Handbook of Proton-NMR Spectra and Data

Volume 3

Edited by

Asahi Research Center

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1985

Academic Press, Inc.
(Harcourt Brace Jovanovich, Publishers)
Tokyo Orlando San Diego New York
London Toronto Montreal Sydney

ACADEMIC PRESS JAPAN, INC.
Hokoku Bldg. 3-11-13, Iidabashi, Chiyoda-ku, Tokyo 102

United States Edition published by ACADEMIC PRESS, INC.
Orlando, Florida 32887

United Kingdom Edition published by ACADEMIC PRESS, INC. (LONDON) LTD.,
24/28 Oval Road, London NW1 7DX

ISBN: 0-12-064503-3
Library of Congress Catalog Card Number: 85-61909

PRINTED IN JAPAN

85 86 87 88 9 8 7 6 5 4 3 2

A User's Guide

This data handbook has been planned as a part of projected open-ended series, with publication of additional data books scheduled upon completion of further data compilation. The handbook consists of proton-NMR spectra and data for 4,000 organic compounds, divided into five volumes with 800 entries each. The handbook is divided into data sections and index sections.

1. Proton-NMR Spectra and Data Sections

All data entries are in the form:

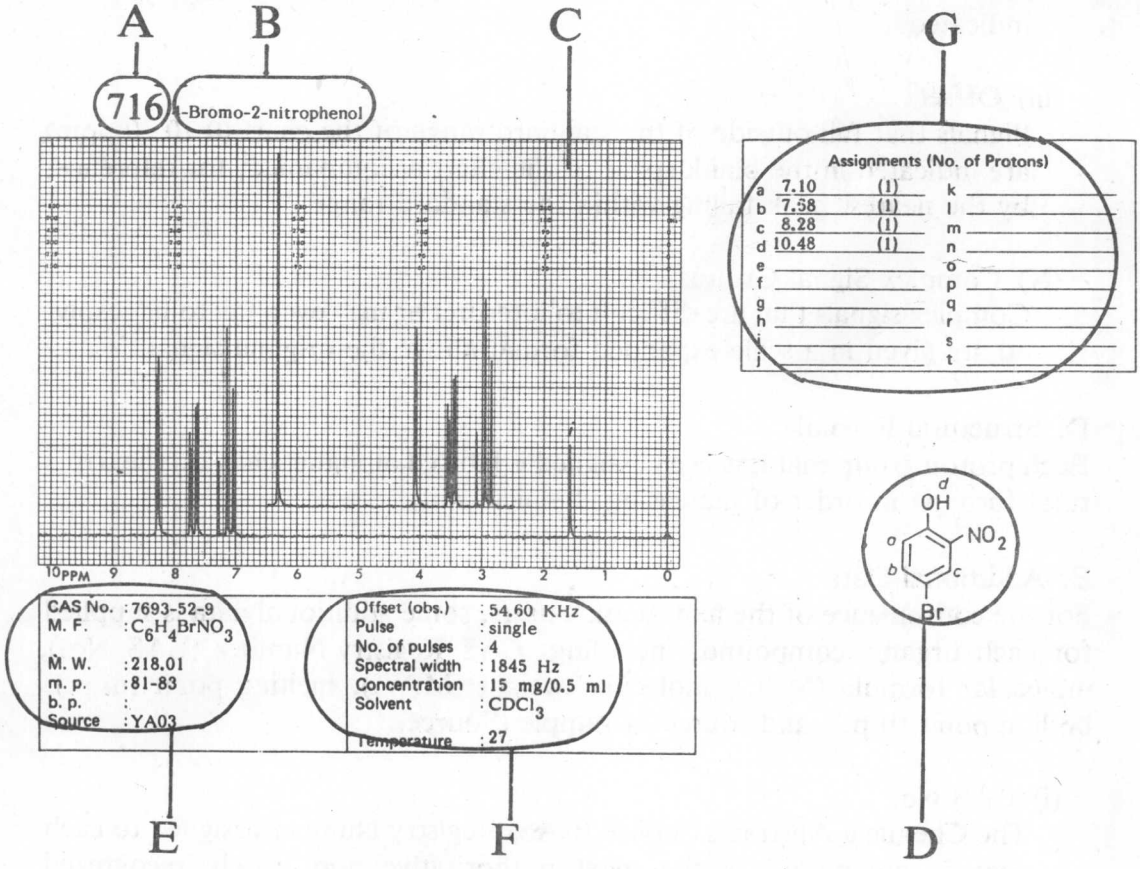

Figure 1. Illustration of Spectral Data

A. Spectrum Number

The organic compounds for which spectral data are provided are arranged in order of molecular complexity, from simpler to more complex. Each entry is assigned a number in sequence which serves as a key for easy indexing and quick reference.

B. Chemical Name

In general, all chemical names are in accord with the IUPAC nomenclature system. There are, however, some compounds that are more frequently referred to by trivial names, such as vanillin. In these cases, the trivial name is used.

C. Spectrum

(i) Units

For easy recognition of peak positions of signals, the smallest unit of the spectrum chart is 0.1 ppm (9 Hz).

(ii) Impurities

Signals resulting from a trace amount of impurities in the sample are indicated by the letter "i" over the signal in question. Signals resulting from impurities in the solvent, however, such as $CHCl_3$ in $CDCl_3$, are not indicated.

(iii) Offset

Signals that fall outside of the standard range of the chart (0-10.20 ppm) are indicated in the blank space of the chart accompanied, for reference, by the nearest peak falling within the standard range.

(iv) Complex Signal Groups

Complex signals that are difficult to interpret or may even fail to be resolved are given in a scale-expanded format above the original signal.

D. Structural Formula

Each proton group that has been assigned is labeled alphabetically on the structural formula in order of increasing chemical shift.

E. Additional Data

For the convenience of the handbook's users, some additional data is supplied for each organic compound, including: CAS Registry Number (CAS No.), molecular formula (M.F.), molecular weight (M.W.), melting point (m.p.), boiling point (b.p.), and source of sample (Source).

(i) CAS No.

The Chemical Abstracts Service (CAS) Registry Number assigned to each organic compound is the most authoritative and widely recognized chemical identification number. As a result, it is extremely helpful as a link

to information available in many other database systems such as CAS-ONLINE and CIS, among others.

(ii) Molecular Formula

Molecular formulas are arranged according to the Hill system, that is, C before H, with all other elements in alphabetical order.

(iii) Molecular Weight

Average molecular weights derived from average atomic weights are given.

(iv) Melting and Boiling Points

Both values are recorded in Celsius, based on the literature or data recorded by sample suppliers. In the case of compounds that decompose, the decomposition point is given, as, for example, 250 dec.

(v) Source of Sample

Sample suppliers are recorded in a four-letter code. Full identification of suppliers is provided in Chart 5.

F. Spectrum Measurement

(i) Spectrometer

The spectrometer used for all measurements is an FX-90Q manufactured by JEOL Ltd. This is a modern Pulse Fourier Transform spectrometer. The 90 MHz spectrometer is the most widely used spectrometer at present.

(ii) Specifications

The specifications for the spectrometer are as follows:

- Magnetic field — 21100 gauss
- Observation frequency — 89.55-89.65 MHz
- NMR lock — D2 internal lock
- Insert coil — 5 mm diameter
- Resolution — $^1H \leqq 0.2$ Hz
- Pulse mode — Single
- Accumulation times — Four (average)
- Data points — 16 K

(iii) Measurement Conditions

Spectra measurements are carried out under constant conditions as much as possible. Measurement is carried out, as a rule, at 27°C. In most cases, the solvent used is $CDCl_3$; D_2O, DMSO-d_6, or polysol, a mixture of $CDCl_3$ and DMSO-d_6 which is used as a solvent for compounds that do not dissolve in $CDCl_3$. Tetramethylsilane (TMS) is employed as the internal standard except when the solvent is D_2O, in which case 3-(trimethylsilyl)propionic acid-d_4 sodium salt (TSP-d_4) is employed.

G. Assignment

Assignment is carried out in order of increasing chemical shift relative to TMS or TSP-d_4. Related proton groups are identified with letters of the alphabet for easy correlation.

Integration curves have been omitted from the spectra chart because of the problem of poor legibility. The number of assigned protons is recorded instead in parentheses following the chemical shift value.

Determination of the chemical shift value has been carried out by standard methods. In addition, digital output from the spectrometer has been referred to. For those multiplets for which first-order approximation is sufficient, the center of the multiplets has been regarded as the chemical shift. For those which clearly exhibit a second-order signal pattern, when all the signals constituting the multiplet can be positively identified, the first approximation or the center of the multiplet is regarded as the chemical shift.

Spin-spin coupled multiplets with complex overlapping are represented by the appropriate signal range, as, for example, 7.22-8.54.

When assignment is difficult because of similar chemical environments of proximate molecular structures or overlapping signals, the several alternative assignment values are each marked with an asterisk and a number which indicates that other asterisked values of the same number may be interchangeable.

When no appropriate signal is observable throughout the entire spectrum, the proton group is marked u.o. (unobserved). When the appropriate signal clearly overlaps with another signal and the chemical shift value is difficult to determine, the proton group is marked u.d. (undetermined). When the precise chemical shift value cannot be determined but an extremely close approximation is possible, the value is marked with the prefix ca. (circa).

2. Index Sections

Thorough, carefully prepared indexes are crucial tools for effective use of any data collection. Four types of exhaustive indexes accompany the present handbook, designed for quick and convenient cross checking, in a handy format that provides extremely useful combinations of data at a glance and greatly enhances the use of the entire handbook. The indexes and the data they contain are as follows:

Table 1

Index Name	First Column	Second Column	Third Column
Chemical Name Index	Chemical name	Spectrum No.	
Molecular Formula Index	Molecular formula	Chemical name	Spectrum No.
Substructure Index	Substructure	Chemical shift	Spectrum No.
Chemical Shift Index	Chemical shift	Substructure	Spectrum No.

A. Chemical Name Index

All chemical names are in alphabetical order. Numerals, Greek characters,

and codes indicating substitution positions (such as 1-, beta-, N-, etc.) and geometrical, stereochemical, and optical isomeric prefixes (such as cis-, endo-, levo-, etc.) are disregarded in alphabetization. Each name is followed by a spectrum number, as can be seen in the sample page of the Chemical Name Index (Chart 1).

B. Molecular Formula Index

When the desired organic compound cannot be found in the Chemical Name Index or its nomenclature is unclear, it becomes necessary to look for a compound by means of its molecular formula. This is just the case for which the Molecular Formula Index was designed. Molecular formulas are listed following the Hill system, in order of complexity. When several compounds have the same molecular formula, the different compounds are listed in alphabetical order, as can be seen in the sample page of the Molecular Formula Index (Chart 2). The spectrum number is also provided for easy cross reference to the data handbook.

C. Substructure Index

Determining what sorts of proton correspond to the various signals within a spectrum, investigating their chemical environments, and suggesting models for their structure are all very important parts of spectral analysis.

A unique notation system for representing substructure has been developed in the Substructure Index to allow easy correlation of the chemical environments of protons and chemical shift, and at the same time permit fast consideration of a wide variety of model structures.

In the substructure notation of the index, the proton group which is assigned as the TARGET is grouped with its neighbors (e.g. α position) and next nearest neighbors (e.g. ß position). The TARGET occupies the head position of the substructure notation, as can be seen in Fig. 2. It is followed by the neighboring atoms, given outside parentheses; the next-nearest atoms are written inside parentheses.

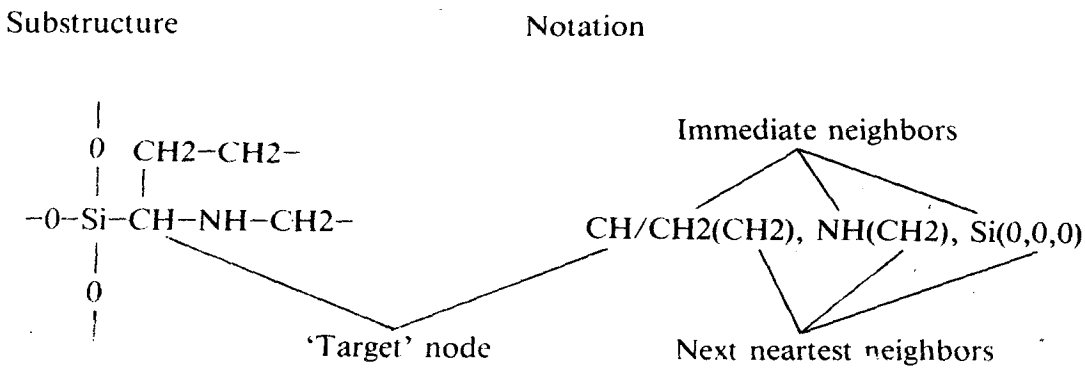

Figure 2. Substructure Notation

All non-identical substructures relating to a particular TARGET are cited in the index. In order to simplify the substructure notation, single bonds have not been represented. Code for other atomic groups is found in Chart 3-1, as is their order of priority. Chart 3-2 shows a sample page of the Substructure Index. For the user's convenience, chemical shift value and spectrum number are also provided for each entry.

D. Chemical Shift Index

Entries on the Chemical Shift Index are arranged in order of increasing delta value (ppm). For easy correlation of chemical shift with substructure, substructure notations are listed for each entry as well. Chart 4 shows a sample page of the Chemical Shift Index.

Chart 1. The Chemical Name Index

Chart 2. The Molecular Formula Index

Chart 3-1. The Code Table of Substructure Notation

Priority	Code	Substructure	Priority	Code	Substructure
1	CH3	$-CH_3$	25	=N=	=N=
2	CH2	$-CH_2-$	26	N〔*	aromatic nitrogen
3	CH	-CH<	27	NO2	$-NO_2$
4	C	>C<	28	#N	≡N
5	CH2=	$=CH_2$	29	OH	-OH
6	CH=	=CH-	30	O	-O-
7	CH=〔E〕	=CH- a〕	31	=O	=O
8	CH=〔Z〕	=CH- b〕	32	SH	-SH
9	C=	=C<	33	S	-S-
10	=C=	=C=	34	=S	=S or =S<
11	#CH	≡CH			
12	C#	≡C-	35	SO2	$-SO_2$
13	AH	c〕	36	P	-P<
14	A	d〕	37	PH=	=PH
15	TPL	e〕	38	P=	-P= or >P=
16	CHO	-CHO	39	F	-F
17	C=O	>C=O	40	CL	-Cl
18	=C=O	=C=O	41	BR	-Br
19	$NH3^+$	ammonium cation	42	I	-I
20	NH2	$-NH_2$	43	AS	>As-
21	NH	>NH	44	AS=	=As-
22	N	>N-	45	SI	>Si<
23	=NH	=NH	46	+	cation
24	N=	-N=	47	-	anion
			48	·	radical
			49	/	chelation
			50 f〕	X	other atoms

a) Entgegen b) Zusammen c) Aromatic carbon with proton
d) Aromatic carbon without proton e) -C(OH)-C(O)- in troponoid
f) Other element symbols are listed in alphabetical order.

Chart 3-2. The Substructure Index

substructure	chemical shift	No.	substructure	chemical shift	No.
CH=/CH=(C=O),N=(C=)	7.43	254	AH/AH(AH),AH(AH)	7.31	778
CH=/CH=(NH),N=(CH=)	7.15	120	AH/AH(AH),AH(AH)	7.32	490
CH=/CH=(NH),N=(C=)	6.98	283	AH/AH(AH),AH(AH)	7.63	797
CH=/CH=(NH),N=(C=)	7.01	525	AH/AH(AH),AH(AH)	7.69	487
CH=/CH=(N),N=(CH=)	6.88	282	AH/AH(AH),AH(AH)	ca. 7.77	786
CH=/CH=(N),N=(CH=)	6.93	524	AH/AH(AH),AH(AH)	7.85	795
CH=/CH=(N),N=(CH=)	7.05	524	AH/AH(AH),AH(A)	6.49	758
CH=/CH=(N),N=(CH=)	7.12	502	AH/AH(AH),AH(A)	6.77	774
CH=/CH=(N),N=(CH=)	7.12	501	AH/AH(AH),AH(A)	6.80- 7.22	723
CH=/CH=(N),N=(CH=)	7.20	501	AH/AH(AH),AH(A)	6.87- 7.37	712
CH=/CH=(N),N=(C=)	6.84	522	AH/AH(AH),AH(A)	6.92	726
CH=/CH=(S),N=(C=)	6.52	123	AH/AH(AH),AH(A)	7.00	781
CH=/CH=(CH=),O(CH=)	7.48	258	AH/AH(AH),AH(A)	7.00- 7.30	773
CH=/CH=(CH=),O(C=)	7.27	506	AH/AH(AH),AH(A)	7.14	707
CH=/CH=(CH=),O(C=)	7.71	479	AH/AH(AH),AH(A)	7.15	711
CH=/CH=(CH=),O(C=)	7.94	482	AH/AH(AH),AH(A)	7.20	737
CH=/CH=(CH=),O(N=)	8.51	102	AH/AH(AH),AH(A)	7.22	774
CH=/CH=(CH=),S(C=)	7.08	512	AH/AH(AH),AH(A)	7.28	726
CH=/CH=(CH=),S(C=)	7.10	242	AH/AH(AH),AH(A)	7.29	707
CH=/CH=(CH=),S(C=)	7.67	480	AH/AH(AH),AH(A)	7.29	753
CH=/CH=(CH=),S(C=)	7.91	241	AH/AH(AH),AH(A)	7.30- 7.63	729
CH=/CH=(C=),S(CH=)	ca. 7.26	240	AH/AH(AH),AH(A)	7.31	778
CH=/CH=(C=),S(C=)	7.28	232	AH/AH(AH),AH(A)	7.33	781
CH=/CH=(N=),S(C=)	7.09	123	AH/AH(AH),AH(A)	7.35	758
CH=/C=(CH3,NH),C=(CH3,N=)	5.82	523	AH/AH(AH),AH(A)	7.38- 7.70	473
CH=/C=(CH3,O),C=(NH2,N=)	5.56	287	AH/AH(AH),AH(A)	7.40	495
CH=/C=(CH=,N=),C=(C=O,BR)	7.79	669	AH/AH(AH),AH(A)	7.52	753
CH=/C=(CH=,N=),C=(C=O,BR)	8.28	669	AH/AH(AH),AH(A)	7.63	797
CH=/C=(C=,BR),C=(S,BR)	6.92	230	AH/AH(AH),AH(A)	ca. 7.66	786
CH=/C=(CH3,C=O),C=O(OH)	6.00	509	AH/AH(AH),AH(A)	7.68	476
CH=/C=(CH3,NH),C=O(NH)	5.69	504	AH/AH(AH),AH(A)	7.70- 8.00	733
CH=/C=(CH2,NH),C=O(NH)	5.67	485	AH/AH(AH),AH(A)	7.72	795
CH=/C=(C,OH),C=O(CH3)	5.95	486	AH/AH(AH),AH(A)	7.88	761
CH=/C=(C=O,OH),C=O(C=)	5.85	771	AH/AH(AH),AH(A)	7.88	756
CH=/C=(C=O,CL),C=O(CH=)	7.04	673	AH/AH(AH),AH(N(*)	6.60	495
CH=/C=(C=O,CL),C=O(C=)	7.17	672	AH/AH(AH),AH(N(*)	7.21	476
CH=/C=(C=O,BR),C=O(O)	7.20	229	AH/AH(AH),AH(N(*)	7.28	473
CH=/C=(CH3,N=),NH(CH=)	6.78	284	AH/AH(AH),AH(N(*)	7.29	487
CH=/C=(C=O,F),NH(C=O)	7.76	243	AH/AH(AH),AH(N(*)	7.32	490
CH=/C=(N,NO2),N=(C=)	7.92	517	AH/AH(AH),AH(N(*)	7.54	250
CH=/C=(NO2,S),N=(C=)	8.26	107	AH/AH(AH),AH(N(*)	7.58	761
CH=/C=(CH=,C=O),O(C=O)	8.38	772	AH/AH(A),AH(A)	6.60	791
CH=/C=(CH=,BR),S(CH=)	ca. 7.26	240	AH/AH(A),AH(A)	6.70	721
CH=/C=O(NH),N=(NH)	7.46	106	AH/AH(A),AH(A)	6.78- 7.44	724
CH=/NH(CH=),N=(CH=)	7.73	120	AH/AH(A),AH(A)	6.81	744
CH=/NH(CH=),N=(C=)	7.57	284	AH/AH(A),AH(A)	6.88- 7.17	741
CH=/NH(A),N=(A)	8.72	469	AH/AH(A),AH(A)	6.90	690
CH=/NH(A),N=(A)	8.78	469	AH/AH(A),AH(A)	6.94	788
CH=/NH(N=),N=(C=)	7.48	51	AH/AH(A),AH(A)	7.00- 7.50	683
CH=/N(CH3,CH=),N=(CH=)	7.42	282	AH/AH(A),AH(A)	7.02	727
CH=/N(CH2,CH=),N=(CH=)	7.49	524	AH/AH(A),AH(A)	7.07	682
CH=/N(CH=,CH=),N=(CH=)	7.68	501	AH/AH(A),AH(A)	7.08	775
CH=/N(CH=,C=O),N=(CH=)	8.17	502	AH/AH(A),AH(A)	7.10	719
CH=(E)/CH3,CH=(E)(CH2)	5.68	361	AH/AH(A),AH(A)	7.13	708
CH=(E)/CH3,CH=(E)(C=O)	7.10	296	AH/AH(A),AH(A)	7.13	799
CH=(E)/CH2(OH),CH=(E)(CH3)	5.68	361	AH/AH(A),AH(A)	7.13	697
CH=(E)/CH2(OH),CH=(E)(C=O)	7.07	539	AH/AH(A),AH(A)	7.18	768
CH=(E)/CH2(CL),CH=(E)(CH2)	5.95	278	AH/AH(A),AH(A)	7.20	782
CH=(E)/CH2(BR),CH=(E)(CH2)	5.99	274	AH/AH(A),AH(A)	7.25	738
CH=(E)/CH=(E)(C#),C#(#N)	6.31	235	AH/AH(A),AH(A)	7.30	754
CH=(E)/CH=(E)(CH3),C=O(OH)	5.85	296	AH/AH(A),AH(A)	7.40	691
CH=(E)/CH=(E)(CH2),C=O(O)	6.12	539	AH/AH(A),AH(A)	7.45	467
CH=(E)/CH=(E)(C=O),C=O(O)	6.55	236	AH/AH(A),AH(A)	7.52	730
CH=(E)/CH=(E)(CL),CL	6.37	25	AH/AH(A),AH(A)	7.58	751
CH=(Z)/CH=(Z)(C=O),C=O(O)	6.02	237	AH/AH(A),AH(A)	7.85	764
CH=(Z)/CH=(Z)(CL),CL	6.45	26	AH/AH(A),AH(A)	7.91	734
#CH/C#(CH2)	2.06	290	AH/AH(A),AH(N(*)	6.08	492
#CH/C#(CH2)	2.33	529	AH/AH(A),AH(N(*)	7.08	496
#CH/C#(CH2)	2.50	124	AH/AH(A),AH(N(*)	7.19	488
#CH/C#(CH2)	2.52	98	AH/AH(A),AH(N(*)	7.20	474
#CH/C#(CH2)	2.53	99	AH/AH(A),AH(N(*)	7.22	494
#CH/C#(CH)	2.47	528	AH/AH(A),AH(N(*)	7.27	477
#CH/C#(C)	2.42	527	AH/AH(A),AH(N(*)	7.48	763
#CH/C#(C=O)	2.88	507	AH/AH(A),AH(S)	6.97	239
#CH/C#(C=O)	3.05	97	AH/AH(N(*),AH(N(*)	6.60	271
AH/AH(AH),AH(AH)	7.00- 7.30	773	AH/AH(N(*),AH(N(*)	6.83	253

Chart 4. The Chemical Shift Index

chemical shift	substructure	No.
ca. 5.87	NH/CH3,C=O(CH2)	401
5.87	OH/A(A,A)	687
5.90	CH/CH3,CL,CL	47
5.90	CH2=/C=(CH2,C=O)	510
5.90	CH=/CH2(O),CH=(CH2)	291
5.90	OH/A(A,A)	721
5.92	CH=/CH2(O),CH2=	292
5.93	CH2=/CH=(C=O)	508
5.93	CH=/CH(CH3,OH),CH2=	362
5.93	CH=/CH(CH3,CL),CH2=	318
5.94	CH=/CH2(O),CH2=	531
5.94	NH/C=O(O),NH2	621
5.95	CH=/CH=(CH=),C=(CH3,O)	506
5.95	CH=/C=(C,OH),C=O(CH3)	486
5.95	CH=(E)/CH2(CL),CH=(E)(CH2)	278
5.96	CH=/CH2(NH2),CH2=	190
5.96	CH=/CH2(CL),CH2=	134
5.97	AH/AH(A),A(AH,O)	759
5.98	CH/CH(CL,CL),CL,CL	31
5.98	CH/C=O(O),CL,CL	116
5.98	CH=/CH=(N=),C=(CH3,O)	266
5.99	CH=(E)/CH2(BR),CH=(E)(CH2)	274
ca. 5.99	NH/CH3,C=O(CH3)	193
6.00	CH=/CH2(OH),CH2=	169
6.00	CH=/C=(CH3,C=O),C=O(OH)	509
6.00- 9.90	OH/C=O(CH2)	309
6.00- 9.90	OH/C=O(CH)	309
6.01	CH=/C(CH3,CH3,OH),CH2=	577
6.02	CH/C=O(OH),CL,CL	28
6.02	CH=/CH2(BR),CH2=	128
6.02	CH=(Z)/CH=(Z)(C=O),C=O(O)	237
6.06	CH/C(O,F,F),F,CL	110
6.07	CH/C=O(O),CL,CL	19
6.07	CH=/CH=(NH),C=(CH3,N=)	285
6.08	CH/CH(BR,BR),BR,BR	23
6.08	CH/C=O(NH2),BR,BR	34
6.08	AH/AH(A),AH(N(*)	492
6.09	CH=/CH2(SO2),CH=(CH2)	302
6.09	NH2/A(AH,A)	779
ca. 6.10	NH2/C=O(C=)	335
6.11	CH2=/CH=(C#)	101
6.12	CH=(E)/CH=(E)(CH2),C=O(O)	539
6.13	CH/C(CL,CL,CL),CL,CL	21
6.13	CH/C=O(CL),CL,CL	20
6.13	CH=/CH2=,C=O(O)	533
6.15	CH2=/C=(C#,CL)	93
6.15	CH=/CH2=,C=O(O)	299
6.15	NH/CH2(CH3),C=(NH,=S)	623
6.17	CH/CH(CH2,CL),CL,CL	118
6.17	NH2/C=O(NH)	413
6.20	CH2=/CH=(C=O)	100
6.22	AH/AH(N(*),A(AH,OH)	489
6.24	CH2=/C=(C#,CL)	93
6.24	OH/A(AH,A)	731
ca. 6.25	CH=/CH2=,C=O(O)	508
6.25	CH=/CH=(C=),CH=(O)	506
6.26	CH/C(CH,CL,CL),CL,CL	94
6.27	CH2=/CH=(C#)	101
6.27	CH2=/C=(CH3,C=O)	298
6.29	CH2=/CH=(N)	395
6.29	NH2/C=(N=,S)	166
6.30	CH2=/CH=(C=O)	557
6.31	CH=(E)/CH=(E)(C#),C#(#N)	235
6.32	AH/AH(AH),A(A,CL)	781
6.35	CH=/CH=(NH),CH=(N=)	121
6.35	CH=/CH=(C=),C=O(O)	772
6.35	NH/CH3,C=(NH,=S)	206
6.37	CH=/CH2=,C=O(CL)	100
6.37	CH=(E)/CH=(E)(CL),CL	25
6.39	CH2=/CH=(C=O)	299
6.39	CH2=/C=(CH2,C=O)	510
6.40	CH=/CH=(N=),CH=(O)	102
6.40	NH/C=O(O),NH2	205
6.41	CH=/CH=(CH=),CH=(O)	258
6.42	CH/C=O(NH2),CL,CL	36
6.44	AH/AH(A),A(NH2,N(*)	483
6.44	AH/AH(N*),A(AH,NH2)	484
6.45	CH2=/CH=(C=O)	533
6.45	CH=(Z)/CH=(Z)(CL),CL	26
6.47	AH/AH(AH),A(NH2,N(*)	495
6.49	CH=/CH2=,O(CH2)	322
6.49	AH/AH(AH),AH(A)	758
6.50	AH/AH(A),A(AH,NH2)	792
6.50	NH2/C=O(C=O)	341
6.50- 9.00	OH/A(AH,A)	767
6.51	CH/C(C,CL,CL),CL,CL	91
6.52	CH=/CH=(S),N=(C=)	123
6.52	AH/AH(A),A(NH2,N(*)	494
6.53	AH/AH(N(*),A(AH,NH2)	497
6.53	OH/A(A,A)	696
6.55	CH2=/CH=(C=O)	508
6.55	CH=(E)/CH=(E)(C=O),C=O(O)	236
6.55	AH/A(AH,NH2),A(N(*,CL)	484
6.56	AH/A(AH,NH2),A(AH,CL)	793
6.58	AH/AH(AH),A(AH,OH)	799
6.58	AH/AH(AH),A(AH,F)	799
6.60	AH/AH(AH),AH(N(*)	495
6.60	AH/AH(A),AH(A)	791
6.60	AH/AH(N(*),AH(N(*)	271
6.60	AH/A(AH,NH2),A(A,CL)	794
6.62	CH=/CH2=,C=O(N)	557
6.62	CH=/CH2=,N(CH3,CH3)	395
6.63	CH=/CH=(C=),CH=(O)	479
6.63	AH/AH(AH),A(A,NH2)	788
6.64	AH/AH(A),A(A,NH2)	748
6.65	CH2=/CH=(C=O)	100
6.65	AH/AH(A),A(A,NH2)	777
6.65	AH/A(AH,OH),A(AH,F)	799
6.68	CH=/CH=(C=),CH=(O)	482
6.68	AH/AH(AH),A(AH,OH)	799
6.68	AH/AH(AH),A(AH,F)	799
6.68	AH/AH(A),A(AH,CL)	790
6.70	AH/AH(A),AH(A)	721
6.70	AH/AH(A),A(A,NH2)	789
6.71	AH/A(A,OH),A(A,OH)	747
6.73	CH=/CH=(C=O),C=O(NH)	245
6.73	AH/AH(AH),A(A,OH)	492
6.73	AH/AH(A),A(AH,OH)	776
6.73	AH/A(AH,CL),A(AH,CL)	793
6.74	AH/AH(A),A(AH,OH)	784
6.75- 7.11	AH/AH(A),A(AH,NH2)	798
6.75- 7.11	AH/AH(A),A(A,F)	798
6.77	AH/AH(AH),AH(A)	774
6.77	AH/AH(AH),A(AH,OH)	782
6.77	AH/AH(A),A(AH,F)	800
6.77	AH/A(AH,OH),A(AH,CL)	745
6.77	AH/A(AH,CL),A(A,NH2)	790
6.78	CH=/CH=(CH=),C=(CH3,S)	512
6.78	CH=/C=(CH3,N=),NH(CH=)	284
6.78	AH/AH(AH),A(AH,BR)	775
6.78	AH/AH(A),A(AH,OH)	783
6.78	AH/A(AH,NH2),A(A,CL)	792
6.78	NH2/SO2(CH3)	16
6.78- 7.44	AH/AH(A),AH(A)	724
6.78- 7.44	AH/AH(AH),A(AH,F)	724
6.78- 7.44	AH/AH(AH),A(AH,CL)	724
6.78- 7.44	AH/A(AH,F),A(AH,CL)	724
6.79	AH/AH(A),A(A,NH2)	779
6.80	AH/AH(AH),A(A,O)	758
6.80	AH/AH(A),A(A,OH)	785
6.80	AH/A(AH,CL),A(A,OH)	785
6.80	AH/A(A,NH2),A(A,CL)	739
6.80- 7.22	AH/AH(AH),AH(A)	723
6.81	AH/AH(A),AH(A)	744
6.82	AH/AH(AH),A(A,CL)	788
6.82	AH/A(A,NH2),A(A,CL)	796
6.82	AH/A(A,O),A(A,CL)	677
6.83	AH/AH(N(*),AH(N(*)	253
6.83	AH/AH(AH),A(AH,OH)	491
6.84	CH=/CH=(N=),N(CH3,C=)	522
6.84	CH=/CH=(N),N=(C=)	522
6.85	AH/AH(AH),N(*(A)	492

Chart 5. Code Table of Sample Suppliers

Code	Name	Appliation
AB01	Abe, Nobuo	Akita University
AB02	Abe, Yoshio	Keio University
AD01	Adachi, Kazuo	Osaka Institute of Technology
AL		Aldrich Chemical Co.
AN01	Ando, Masayoshi	Tohoku University
AR01	Arai, Mannosuke	Tohoku University
AS01	Asao, Toyonobu	Tohoku University
FU01		Kao Corporation
FU02	Fujise, Yutaka	Tohoku University
GO01	Goromaru, Tsuyoshi	The University of Tokushima
HA01	Hamada, Yoshiki	Meijo University
HA02	Hamada, Keinosuke	Nagasaki University
HA03	Harada, Nobuyuki	Tohoku Universtiy
HA04	Hagiwara, Hisahiro	Tohoku University
HI01	Hirose, Yoshiyuki	Science University of Tokyo
HI02	Hirota, Hiroshi	The University of Tokyo
HO01	Horiike, Michio	Kochi University
II01	Iino, Masashi	Tohoku University
IK01	Ikeda, Masazumi	Osaka University
IK02	Ikariya, Takao	The University of Tokyo
IS01	Ishida, Shin-ichiro	Kanazawa University
IS02	Ishikawa, Yukihiro	Tottori University
IT01	Ito, Kenji	Toyohashi University of Technology
IT02	Ito, Takashi	Yokohama National University
KA		Kanto Chemical Co., Inc.
KA01	Kan, Takayuki	Hiroshima University
KA02	Kasahara, Akira	Yamagata University
KA03	Kakei, Shoichi	Shinshu University
KA04	Kanno, Shunroku	Yamagata University
KA05	Karube, Akio	Akita National College of Technology
KA06		Konishiroku Photo Ind. Co., Ltd.
KA07	Kato, Norimoto	Tohoku University
KI01	Kimura, Yoshiharu	Kyoto University of Industrial Art and Textile
KI02	Kido, Hideo	Tohoku University
KO01	Kosugi, Hiroshi	Tohoku University
KO02	Komiya, Sanshiro	Tokyo University of Agriculture and Technology
KO03	Koga, Gen	Ibaraki University
KU01	Kusuyama, Yoshiaki	Wakayama University
KU02	Kurosawa, Kazu	Kumamoto University
MA01	Matoba, Katsuhide	Toyama Medical and Pharmaceutical University
MA02	Machida, Katsunosuke	Kyoto University
MA03	Maruyama, Masao	Miyagi University of Education
MA04	Matsueda, Sumu	Hirosaki University
MA05	Maruyama, Kazuhiro	Kyoto University
MO01	Mochida, Kunio	Gakushuin University
MO02		Fujisawa Pharmaceutical Co., Ltd.
MO03	Morita Yasuo	Tohoku Pharmaceutical College
NA01	Nakasuga, Noriyuki	Nagoya University
NA02	Nakagawa, Shigeki	Nippon University
NA03	Hoshino, Masamatsu	Saitama University
NI01	Nishimura, Jun	Kyoto University of Industrial Art and Textile
NI02	Nishiyama, Shigeru	Keio University
NO01	Nonaka, Tsutomu	Tokyo Institute of Technology
NU01		Numazu College of Technology
OG01	Ogino, Hiroshi	Tohoku University
OJ01	Ojima, Juro	Toyama University
OO01	Osawa, Keisuke	Tohoku Pharmaceutical College
OO02	Onuma, Hiroshi	Akita University
OO03	Omura, Satoshi	Kitasato University
OZ01	Ozawa, Fumiyuki	Tokyo Institute of Technology
SA01	Sato, Gen	Sophia University
SA02		Fuji Photo Film Co., Ltd.
SA03	Sato, Masaru	Saitama University
SA04		Konishiroku Photo Ind. Co., Ltd.
SA05	Minabe, Masahiro	Utsunomiya University
SE01	Senda, Yasuhisa	Tohoku University
SI01	Shibata, Hisao	Shinshu University
SU01	Suzuki, Minoru	Hokkaido University
SU02	Suzuki, Toshio	Akita University
SU03	Suzuki, Kanji	Tokyo Institute of Technology
TA01	Takatori, Masayuki	Fukushima University
TA02	Tabei, Katsumi	Tokyo College of Pharmacy
TA03		Zeria Pharmaceutical Co., Ltd.
TA04	Tanaka, Kuniyoshi	Kinki University
TO		Tokyo Kasei Kogyo Co., Ltd.
TS01		Sumitomo Bakelite Co., Ltd.
TS02	Tsunetsugu, Josuke	Saitama University
UE01	Uehara, Tadao	Tohoku University
YA01	Yasuda, Seiichi	Nagoya University
YA02		Central Glass Co., Ltd.
YA03	Yamato, Masatoshi	Okayama University
YA04	Yamamoto, Yutaka	Tohoku Pharmaceutical College
YA05	Yasunami, Masafumi	Tohoku Univesity
YA06	Yamada, Yoichi	Utsunomiya University
YO01		Maruzen Petrochemical Co., Ltd.
YO02		The Green Cross Corporation

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