

3E Company HazMat Management Web Seminar Series

“Importance of Chemical Classes in the World of
Chemical Regulations”



Ariel

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Web Seminar Instructions



- The preferred screen resolution is 1024 X 768
- If you have popup blockers please disable them to optimize the visual presentation.
- If you do not have access to the internet, please call (US & Canada) 1-877-407-0625 or (International) +1-201-689-8548.
- Click Q&A button to submit your questions. Questions will be answered at the end of the presentation.
- The web seminar will be recorded. The audio and visual presentation link will be sent to you after the web seminar.

Guest Speaker

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Importance of Chemical Classes in the World of Chemical Regulations

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Importance of Chemical Classes in the World of Chemical Regulations

- A simplified view of the regulatory process
- A real-world example – cadmium
- Commonly regulated chemical classes
- Compliance issues
- A computerized solution
- Ariel generics – what do they look like and how do they work
- What generics can and can't do for you
- What should you remember?

A Simplified View of the Regulatory Process

- Researchers conduct experiments on the effects of specific chemical compounds on humans and animals
- Similar chemicals are often evaluated within a single study, or by other researchers
- Once a sufficient body of evidence has been developed, advisory groups (such as IARC and ACGIH) carefully draw generalizations from the data and make overall recommendations, often for entire classes of similar chemicals
- Regulatory bodies tend to rapidly adopt these recommendations as published

Cadmium – A Real-World Example

- In 1994, IARC published a monograph (Volume 58), which included a section on cadmium and cadmium compounds
- Evidence was cited for cadmium metal, 9 specific cadmium compounds, and 4 cadmium/copper alloys
- IARC changed its overall evaluation for cadmium and cadmium compounds from 2A (Probably carcinogenic to humans) to 1 (Carcinogenic to humans)

Cadmium – A Real-World Example

- Also in 1994, ACGIH changed its recommended TWA for cadmium and cadmium compounds from 0.05 mg/m³ to 0.01 mg/m³ for total dust and 0.002 mg/m³ for respirable dust
- Many (but not all) countries have since adopted identical exposure limits – *all based on experimental data for a limited number of compounds*
- Ariel/3E have identified more than 270 cadmium compounds of commercial interest that are regulated as a result

Commonly Regulated Chemical Classes

- Compounds of metals
- Heavy metal compounds
- Salts and/or esters of acids
- Salt forms of pharmaceuticals
- Isomers of certain compounds
- Polychlorinated biphenyls
- Asbestos
- Polychlorinated dibenzodioxins and furans
- Halogenated alkanes
- Steroids
- Nitroso compounds
- Azo dyes
- Organophosphorus pesticides
- Hydrates
- Substances classified as known human carcinogens according to Directive 67/548/EEC

Compliance Problems

- Chemical regulations rarely list all of the chemicals covered but instead include “generic” entries to cover these classes of chemicals
- Determining if a specific chemical is regulated then becomes quite difficult and time-consuming, requiring
 - detailed knowledge of the chemistry of the substance in question
 - broad knowledge of chemistry to determine which, if any, chemical classes are relevant
 - understanding of the difference between “classical” chemistry and “regulatory” chemistry

Compliance Problems

- The 2005 ACGIH TLV list contains 663 entries, several of which do not reference specific CAS numbers
- Of these, Ariel/3E have identified 182 which potentially affect chemicals that are not explicitly listed by CAS number
- For those 182 entries, we have identified more than 8,300 additional CAS numbers which may be covered this list

Compliance Problems

- Annex I of Directive 67/548/EEC lists 3,364 Index Numbers (as of the 29th ATP)
- Approximately 3500 CAS numbers are given in the published list
- Ariel/3E have identified a total of nearly 9,000 chemicals which are affected by this list

A Computerized Solution

- Ariel/3E and others market databases containing regulatory information, searchable primarily by CAS number
- One solution to the compliance problem would be to add all of the identified CAS numbers to each of these databases
- However, maintenance of these databases would be very difficult and there would be massive duplication of data (and opportunities for error)

A Computerized Solution

- A computerized look-up table provides the needed solution
 - Every entry on a list is given an identifier, even if no CAS number is given in the source document
 - For certain chemical classes, a standardized labeling system can be used
 - A look-up table is created for each class identifier, containing the CAS numbers for compounds of commercial interest which have been identified as belonging to that class
 - When searching a database for a particular CAS number, the software must also search the look-up table to see if any of the classes to which that chemical belongs are listed

What do Ariel generics look like?

- Certain types of groups get special standardized identifiers
 - Metal compounds (e.g., cadmium, zinc, etc.)
 - Alkanes (e.g., hexane, nonane, etc.)
 - Derivatives of specific compounds (e.g., salts of pentachlorophenol)
- Any identifier can be a parent, including CAS numbers

What do Ariel generics look like?

- Metal compounds are identified by the symbol for the element (e.g., S~CD~C)
 - S~ says this is a special generic group
 - CD says this is for cadmium
 - ~C says this is for all compounds of cadmium
 - Many other final codes can be used (~I for inorganic compounds, ~A for alkyl compounds, ~W for water-soluble salts)
 - Standard coding system has been established

What do Ariel generics look like?

- Groups of alkanes are identified similarly (e.g., S~ALK6~C)
 - S~ says this is a special generic group
 - ALKn says this is for alkanes with n carbons
 - ~C says this is for all isomers
- Exceptions can also be applied – for example, S~ALK6~CE1 is defined as “Hexane, all isomers except n-Hexane”

What do Ariel generics look like?

- Derivatives of specific compounds are given identifiers based on the CAS number of the compounds (e.g., T87865)
 - 87-86-5 is the CAS number for pentachlorophenol
 - T87865 stands for “salts of pentachlorophenol”
 - Other codes can be used as well (TG = “esters of ...”, TE = “salts and esters of ...”, etc.)

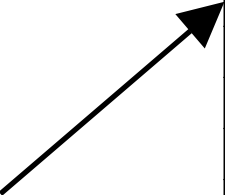
What do Ariel generics look like?

- Any CAS number or other identifier can represent a generic group as well
 - CAS 1319-77-3 is defined as mixed isomers of Cresol, therefore the CAS numbers for all 3 isomers have been linked to this CAS number
 - SEQ101855 has been defined to represent diesel fuel, for which 6 CAS numbers have been identified

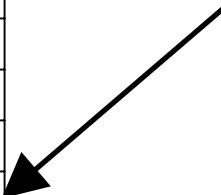
What do Ariel generics look like?

CHI	PAR
547671	S~NI~C
557197	S~NI~C
1271289	S~NI~C
1303226	S~NI~C
1313991	S~NI~C
1314063	S~NI~C
2223952	S~NI~C
3264822	S~NI~C
3333673	S~NI~C
3349062	S~NI~C
3906556	S~NI~C
4454164	S~NI~C
4995919	S~NI~C
6018924	S~NI~C
7580316	S~NI~C
7718549	S~NI~C
7786814	S~NI~C
8007189	S~NI~C

These are CAS numbers of some nickel compounds



S~NI~C is the identifier for "nickel compounds"



How do Ariel generics work?

- Search for Cadmium chloride (10108-64-2)

▼ U.S. Federal, Workplace

ACGIH Threshold Limit Values (2005)

CAS RN: 10108-64-2 regulated as a member of the Generics group for CAS RN: S~CD~C
Generics group name: CADMIUM AND COMPOUNDS, AS CD
Carcinogen Category: A2 (Suspected Human Carcinogen)
The 8-Hour Exposure Limit (TLV-TWA) is 0.01 mg/m3.
Molecular Weight: 112.40
TLV Basis -- Critical Effect(s): Kidney
Note(s): ac24

CAS RN: 10108-64-2 regulated as a member of the Generics group for CAS RN: S~CD~C
Generics group name: CADMIUM AND COMPOUNDS, AS CD, RESPIRABLE FRACTION
Carcinogen Category: A2 (Suspected Human Carcinogen)
The 8-Hour Exposure Limit (TLV-TWA) is 0.002 mg/m3.
Molecular Weight: Varies
TLV Basis -- Critical Effect(s): Kidney
Note(s): ac24

Notes

Code	Explanation
ac24	ACGIH has also assigned Biological Exposure Indices (BEIs) for this substance. BEIA: See BEI for Acetylcholinesterase Inhibiting Pesticides. BEIM: See BEI for Methemoglobin Inducers.

How do Ariel generics work?

- Search for Barium sulfate (7727-43-7)

▼ U.S. Federal, Workplace

ACGIH Threshold Limit Values (2005)

CAS RN: 7727-43-7

Name: BARIUM SULFATE

The 8-Hour Exposure Limit (TLV-TWA) is 10 mg/m³.

Molecular Weight: 233.43

TLV Basis -- Critical Effect(s): Pneumoconiosis (baritosis)

CAS RN: 7727-43-7 regulated as a member of the Generics group for CAS RN: S~BA~D

Generics group name: BARIUM AND SOLUBLE COMPOUNDS, AS BA

Carcinogen Category: A4 (Not Classifiable as a Human Carcinogen)

The 8-Hour Exposure Limit (TLV-TWA) is 0.5 mg/m³.

Molecular Weight: 137.30

TLV Basis -- Critical Effect(s): Irritation; GI; muscles

How do Ariel generics work?

- Search for Cadmium sulfate hydrate (10101-41-4)

Germany. List of Water-Endangering Substances. VwVwV on the Classification of Water-Endangering Substances & KBwS decisions

CAS RN: 7790-84-3 regulated as a member of the Generics group for CAS RN: 10124-36-4

Generics group name: CADMIUMSULFAT

WGK Identification Number: 564

The WGK class is: 3 (severely water-endangering)

Note(s): vwa

Notes

Code	Explanation
vwa	Source: Annex 1 or Annex 2

How do Ariel generics work?

- Search for Cadmium sulfate hydrate (10101-41-4)

EU Directive 67/548/EEC on the classification, packaging, and labelling of dangerous substances, Annex I, as last amended by Directive 2004/73/EC (29th AT)

CAS RN: 7790-84-3 regulated as a member of the Generics group for CAS RN: 10124-36-4

Generics group name: CADMIUM SULPHATE

Annex I EC number: 2333316

Annex I Index number: 048-009-00-9

Risk Phrases: 45, 46, 60, 61, 25, 26, 48/23/25, 50/53

Safety Phrases: 53, 45, 60, 61

Symbols Required: T+, N

Classification on the basis of the specific effects on human health: C2, M2, R2

EU Dangerous Substances Directive Danger Classification: T, T+, T, N

Note(s): Nota E, am29

CAS RN: 7790-84-3 regulated as a member of the Generics group for CAS RN: S~CD~CE3

Generics group name: CADMIUM COMPOUNDS, WITH THE EXCEPTION OF CADMIUM SULPHOSELENIDE (XCDS.YCDSE), MIXTURE OF CADMIUM SULPHIDE WITH ZINC MIXTURE OF CADMIUM SULPHIDE WITH MERCURY SULPHIDE (XCDS.YHGS) ... (0,1%≤C<0,25%)

Annex I Index number: 048-001-00-5

Risk Phrases: 20/21/22

Symbols Required: Xn

Note(s): Nota 1

What can't generics do?

- Resolve situations where regulations give conflicting data
- Determine how to classify a chemical according to a physical property (e.g., solubility)
- Interpret exemptions, special rules, etc., that are particular to a specific regulation (e.g., hydrate exemptions on national inventories)
- Give information on every CAS number in existence (there are more than 25 million of them)

What should you remember?

- Broad conclusions about classes of chemicals are often drawn on the basis of evidence for only a few members of the class
- Generic classes of chemicals are present in nearly every chemical regulation
- A computerized generics database can assist you in finding all of the relevant regulatory information for a specific chemical, even if it is not explicitly listed in a chemical regulation
- A generics database *cannot* answer all questions related to a regulation – ultimately, you as the expert must make the final decision on what data are correct in your particular situation