

D a t a b a s e o f S a f e t y L a w s f o r
C h e m i c a l C o m p o u n d s

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Good afternoon. I would like to speak to you about the database that we are preparing which enables us to search the laws, provisions, and their texts in detail. This work on the database was undertaken as a part of the project of the Science and Technology Agency, with Professor Shizuo Fujiwara as the chairman. In relation to this, I would also like to talk about the database that we are also working on which enables us to find the list of the existing chemicals based on the Japanese Chemical Substances Control Law.

It is important that chemical substances are useful in the human society, but many legal controls have been established in different countries to prevent adverse effects on humans or environment in the processes of research and development of new substances, their manufacture and import, storage and transportation, sales, processing, use, and disposal.

It is important for us to understand the types of laws in effect in different fields to ensure the safety of their use.

However, presently there is no database available in Japan or even anywhere outside Japan for finding out the content of such laws just by searching a chemical by its name.

OHP 1 shows the databases concerning the regulations within and outside Japan.

The Prime Minister's Office Law Reference System is a database in Japanese giving the full text of the law, and so it is difficult to exactly search a chemical substance by its name.

The IRPTC-Legal only provides a brief description of a regulation, and Dialog's CRGS has not been renewed for a long time. The Federal Register Abstracts give the summary of the Federal Register records. The CNIC is known to be in the process of construction, but it has not yet been completed.

In this way the necessity of database is perceived by many, but despite its need it has not yet been constructed and put into practice most probably for the following reasons:

First of all, laws in Japan are arranged in a hierarchial order. Given in the OHP 3 as an example is the Japanese Industrial Safety and Health Law, its supplementary Enforcement Order and Ordinances. Also given in the OHP 5 are some examples of substances which have such a hierarchial structure.

The Structure of the Legal System of Substances.

A substance can be referred to in a variety of ways using different names in the laws. This could be classified as follows:

1. Designated Classification of Substances

This is a concept of classification to refer to the group of substances that are subject to regulation by the law, and it functions to establish a link between specific chemical substances and the control measures.

Examples are, Poisonous Substance, Deleterious Substance, and Class 1 Hazardous Substances.

2. Generic Names of Substances

It is possible to refer to particular chemical substances not by their individual names but by their generic name or category. Included are the following:

o Naming by physical properties

eg) substances with the flash point of less than -30°C .

o Naming by chemical groups

eg) Organic phosphorus compounds, and ketones.

o Naming by composition

eg) agents including -.

o Naming by law

eg) Substances as those given in the table.

3. Legal Names of Substances

These are the individual names of chemical substances given to each as expressed in the law.

eg) acetone

4. Reference Substance Names

When a substance is given in the law by its generic name, not by its individual name, it is possible to input the individual name of a substance contained in it as a reference substance.

For example, in the case of ketones, the reference substance is acetone.

The above four classification groups form a structure as shown below in accordance with each legal system. The arrows indicate the position of the structure that could be referred to.

The Group-1 Substances in the Specified Chemical Substances (OHP 6) are indicated in the Attached Table 3 of the Enforcement Order of Industrial Safety and Health Law but, as in the case of dichlorobenzidine and its salts, or beryllium and its compounds, "generic names", introducing a lot of substances by one name, are found. Also coexisting here is the case where a single substance is given as in benzotrichloride.

That is, The Group-1 Substances

|
beryllium and its compounds
|
beryllium oxide

The name "beryllium oxide" is not mentioned in the text of the regulations; therefore, when we want to know how beryllium oxide is regulated, it is necessary to refer to it as being included in "beryllium and its compounds" and look it up under that name.

Secondly, there is an inconsistency in the way the names of substances are mentioned. In other words, substances are sometimes cited in the provisions but other times cited as "organic solvents" in the provisions. In the latter case we have to refer to the separate table listing the substances

regulated as "organic solvents" or refer to the supplementary ordinances to look them up.

Next, as indicated in OHP 7, there are cases where the same substance is expressed differently in different laws. This occurs in cases where the laws, and accordingly the ministries concerned, differ or in cases where the old ordinances and recently promulgated ordinances differ.

The substances a) and b) in example 1 are identical. a) "phenol" is indicated in katakana which is a phonetic sign. b), on the other hand, is indicated in kanji, which is an ideograph, and this word means coal acid. Likewise, example 2 is a case where a) and b) are identical (oxalic acid), but a) is written in katakana and b) is written in kanji.

Next, comes the most difficult problem. That is, regulation by physical properties. For instance, as indicated in OHP 8, it is expressed: "Inflammable substances whose flash points are lower than -30°C ." According to this definition, all substances having this property are subject to regulation by this law; however, not many substances are cited as examples.

As given above, there exist many difficulties. We have tried our best to overcome these problems, and have worked on preparing a database which enables us to find the text of the regulations and their content by looking up the name of the substance. We have completed the input of a total of 27 laws and regulations, that is, 6 laws and their supplementary ordinances, as indicated in OHP 9.

What we have prepared is a very unique database, where each provision is a piece of document and has its place in the hierarchical structure, and, likewise, each substance mentioned in the provision has its place in the hierarchical structure.

Let us look at what kind of things we can look up using this database (OHP 10).

First of all, we can look up a substance by its name. By doing so, we

can find out all the laws and provisions in which that substance is mentioned. We can also find out if a substance is regulated by a specific law such as the Industrial Safety and Health Law.

Second of all, we can look up a substance by its molecular formula or the CAS Registry Number.

Third of all, we can search a law or provision and find out the names of substances which it regulates. For example, we can look up a law called "the Ordinance on the Prevention of Organic Solvent Poisoning" and find out the organic solvents that it controls.

Fourthly, we can find out about the related provisions or substances subject to control by looking up the keywords taken from one of the provisions. For instance, we can take the words "Production" and "Permission" as keywords for the Fire Protection law, look them up in the database and get the list of provisions related to that Law.

Fifth of all, we can use our database together with other databases prepared by the Science Technology Agency Project.

For example, we can use their database to find out the names of substances with the flash point which is below a certain value, and use our database to find about the measures of control.

I feel that our database is of great value for these reasons and hope you feel the same.

The practical use of our database will be realized when the databases for other laws, besides the six being worked on so far, are completed.

We have expanded the scope of the laws and are working at JICST (Japan Information Center of Science and Technology) in preparation for the practical use of our database.

Let me now talk to you a little about the database that we are also constructing to look up the list of existing chemicals based on the Japanese Chemical Substances Control Law as I told you earlier.

In Japan, the United States, and the EC countries laws have been adopted to prevent environmental and human hazards when a new chemical is manufactured or imported. These are the Japanese Chemical Substances Control Law, the U.S. Toxic Substances Control Law (TSCA) and the EC's Sixth Amendment.

In each country a list of existing chemicals is made to distinguish between new chemicals that require notification by law and old chemicals that do not require such a notification. I have given them to you in the OHP.

In the case of the U.S. TSCA's Inventory List and the EC's EINECS it is possible to look up a substance by its CAS registry number as well as by its molecular formula besides its name. It is also possible to look up using a tape. On the other hand, the Japanese list was made earlier than the two; therefore, it only lists substances under two classifications, that is, by substance name and briefly by their structure. Another thing to mention is that the Japanese list contains a lot of generic names.

We are now working on a database which enables us to look up a substance by its molecular formula and by its CAS registry number with the instruction of the Ministry of International Trade and Industry and supported by the Database Promotion Center. We are hoping to open some part of it to the public some time next year.

Thank you for your attention. If there are any questions, I am happy to answer them now.

OHP 1

Database Related to Laws in Japan and Abroad

1. Prime Minister's Office Law Reference System (Japan)
2. IRPTC-Legal (ECDIN)
3. CRGS (DIALOG)
4. Federal Register Abstracts (DIALOG)
5. FRSS (CIS)
6. CNIC (France)

OHP 3

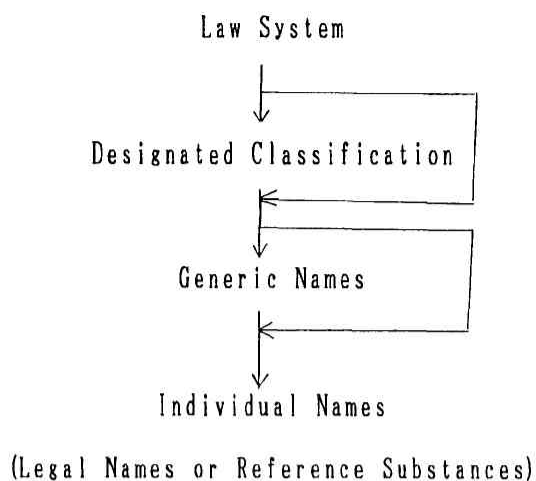
Industrial Safety and Health Law
Enforcement Order of Industrial Safety and Health Law

- Ordinance on Industrial Safety and Health
- Ordinance on the Prevention of Organic Solvent Poisoning
- Ordinance on Prevention of Lead Poisoning
- Ordinance on Prevention of Tetraalkyl Lead Poisoning
- Ordinance on Prevention of Hazards due to Specified Chemical Substances
- Ordinance on Safety and Health of Work Under High Pressure
- Ordinance on Prevention of Ionizing Radiation Hazards
- Ordinance on Prevention of Anoxia
- Ordinance on Health Standards in the Office
- Ordinance on Prevention of Hazards due to Dust
- other Ordinances

OHP 2

- 1) some of the laws and the names of substances have a certain hierarchal structure which is rather complex;
- 2) an inconsistency exists in the way the substances are referred to in the laws in that substances may be cited in the laws themselves or may be cited elsewhere independently;
- 3) a certain chemical substance is sometimes referred to by different names in different sections;
- 4) there are too many generic names;
- 5) the substances are sometimes regulated by physical property;
- 6) expressions as "excluding~" are found;
- 7) the data require a constant renewal;
- 8) there is a danger of some information missing from the database.

OHP 4



OHP 5

- 1 Designated Classification of Substances
ex. Posionous Substances
- 2 Generic Name of Substances
ex. Ketones
- 3 Legally Established Names of Substances
ex. Acetone
- 4 Reference Substance Names
ex. Acetone for ketones

OHP 6

The Group-1 Substnaces in the specified Chemical Substances

- (1) Benzidine and its salts.
- (1)-2 Bis (chloromethyl) ether.
- (2) Beta-naphtylamine and its salts.
- (3) Dichlorobenzidine and its salts.
- (4) Alpha-naphtylamine and its salts.
- (5) O-Tridine and its salts.
- (6) Dianisidine and its salts.
- (7) Beryllium and its compounds.
- (7)-2 Benzo-trichloride

Attached Table 3 of the Enforcement Order of Industrial
Safety and Health Law.

OHP 7

法令中 同一物質が異名の例

例 1 (example 1)

a) フェノール

毒物及び劇物取締法
別表第二(第二条関係)(劇物の指定)

b) 石炭酸

労働安全規則
第十三条 二のル(産業医の選任)

例 2 (example 2)

a) シュウ酸

- 1 食品衛生法 施行規則
別表第二(第三条、第五条関係)
- 2 食品、添加物等の規格基準

b) 砒酸

- 1 毒物及び劇物取締法
別表第二(第二条関係)
- 2 同上 施行規則
別表第二(第四条の三関係)
- 3 同上 同上
別表第四(第十八条の2関係)

OHP 8

Regulation by Physical Properties

example

Chemical Substances whose flash points
are lower than -30℃

OHP 9

1. Industrial Safety and Health Law

2. Fire Defence Law

3. Chemical Substances Control Law

4. Food Sanitation Law

5. Poisonous and Deleterious Substances
Control Law6. Law for the Control of Household
Products Containing Harmful Substances

OHP 10

1. Searching by chemical name, molecular
formula or the CAS Registry Number2. Chemical Substances regulated by a
specific law3. Keyword Searching
ex "Production" and Permission4. Connecting Searching together with
another databases

Structure of Subfile

Input Data Volume

Chemical Substances File

CAS Registry Number
 NIOSH Number
 Molecular Formula
 Japanese Chemical Substances Dictionary
 Number

1 Number of Laws and Regulations
 27
 2 Number of Substances
 1,143
 3 Capacity of Data
 2.5MB

Legal System of Substances File

Designated Classification
 Generic Names
 Legal Names
 Reference Names

Amount of Data Input

1 Bibliographic Index
 8057

Law Contents File

Name of Laws
 Law Number
 Promulgated date
 Section, Sub-section, Clause, Sub-clause

2 Substance Name Index
 5958
 3 Subject Index
 3759
 4 Others
 4289

TSCA INVENTORY: 1985 EDITION

CHEMICAL SUBSTANCE IDENTITIES

50-00-0
 Formaldehyde CH_2O
 50-01-1
 Guanidine, monohydrochloride $\text{CH}_5\text{N}_3\text{ClH}$
 50-02-2
 Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-trihydroxy-16-meth-
 yl-, (11 β ,16 α)- $\text{C}_{22}\text{H}_{28}\text{FO}_5$
 50-07-7
 Azirino[2',3':3,4]pyrrolo[1,2-*a*]indole-4,7-dione, 6-amino-8-[[[amino-
 carbonyl]oxy]methyl]-1,1a,2,8,8a,8b-hexahydro-8a-methoxy-5- α -
 methyl-, [1a*S*-(1a α ,8 β ,8a α ,8b α)]- $\text{C}_{16}\text{H}_{18}\text{N}_4\text{O}_5$
 50-14-6
 9,10-Secoergosta-5,7,10(19),22-tetraen-3-ol, (3 β ,5*Z*,7*E*,22*E*)-
 $\text{C}_{28}\text{H}_{44}\text{O}$
 50-21-5
 Propanoic acid, 2-hydroxy- $\text{C}_3\text{H}_6\text{O}_3$
 50-23-7
 Pregn-4-ene-3,20-dione, 11,17,21-trihydroxy-, (11 β)- $\text{C}_{21}\text{H}_{30}\text{O}_5$
 50-24-8
 Pregna-1,4-diene-3,20-dione, 11,17,21-trihydroxy-, (11 β)-
 $\text{C}_{21}\text{H}_{28}\text{O}_5$
 50-29-3

51-17-2
 1*H*-Benzimidazole $\text{C}_7\text{H}_6\text{N}_2$
 51-20-7
 2,4(1*H*,3*H*)-Pyrimidinedione, 5-bromo- $\text{C}_4\text{H}_3\text{BrN}_2\text{O}_2$
 51-21-8
 2,4(1*H*,3*H*)-Pyrimidinedione, 5-fluoro- $\text{C}_4\text{H}_3\text{FN}_2\text{O}_2$
 51-28-5
 Phenol, 2,4-dinitro- $\text{C}_6\text{H}_4\text{N}_2\text{O}_5$
 51-35-4
 L-Proline, 4-hydroxy-, *trans*- $\text{C}_5\text{H}_9\text{NO}_3$
 51-43-4
 1,2-Benzenediol, 4-[1-hydroxy-2-(methylamino)ethyl]-, (*R*)-
 $\text{C}_6\text{H}_{13}\text{NO}_3$
 51-44-5
 Benzoic acid, 3,4-dichloro- $\text{C}_7\text{H}_4\text{Cl}_2\text{O}_2$
 51-45-6
 1*H*-Imidazole-4-ethanamine $\text{C}_6\text{H}_9\text{N}_3$
 51-46-7
 1,3,6,8-Tetraazatricyclo[4.4.1.1^{3,6}]dodecane $\text{C}_8\text{H}_{16}\text{N}_4$
 51-48-9
 L-Tyrosine, *O*-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-
 $\text{C}_{16}\text{H}_{11}\text{I}_2\text{NO}_4$
 51-52-5

EUROPEAN INVENTORY
OF
EXISTING COMMERCIAL CHEMICAL SUBSTANCES

MASTER INVENTORY

2000018	Formaldehyde	CH ₂ O	50-00-0	2000243	Benzene, 1,1'-(2,2,2-trichloroethylidene)bis[4-chloro-	50-29-3
2000023	Guanidine, monohydrochloride	CH ₅ N ₃ .ClH	50-01-1		C ₁₄ H ₉ Cl ₅	
2000039	Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-trihydroxy-16- methyl-, (11 β ,16 α)-	C ₂₂ H ₂₉ FO ₆	50-02-2	2000259	Benzoic acid, 2,6-dichloro-	50-30-6
2000044	Pregn-4-ene-3,20-dione, 21-(acetyloxy)-11,17-dihydroxy-, (11 β)-	C ₂₃ H ₃₂ O ₆	50-03-3	2000264	Benzoic acid, 2,3,6-trichloro-	50-31-7
2000065	Pregn-4-ene-3,11,20-trione, 21-(acetyloxy)-17-hydroxy-	C ₂₃ H ₃₀ O ₆	50-04-4	2000285	Benzo[a]pyrene	50-32-8
2000070	2,4,6-(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>)-Pyrimidinetrione, 5-ethyl-5-phenyl-	C ₁₂ H ₁₂ N ₂ O ₃	50-06-6	2000290	3,5-Pyrazolidinedione, 4-butyl-1,2-diphenyl-	50-33-9
2000086	Azirino[2'3':3,4]pyrrolo[1,2- <i>a</i>]indole-4,7-dione, 6-amino-8- \equiv		50-07-7	2000306	2-Propanaminium, <i>N</i> -methyl- <i>N</i> -(1-methylethyl)- <i>N</i> -[2-[(9 <i>H</i> - \equiv xanthen-9-ylcarbonyl)oxy]ethyl]-, bromide	50-34-0
				2000311	1 <i>H</i> -Isoindole-1,3(2 <i>H</i>)-dione, 2-(2,6-dioxo-3-piperidinyl)-	50-35-1
					C ₁₃ H ₁₀ N ₂ O ₄	
				2000397		50-36-2

Section 2
Low Molecular Chain-like Organic
Compounds

Section-Structure
NumberClass-Reference
Number
in The Gazette List

B 1 Hydrocarbons

B 11 Saturated hydrocarbons

C_nH_{2n+2}

1	Methane	1
2	Ethane	2
3	Propane	3
4	Butane	4
5	Pentane	5
6	Hexane	6
7	Heptane	7
8	Octane	8
9	Nonane	9
10	Alkane (C 10-29)	10
11	Squalane	9-762
12	2, 6, 10, 15, 19, 23-Hexamethyltetra- cosane	9-1317