/%C,C/C,=OO)	71.4 # 0.6 PPM		2 LINES	(71.8 -	71.0 PPM)	
%CC(C,=C/=CS,/C,C)	93.2 # 0. PPM		1 LINES	(93.2 -	93.2 PPM)	
%CC(C,=C/=C,CC/CC,=C,)	99.0 # 2.7 PPM	(98.4 # 0.7 PPM)	12 LINES	(107.2 -	96.9 PPM)	
%CC(C,=C/=C,CC/CC,=O,)	93.4 # 1.1 PPM		2 LINES	(94.2 -	92.6 PPM)	
%CC(C,=C/=C,C/C,&)	116.3 # 0. PPM		2 LINES	(116.3 -	116.3 PPM)	
%CC(C,=C/CCC,C/,,,=C)	78.1 # 0.1 PPM		2 LINES	(78.2 -	78.1 PPM)	
%CC(C,=C/CCN,C/,,,CCN)	97.8 # 0. PPM		1 LINES	(97.8 -	97.8 PPM)	
%CC(C,=C/C,C/C,C)	78.6 # 0. PPM		1 LINES	(78.6 -	78.6 PPM)	
%CC(C,=C/C,C/C,&)	94.5 # 0. PPM		1 LINES	(94.5 -	94.5 PPM)	
%CC(C,=C/,O/C)	74.4 # 0. PPM		1 LINES	(74.4 -	74.4 PPM)	
%CC(C,=OC/%C,,*C*C/C,*C,*C)	70.8 # 0. PPM		1 LINES	(70.8 -	70.8 PPM)	
%CC(C,=OC/%C,,CCC/C,,,)	71.6 # 0.8 PPM		2 LINES	(72.1 -	71.0 PPM)	
%CC(C,=OC/*C*C,,CC/*C,*C,CC,	54.4 # 0. PPM		1 LINES	(54.4 -	54.4 PPM)	
%CC(C,=OC/*C*C,,/*C,*C)	88.0 # 0. PPM		1 LINES	(88.0 -	88.0 PPM)	
%CC(C,=OO/=OO,,C/,C,C)	74.7 # 0. PPM		2 LINES	(74.7 -	74.7 PPM)	
%CC(C,=OO/=OO,,/,)	75.6 # 0. PPM		2 LINES	(75.6 -	75.6 PPM)	
%CC(C,=OO/*C*C,,C/*C,*C,C)	80.9 # 0. PPM		1 LINES	(80.9 -	80.9 PPM)	
%CC(C,=OO/*C*C,,/*C,*C)	81.3 # 0. PPM		1 LINES	(81.3 -	81.3 PPM)	

%CC(C,=OO/CO,,C/CO,C,	78.5 # 0.8 PPM	(78.1 # 0.3 PPM)	4 LINES (79.7 - 77.9 PPM)
%CC(C,=OO/CO,,C/CO,,)	77.1 # 0. PPM		1 LINES (77.1 - 77.1 PPM)
%CC(C,=ON/*C*C,,/*C,*C)	82.0 # 0. PPM		1 LINES (82.0 - 82.0 PPM)
%CC(C,=OF/*C*C,,/*C,*C)	83.8 # 0. PPM		1 LINES (83.8 - 83.8 PPM)
%CC(C,=OF/,,/)	67.4 # 0. PPM		1 LINES (67.4 - 67.4 PPM)
%CC(C,=O/%C,/C)	75.1 # 0.3 PPM		2 LINES (75.3 - 74.9 PPM)
%CC(C,=O/*C*C,/*C,*C)	87.6 # 0. PPM		1 LINES (87.6 - 87.6 PPM)
%CC(C,*C*C/%C,*C,*C/C,*C,*&)	81.4 # 0.4 PPM	(81.6 # 0.1 PPM)	5 LINES (81.7 - 80.8 PPM)
%CC(C,*C*C/=OC,*C,*C/,CC,*C,*	105.7 # 0. PPM		1 LINES (105.7 - 105.7 PPM)
%CC(C,*C*C/=OC,*C,*C/,,*C,*&)	91.8 # 0. PPM		1 LINES (91.8 - 91.8 PPM)
%CC(C,*C*C/=OO,*C,*C/,C,*C,*	85.3 # 0. PPM		1 LINES (85.3 - 85.3 PPM)
%CC(C,*C*C/=OO,*C,*C/,,*C,*&	85.4 # 0. PPM		1 LINES (85.4 - 85.4 PPM)
%CC(C,*C*C/=ON,*C,*C/,,*C,*&	88.0 # 0. PPM		1 LINES (88.0 - 88.0 PPM)
%CC(C,*C*C/=OF,*C,*C/,,*C,*&	94.9 # 0. PPM		1 LINES (94.9 - 94.9 PPM)
%CC(C,*C*C/=O,*C,*C/,*C,*&)	97.0 # 0. PPM		1 LINES (97.0 - 97.0 PPM)
%CC(C,*C*C/*C*C,*C,*C/*C,*C,*C,*&	89.6 # 0. PPM		2 LINES (89.6 - 89.6 PPM)
%CC(C,*C*C/CCC,*C,*C/=CC,CC&	83.7 # 0.6 PPM	(83.8 # 0.6 PPM)	8 LINES (84.4 - 82.9 PPM)
%CC(C,*C*C/CCC,*C,*C/*C*C,CCC,,)	85.8 # 0. PPM		2 LINES (85.8 - 85.8 PPM)
%CC(C,*C*C/CCO,*C,*C/*C*C,*C*C,,)	86.9 # 0.5 PPM		2 LINES (87.3 - 86.6 PPM)
%CC(C,*C*C/CCO,*C,*C/*C*C,,,*C,)	84.2 # 0. PPM		1 LINES (84.2 - 84.2 PPM)
%CC(C,*C*C/CCO,*C,*C/,,,*C,*&,	82.9 # 0. PPM		1 LINES (82.9 - 82.9 PPM)
%CC(C,*C*C/CO+,*C,*C/,.*C,*	134.0 # 0. PPM		1 LINES (134.0 - 134.0 PPM)
%CC(C,*C*C/CN,*C,*C/=CC,CC,	85.8 # 0. PPM		1 LINES (85.8 - 85.8 PPM)
%CC(C,*C*C/C,*C,*C/C,*C,*&)	89.8 # 0. PPM		1 LINES (89.8 - 89.8 PPM)
%CC(C,*C*C/OO+,*C,*C/C,,*C	109.5 # 0. PPM		1 LINES (109.5 - 109.5 PPM)
%CC(C,*C*C/OO+,*C,*C/,.*C,	112.5 # 0. PPM		1 LINES (112.5 - 112.5 PPM)
%CC(C,*C*C/OO,*C,*C/C,C,*C,	84.7 # 0. PPM		1 LINES (84.7 - 84.7 PPM)
%CC(C,*C*C/ON+,*C,*C/,.*C,	106.4 # 0. PPM		1 LINES (106.4 - 106.4 PPM)
%CC(C,*C*C/O+,*C,*C/,*C,*&)	143.7 # 0. PPM		1 LINES (143.7 - 143.7 PPM)
%CC(C,CCC/%C,,,/C)	88.5 # 4.4 PPM	(88.7 # 1.6 PPM)	11 LINES (96.9 - 78.2 PPM)
%CC(C,CCC/=C,,,/C)	104.4 # 4.3 PPM		2 LINES (107.5 - 101.4 PPM)
%CC(C,CCC/*C*C,=CC,CC&,/*C,	92.9 # 0.8 PPM	(92.7 # 0.8 PPM)	8 LINES (94.0 - 91.8 PPM)
%CC(C,CCC/*C*C,*C*C,CCC,/*C,*C,)	94.1 # 0. PPM		2 LINES (94.1 - 94.1 PPM)
%CC(C,CCC/CCC,=CC,CC&,/,,	80.6 # 0. PPM		2 LINES (80.6 - 80.6 PPM)
%CC(C,CCC/CCC,C,C,C/C,C,C,	87.7 # 0. PPM		2 LINES (87.7 - 87.7 PPM)
%CC(C,CCC/CCC,S,,/&,,,&	108.5 # 0. PPM		2 LINES (108.5 - 108.5 PPM)
%CC(C,CCC/CCC,,,/=CC,CC&,	92.3 # 0. PPM		2 LINES (92.3 - 92.3 PPM)
%CC(C,CCC/,=CC,CC&,/C&,	81.2 # 0. PPM		2 LINES (81.2 - 81.2 PPM)
%CC(C,CCO/%C,CC,,/C,,)	72.3 # 0. PPM		2 LINES (72.3 - 72.3 PPM)
%CC(C,CCO/%C,C,C,/C,C,&,	83.1 # 0. PPM		2 LINES (83.1 - 83.1 PPM)
%CC(C,CCO/%C,C,,/C,)	82.9 # 0.0 PPM	(82.9 # 0.0 PPM)	6 LINES (83.0 - 82.9 PPM)
%CC(C,CCO/%C,,,/C)	84.1 # 0. PPM		2 LINES (84.1 - 84.1 PPM)
%CC(C,CCO/*C*C,*C*C,*C*C,/*C,*C,)	91.6 # 0.2 PPM		2 LINES (91.8 - 91.5 PPM)
%CC(C,CCO/*C*C,*C*C,,/*C,*C,*C,)	92.5 # 0. PPM		1 LINES (92.5 - 92.5 PPM)
%CC(C,CCO/*C*C,,,/*C,*C)	95.4 # 0. PPM		1 LINES (95.4 - 95.4 PPM)
%CC(C,CCO/CCO,C,C,/C,C,)	88.0 # 0. PPM		2 LINES (88.0 - 88.0 PPM)
%CC(C,CCO/CCO,C,,/C,,,CC,)	87.8 # 0. PPM		2 LINES (87.8 - 87.8 PPM)
%CC(C,CCO/CCO,C,,/C,,,C,)	86.9 # 0. PPM		2 LINES (86.9 - 86.9 PPM)
%CC(C,CCO/CCO,C,,/C,,,,)	87.3 # 0. PPM		2 LINES (87.3 - 87.3 PPM)
%CC(C,CCO/CCO,,,/,,)	87.4 # 0. PPM		2 LINES (87.4 - 87.4 PPM)
%CC(C,CCO/CC,*C*C,,/,,*C,*C,)	83.2 # 0. PPM		1 LINES (83.2 - 83.2 PPM)
%CC(C,CCO/CO,CCC,CC,/,C,)	83.5 # 0. PPM		1 LINES (83.5 - 83.5 PPM)
%CC(C,CCO/.*C*C,*C*C,/*C,*C,*C,)	82.3 # 0. PPM		1 LINES (82.3 - 82.3 PPM)
%CC(C,CCO/,,,/)	84.6 # 0. PPM		1 LINES (84.6 - 84.6 PPM)
%CC(C,CCN/=C,,,/C)	77.7 # 0. PPM		1 LINES (77.7 - 77.7 PPM)
%CC(C,CC/CCO,,/*C*C,,)	91.3 # 0. PPM		1 LINES (91.3 - 91.3 PPM)
%CC(C,CC/CC,=C,C/=C,C,C,	83.1 # 0. PPM		1 LINES (83.1 - 83.1 PPM)
%CC(C,CC/CC,=C,C/=C,C,&	82.5 # 0. PPM		1 LINES (82.5 - 82.5 PPM)
%CC(C,CC/CC,C,C/,,C,&)	85.7 # 0. PPM		1 LINES (85.7 - 85.7 PPM)
%CC(C,CC/CC,,/C,C)	83.4 # 0. PPM		1 LINES (83.4 - 83.4 PPM)
%CC(C,CC/C,C,C/C,C,&)	84.4 # 0. PPM		1 LINES (84.4 - 84.4 PPM)
%CC(C,CO+/*C*C,,/*C,*C)	91.5 # 0. PPM		1 LINES (91.5 - 91.5 PPM)
%CC(C,CO/%C,=C,/C,C)	79.3 # 0. PPM		2 LINES (79.3 - 79.3 PPM)
%CC(C,CO/%C,*C*C,/C,*C,*C)	77.9 # 3.2 PPM		3 LINES (79.7 - 74.2 PPM)
%CC(C,CO %C,CCC,/C,,,)	77.2 # 0.6 PPM		2 LINES (77.6 - 76.8 PPM)
%CC(C,CO/%C,C,/C,C)	81.6 # 0.2 PPM		2 LINES (81.7 - 81.4 PPM)
%CC(C,CO/%C,,/C)	80.0 # 2.3 PPM		3 LINES (81.3 - 77.4 PPM)
%CC(C,CO/=OO,CO,C/,C,	84.3 # 0.9 PPM	(84.7 # 0.0 PPM)	4 LINES (84.8 - 83.0 PPM)
%CC(C,CO/=OO,CO,/,C,C	86.9 # 0. PPM		1 LINES (86.9 - 86.9 PPM)
%CC(C,CO/CCO,,C/CCC,CC,)	90.6 # 0. PPM		1 LINES (90.6 - 90.6 PPM)
%CC(C,CN/*C*C,=CC,CC/*C,*C,	86.6 # 0. PPM		1 LINES (86.6 - 86.6 PPM)
%CC(C,CY/CY,CCC,/CCC,,,,	85.6 # 0. PPM		2 LINES (85.6 - 85.6 PPM)
%CC(C,C/%C,CO/C,C,)	77.9 # 0. PPM		2 LINES (77.9 - 77.9 PPM)
%CC(C,C/%C,C/C,C)	76.1 # 2.5 PPM	(76.6 # 0.7 PPM)	38 LINES (78.3 - 66.7 PPM)
%CC(C,C/%C,C/C,)	80.8 # 5.9 PPM	(78.5 # 3.4 PPM)	5 LINES (90.0 - 75.6 PPM)
%CC(C,C/%C,O/C,C)	73.6 # 0. PPM		2 LINES (73.6 - 73.6 PPM)
%CC(C,C/%C,/C)	77.9 # 0.6 PPM	(77.8 # 0.6 PPM)	4 LINES (78.5 - 77.4 PPM)
%CC(C,C/=C,C/C,C)	95.4 # 0. PPM		1 LINES (95.4 - 95.4 PPM)
%CC(C,C/=C,C/C,&)	114.5 # 0. PPM		1 LINES (114.5 - 114.5 PPM)
%CC(C,C/*C*C,C/*C,*C,)	80.7 # 0. PPM		1 LINES (80.7 - 80.7 PPM)
%CC(C,C/CC,C/C,C,)	79.6 # 0. PPM		1 LINES (79.6 - 79.6 PPM)
%CC(C,C/C,%C/%C,C)	74.0 # 0.3 PPM	(74.1 # 0.3 PPM)	4 LINES (74.3 - 73.7 PPM)
%CC(C,C/C,%C/C,C)	80.5 # 0. PPM		2 LINES (80.5 - 80.5 PPM)
%CC(C,C/C,%C/C,)	75.0 # 0. PPM		1 LINES (75.0 - 75.0 PPM)
%CC(C,C/C,C/%C,C)	80.9 # 0. PPM		2 LINES (80.9 - 80.9 PPM)
%CC(C,C/C,C/%C,S)	78.5 # 0. PPM		1 LINES (78.5 - 78.5 PPM)
%CC(C,C/C,C/C,%C)	80.1 # 0. PPM	(80.1 # 0. PPM)	6 LINES (80.1 - 80.1 PPM)
%CC(C,C/C,C/C,C)	80.4 # 0.5 PPM	(80.4 # 0.2 PPM)	70 LINES (81.5 - 78.9 PPM)
%CC(C,C/C,C/C,&)	94.4 # 0. PPM		2 LINES (94.4 - 94.4 PPM)
%CC(C,C/C,C/C,)	79.4 # 0.5 PPM	(79.3 # 0.5 PPM)	8 LINES (80.1 - 78.9 PPM)
%CC(C,C/C,C/O,C)	82.0 # 0.1 PPM		2 LINES (82.1 - 81.9 PPM)
%CC(C,C/C,C/,C)	79.6 # 1.3 PPM	(79.3 # 1.0 PPM)	6 LINES (81.5 - 78.2 PPM)
%CC(C,C/C,C/,)	79.3 # 1.3 PPM		2 LINES (80.2 - 78.4 PPM)
%CC(C,C/C,O/C,)	76.8 # 0.1 PPM		2 LINES (76.9 - 76.7 PPM)
%CC(C,C/C,/C)	80.3 # 1.2 PPM	(80.6 # 1.0 PPM)	8 LINES (81.9 - 78.3 PPM)
%CC(C,C/C,/)	80.3 # 0.5 PPM	(80.2 # 0.5 PPM)	6 LINES (81.0 - 79.9 PPM)
%CC(C,C/O,C/,C)	78.7 # 0. PPM		1 LINES (78.7 - 78.7 PPM)
%CC(C,C/N,C/CC,N)	81.3 # 5.7 PPM		3 LINES (84.7 - 74.7 PPM)
%CC(C,C/,C/%C)	77.7 # 0. PPM		2 LINES (77.7 - 77.7 PPM)
%CC(C,C/,C/C)	78.5 # 0.8 PPM	(78.6 # 0.7 PPM)	8 LINES (79.4 - 77.6 PPM)
%CC(C,C/,C/)	77.7 # 1.3 PPM		3 LINES (79.2 - 76.9 PPM)
%CC(C,C/,/)	80.3 # 0. PPM		1 LINES (80.3 - 80.3 PPM)
%CC(C,OO+/*C*C,C,/*C,*C,C	79.5 # 0. PPM		1 LINES (79.5 - 79.5 PPM)
%CC(C,OO+/*C*C,,/*C,*C)	76.8 # 0. PPM		1 LINES (76.8 - 76.8 PPM)
%CC(C,OO/=CS,C,C/C,C,	87.8 # 0. PPM		1 LINES (87.8 - 87.8 PPM)
%CC(C,OO/*C*C,C,C/*C,*C,C,	85.2 # 0. PPM		1 LINES (85.2 - 85.2 PPM)
%CC(C,ON+/*C*C,,/*C,*C)	75.0 # 0. PPM		1 LINES (75.0 - 75.0 PPM)
%CC(C,O+/*C*C,/*C,*C)	95.1 # 0. PPM		1 LINES (95.1 - 95.1 PPM)

%CC(C,O/%C,C/C,=OC)	75.4 #	4.0 PPM	(73.7 # 0.4 PPM)	6 LINES (83.5 - 73.1 PPM)	
%CC(C,O/%C,C/C,CO)	79.1 #	6.5 PPM		3 LINES (86.6 - 75.1 PPM)	
%CC(C,O/%C,/C)	76.8 #	2.1 PPM	(77.4 # 1.6 PPM)	8 LINES (78.6 - 73.1 PPM)	
%CC(C,O/%C,/)	74.7 #	0. PPM		2 LINES (74.7 - 74.7 PPM)	
%CC(C,O/=CS,C/C,C,=OC)	87.8 #	0. PPM		1 LINES (87.8 - 87.8 PPM)	
%CC(C,O/C,/C)	86.0 #	0. PPM		1 LINES (86.0 - 86.0 PPM)	
%CC(C,O/O,C/C,=OC)	80.8 #	0. PPM		2 LINES (80.8 - 80.8 PPM)	
%CC(C,O/O,/)	84.4 #	0. PPM		2 LINES (84.4 - 84.4 PPM)	
%CC(C,O/,/)	80.8 #	1.1 PPM		2 LINES (81.6 - 80.0 PPM)	
%CC(C,N/%C,CC/C,C,C)	73.5 #	0. PPM		2 LINES (73.5 - 73.5 PPM)	
%CC(C,N/C,CC/C,C,C)	78.5 #	6.0 PPM		3 LINES (85.4 - 74.6 PPM)	
%CC(C,N/N,CC/CC,=OC,C)	80.6 #	0. PPM		1 LINES (80.6 - 80.6 PPM)	
%CC(C,N/N,CC/CC,C,C)	79.1 #	0.1 PPM		3 LINES (79.2 - 79.0 PPM)	
%CC(C,N/N,CC/CC,,)	80.0 #	0. PPM		2 LINES (80.0 - 80.0 PPM)	
%CC(C,N/N,C/C,C)	81.4 #	0. PPM		2 LINES (81.4 - 81.4 PPM)	
%CC(C,S/,=O=OC/,,"C"C)	76.9 #	0. PPM		1 LINES (76.9 - 76.9 PPM)	
%CC(C,X/X,/)	81.2 #	0. PPM		2 LINES (81.2 - 81.2 PPM)	
%CC(C,/%C/C)	80.4 #	0.6 PPM	(80.7 # 0.2 PPM)	5 LINES (80.9 - 79.4 PPM)	5 %
	73.4 #	1.6 PPM	(72.9 # 1.6 PPM)	4 LINES (74.8 - 72.0 PPM)	46 %
%CC(C,/=CC/C,)	93.6 #	0. PPM		1 LINES (93.6 - 93.6 PPM)	
%CC(C,/=CS/C,C)	91.6 #	0. PPM		1 LINES (91.6 - 91.6 PPM)	
%CC(C,/=C/O)	88.8 #	0. PPM		1 LINES (88.8 - 88.8 PPM)	
%CC(C,/=OF/,)	94.4 #	0. PPM		1 LINES (94.4 - 94.4 PPM)	
%CC(C,/CCC/=CC,CC&,)	78.8 #	0. PPM		2 LINES (78.8 - 78.8 PPM)	
%CC(C,/CCO/"C"C,"C"C,)	83.4 #	0. PPM		1 LINES (83.4 - 83.4 PPM)	
%CC(C,/CCO/,,)	77.7 #	0. PPM		1 LINES (77.7 - 77.7 PPM)	
%CC(C,/C/C)	74.8 #	0.8 PPM	(74.8 # 0.7 PPM)	13 LINES (75.8 - 73.7 PPM)	
%CC(C,/C/)	74.2 #	0. PPM		1 LINES (74.2 - 74.2 PPM)	
%CC(C,/O/)	78.4 #	0.7 PPM		2 LINES (78.9 - 77.9 PPM)	
%CC(C,/S/=O=OC)	76.9 #	0. PPM		1 LINES (76.9 - 76.9 PPM)	
%CC(C,//)	76.9 #	3.8 PPM	(75.8 # 3.8 PPM)	4 LINES (80.2 - 73.6 PPM)	
%CC(N,/CC/"C"C,)	61.8 #	0. PPM		1 LINES (61.8 - 61.8 PPM)	
%CC(N,/CC/C,C)	57.6 #	0. PPM		1 LINES (57.6 - 57.6 PPM)	
%CC(P,/=OCC/,%C,%C)	101.4 #	0. PPM		3 LINES (101.4 - 101.4 PPM)	
%CC(P,/=OCC/,"C"C,"C"C)	105.3 #	0. PPM		1 LINES (105.3 - 105.3 PPM)	
%CC(P,/=OOO/,C,C)	98.1 #	0. PPM		1 LINES (98.1 - 98.1 PPM)	
%CC(P,/=ONN/,CC,CC)	98.5 #	0. PPM		1 LINES (98.5 - 98.5 PPM)	
%CC(P,/=OXX/,,)	105.9 #	0. PPM		1 LINES (105.9 - 105.9 PPM)	
%CC(P,/CCC+/"C"C,"C"C,"C"C)	121.8 #	0. PPM		1 LINES (121.8 - 121.8 PPM)	
%CC(P,/CC/%C,%C)	102.9 #	0. PPM		3 LINES (102.9 - 102.9 PPM)	
%CC(P,/CC/"C"C,"C"C)	105.8 #	0. PPM		1 LINES (105.8 - 105.8 PPM)	
%CC(P,/OO/C,C)	101.6 #	0. PPM		1 LINES (101.6 - 101.6 PPM)	
%CC(P,/NN/CC,CC)	101.4 #	0. PPM		1 LINES (101.4 - 101.4 PPM)	
%CC(X,=CX/,XX,/,)	63.9 #	0. PPM		1 LINES (63.9 - 63.9 PPM)	
%CC(Y,"C"C/,"C,"C/"C,"&)	80.0 #	0. PPM		1 LINES (80.0 - 80.0 PPM)	
%CC(Y,CC/,CC&,C&/,,=O	76.5 #	0. PPM		1 LINES (76.5 - 76.5 PPM)	
%CC(I,CO/,C,/C)	95.7 #	0. PPM		2 LINES (95.7 - 95.7 PPM)	
%CC('W',"C"C/+)C)C:C:	127.4 #	0. PPM		1 LINES (127.4 - 127.4 PPM)	
%CC('B',C/OO,C/C,C,C)	104.9 #	0. PPM		1 LINES (104.9 - 104.9 PPM)	
%CC(,%C/C/O)	67.5 #	0. PPM		2 LINES (67.5 - 67.5 PPM)	
%CC(,=CC/CC,CC/%C,CC,C,C	81.2 #	1.1 PPM	(81.5 # 1.1 PPM)	4 LINES (82.1 - 80.3 PPM)	
%CC(,=CC/C,/OO)	81.3 #	0. PPM		1 LINES (81.3 - 81.3 PPM)	
%CC(,=CC/C,/O)	82.0 #	0. PPM		1 LINES (82.0 - 82.0 PPM)	
%CC(,=C/C/=O)	88.9 #	0. PPM		1 LINES (88.9 - 88.9 PPM)	
%CC(,=C/C/C)	77.6 #	2.9 PPM		2 LINES (79.6 - 75.5 PPM)	
%CC(,=C/O/C)	78.6 #	0. PPM		1 LINES (78.6 - 78.6 PPM)	
%CC(,=OC/,CC/=OO,CC)	81.8 #	0. PPM		1 LINES (81.8 - 81.8 PPM)	
%CC(,=OC/,/)	81.9 #	0. PPM		1 LINES (81.9 - 81.9 PPM)	
%CC(,=OO/,C/C)	74.8 #	0. PPM		1 LINES (74.8 - 74.8 PPM)	
%CC(,=OO/,/)	74.0 #	0. PPM		1 LINES (74.0 - 74.0 PPM)	
%CC(,=ON/,C/)	75.2 #	0. PPM		1 LINES (75.2 - 75.2 PPM)	
%CC(,=OF/,/)	69.1 #	0. PPM		1 LINES (69.1 - 69.1 PPM)	
%CC(,=O+//)	48.9 #	0. PPM		1 LINES (48.9 - 48.9 PPM)	
%CC(,"C"C/"CC,"C/"C,CC,"&)	82.3 #	0. PPM		1 LINES (82.3 - 82.3 PPM)	
%CC(,"C"C/"CC,"C/"C,C,"&)	82.3 #	0. PPM		1 LINES (82.3 - 82.3 PPM)	
%CC(,"C"C/"C,"C/"CC,"&)	83.9 #	0. PPM		1 LINES (83.9 - 83.9 PPM)	
%CC(,"C"C/"C,"C/"C,"&)	83.8 #	0.7 PPM	(84.0 # 0.5 PPM)	6 LINES (84.9 - 82.6 PPM)	
%CC(,CCC/=CC,CC&,/C&,,=	85.9 #	0. PPM		2 LINES (85.9 - 85.9 PPM)	
%CC(,CCC/C&,YY&,/,,)	81.9 #	0. PPM		1 LINES (81.9 - 81.9 PPM)	
%CC(,CCC/C&,Y&,/,)	83.2 #	0. PPM		1 LINES (83.2 - 83.2 PPM)	
%CC(,CCC/C&,&,/)	87.5 #	0. PPM		1 LINES (87.5 - 87.5 PPM)	
%CC(,CCC/C,C,C/CC,C&,&:	92.3 #	0. PPM		1 LINES (92.3 - 92.3 PPM)	
%CC(,CCC/YY&,&,/,)	84.5 #	0. PPM		1 LINES (84.5 - 84.5 PPM)	
%CC(,CCC/Y&,&,/)	86.3 #	1.1 PPM		2 LINES (87.0 - 85.5 PPM)	
%CC(,CCC/&,&,/)	90.2 #	0. PPM		1 LINES (90.2 - 90.2 PPM)	
%CC(,CCO/=CC,,/C,=OO)	86.2 #	0. PPM		1 LINES (86.2 - 86.2 PPM)	
%CC(,CCO/CC,C,/C,,&)	86.9 #	2.6 PPM		2 LINES (88.7 - 85.1 PPM)	
%CC(,CCO/C,C,/C,&)	88.2 #	0. PPM		1 LINES (88.2 - 88.2 PPM)	
%CC(,CCO/C,C,/&,&)	88.1 #	0. PPM		1 LINES (88.1 - 88.1 PPM)	
%CC(,CCO/C,,/CC)	88.6 #	0. PPM		1 LINES (88.6 - 88.6 PPM)	
%CC(,CCO/C,,/C)	87.6 #	0. PPM		1 LINES (87.6 - 87.6 PPM)	
%CC(,CCO/C,,/)	87.9 #	0.1 PPM		2 LINES (88.0 - 87.8 PPM)	
%CC(,CCO/,,/)	89.2 #	0.3 PPM		3 LINES (89.6 - 89.0 PPM)	
%CC(,CCN/C,C,/C,&)	90.4 #	0. PPM		1 LINES (90.4 - 90.4 PPM)	
%CC(,CC/CCC,/=C,=OC,)	85.2 #	0.3 PPM		3 LINES (85.4 - 84.9 PPM)	
%CC(,CC/C&,&/=O)	81.0 #	0. PPM		1 LINES (81.0 - 81.0 PPM)	
%CC(,CC/C&,&/=N)	32.9 #	0. PPM		1 LINES (32.9 - 32.9 PPM)	
%CC(,CC/C,C/C,&)	89.0 #	0. PPM		1 LINES (89.0 - 89.0 PPM)	
%CC(,CC/&,&/)	87.5 #	0. PPM		1 LINES (87.5 - 87.5 PPM)	
%CC(,CC/,/)	89.3 #	0.1 PPM		2 LINES (89.3 - 89.2 PPM)	
%CC(,CO/CO,C/O&,C,C:	81.7 #	0. PPM		1 LINES (81.7 - 81.7 PPM)	
%CC(,CO/C&,&/=C)	78.6 #	0. PPM		1 LINES (78.6 - 78.6 PPM)	
%CC(,CO/C,C/C,=OC)	80.1 #	0. PPM		1 LINES (80.1 - 80.1 PPM)	
%CC(,CO/C,Q/C,CCC)	85.4 #	0.2 PPM		2 LINES (85.6 - 85.3 PPM)	
%CC(,CO/C,/C)	85.3 #	0.1 PPM	(85.4 # 0.0 PPM)	4 LINES (85.4 - 85.1 PPM)	
%CC(,CO/C,/)	85.2 #	0. PPM		1 LINES (85.2 - 85.2 PPM)	
%CC(,CN/C&,C&/=C,CCC)	82.0 #	0. PPM		1 LINES (82.0 - 82.0 PPM)	
%CC(,C/%C/C)	79.3 #	0. PPM		1 LINES (79.3 - 79.3 PPM)	
%CC(,C/CCC/=CC,=OC,)	80.0 #	0. PPM		1 LINES (80.0 - 80.0 PPM)	
%CC(,C/CCC/=C,=OC,)	80.4 #	0. PPM		1 LINES (80.4 - 80.4 PPM)	
%CC(,C/C/C)	83.8 #	0.7 PPM	(83.8 # 0.6 PPM)	37 LINES (85.2 - 82.4 PPM)	
%CC(,C/C/S)	82.4 #	0. PPM		1 LINES (82.4 - 82.4 PPM)	
%CC(,C/C/)	83.4 #	0.8 PPM		3 LINES (84.0 - 82.5 PPM)	
%CC(,C/O/)	81.6 #	0. PPM		1 LINES (81.6 - 81.6 PPM)	
%CC(,C//)	85.4 #	0.7 PPM		3 LINES (86.0 - 84.7 PPM)	
%CC(,O/C/=OC)	78.4 #	0. PPM		1 LINES (78.4 - 78.4 PPM)	
%CC(,O/C/)	79.9 #	0. PPM		1 LINES (79.9 - 79.9 PPM)	
%CC(,O/N/=C)	79.5 #	0. PPM		2 LINES (79.5 - 79.5 PPM)	