

GHS data for solutions

Experimental data for solutions are available for relatively few chemicals, apart from the most common industrial chemicals, such as sodium hydroxide and sulfuric acid. In the absence of experimental data, RiskAssess applies the rules in the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) [1] to estimate the hazardous properties of solutions based on those of the pure chemicals. In general, these rules are conservative, but provide a general guide.

RiskAssess provides solution data only for aqueous solutions. If a solvent other than water is used, the user needs to consider the hazardous properties of the solvent (e.g. flammability), using the GHS rules. The concentrations of aqueous solutions are often limited by the solubility of the chemical in water at room temperature ($\sim 20^{\circ}\text{C}$). RiskAssess provides solubility data when appropriate.

Chemicals are classified in categories and sub-categories in the GHS system. RiskAssess does not show these categories and sub-categories, since most people will be interested only in the signal words, pictograms and hazard statements. Classification information is available from manufacturers' safety data sheets (SDSs), Safe Work Australia [2], the European Chemicals Agency (ECHA) [3] and numerous other sources.

Once a chemical solution has been classified, the set of rules in the GHS [1] prescribes the manner in which the solution should be labelled, using a signal word, pictogram(s) and hazard statement(s). Precautionary statements are also defined and can be found in the SDS and in the original labelling of a chemical. Many of the precautionary statements are not appropriate to the school situation. To better assist users, RiskAssess provides information about "Potential Hazards" and "Standard Handling Procedures" for each chemical. These are tailored to the school situation, based on chemical experience and authoritative sources. RiskAssess also converts the GHS solution data defined in % wt/wt to molarity, since this is the unit most commonly used in schools.

The GHS [1] classifies physical, health and environmental hazards. Solutions posing health or environmental hazards have specific hazards that can be estimated using rules in the GHS on the basis of the hazardous properties of the pure chemical. However, no GHS rules are provided for solutions posing physical hazards (e.g. flammability); classification is solely on the basis of experimental measurements of their physical properties.

The following descriptions of solution classifications are summaries and simplifications from the GHS [1], which should be consulted for more detailed information.

Acute toxicity

Acute toxicity has five ranges according to the GHS based on oral toxicity (lethal dose for 50% of the population):

- Category 1 <5 mg/kg bodyweight
- Category 2 5-50 mg/kg bodyweight
- Category 3 50-300 mg/kg bodyweight
- Category 4 300-2000 mg/kg bodyweight
- Category 5 2000-5000 mg/kg bodyweight

Similar ranges are defined on the basis of skin absorption and inhalation, but these are rarely relevant to the school situation.

Category 5 is rarely used by authorities in the classification of pure chemicals. Chemicals less acutely toxic than 5000 mg/kg bodyweight can be classified only if reliable evidence is available indicating a human effect.

Experimental data for acute toxicity are variable, but there is usually agreement as to the category. Highly toxic chemicals, in Category 1 and Category 2, are rarely found in schools. Most acutely toxic chemicals used in schools are Category 3 or Category 4.

In calculating the acute toxicity of solutions, water acts as an inert diluent. For example, a 10% wt/wt solution of a chemical with an acute toxicity of 60 mg/kg bodyweight (Category 3) would be regarded as having an acute toxicity of 600 mg/kg (Category 4).

Solution data for acute toxicity in RiskAssess are based on the most conservative estimates of dilution needed to reduce the acute toxicity to the next (less toxic) category. Hazard statements appropriate to the more concentrated solution are maintained until the most conservative estimate of dilution ensures that the lower level of acute toxicity has been reached. For example, a Category 3 chemical is assumed to have a toxicity of 50 mg/kg bodyweight (the most toxic limit of the range) and its solutions maintain the hazard warnings of the original chemical until it has been diluted 1/6, to a maximum toxicity of 300 mg/kg bodyweight (17% wt/wt). After that, hazard warnings for Category 4 are maintained until the original chemical has been diluted 1/40, to a maximum toxicity of 2000 mg/kg bodyweight (2.5% wt/wt). Then, hazard warnings for Category 5 are maintained until the original chemical has been diluted 1/100 (1% wt/wt). At dilutions greater than 1/100 (less acutely toxic than 5000 mg/kg), the chemical is not classified by GHS and no warnings are given regarding acute toxicity.

Category of pure substance	% wt/wt in solution	Category of solution
Category 1 (1 mg/kg)	100 - 20	Category 1
	20 - 2	Category 2
	2 - 0.3	Category 3
	0.3 - 0.05	Category 4
	0.05 - 0.02	Category 5
	<0.02	not classified
Category 2	100 - 10	Category 2
	10 - 2	Category 3
	2 - 0.25	Category 4
	0.25 - 0.1	Category 5
	<0.1	not classified
Category 3	100 - 17	Category 3
	17 - 2.5	Category 4
	2.5 - 1	Category 5
	<1	not classified
Category 4	100 - 15	Category 4
	15 - 6	Category 5
	<6	not classified
Category 5	100 - 40	Category 5
	<40	not classified

These assignments of solution toxicity are highly conservative and may be revised as better experimental data become available in the future.

Skin corrosion/irritation

Skin corrosion/irritation has three categories according to the GHS:

- Category 1 skin corrosion
- Category 2 skin irritation
- Category 3 mild skin irritation

A crucial division is between "corrosion" and "irritation". Skin "irritation" is reversible, but "corrosion" results in permanent skin damage.

Experimental data for skin corrosion/irritation are highly variable. There is frequently disagreement about whether a chemical is Category 1 (causing permanent skin damage) or Category 2 (causing reversible irritation). In RiskAssess, the more conservative assignments have generally been used for the pure chemicals, with the result that solution data are also conservative.

For solutions of chemicals for which experimental data are not available, the following rules are provided by GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1	100 - 5 5 - 1 <1	Category 1 Category 2 not classified
Category 2	100 - 10 10 - 1 <1	Category 2 Category 3 not classified
Category 3	100 - 10 <10	Category 3 not classified

There is a special situation for strongly acidic or alkaline solutions: solutions of acids with a pH < 2 or solutions of bases with pH > 11.5 are regarded as Category 1.

Serious eye damage/irritation

Serious eye damage/irritation has two categories according to the GHS:

Category 1 serious eye damage (irreversible effects on the eye)

Category 2 eye irritation (reversible effects on the eye)

Experimental data for serious eye damage/irritation are variable.

In RiskAssess, the more conservative assignments have generally been used for the pure chemicals, with the result that solution data are also conservative.

For solutions of chemicals for which experimental data are not available, the following rules are provided by GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1	100 - 3 3 - 1 <1	Category 1 Category 2 not classified
Category 2	100 - 10 <10	Category 2 not classified

There is a special situation for strongly acidic or alkaline solutions: acids with a pH < 2 or bases with pH >11.5 at concentrations >1% wt/wt are regarded as Category 1.

Respiratory or skin sensitisation

For both respiratory sensitisation and skin sensitisation there is only one category (Category 1) and it has two sub-categories:

- Sub-category 1A High frequency in humans (or probably, from animal studies)
- Sub-category 1B Moderate to low frequency in humans (or probably, from animal studies)

There is disagreement between authorities as to the concentration below which a solution containing a sensitiser should no longer be classified when experimental data are not available. RiskAssess adopts the most conservative view and maintains classification as a respiratory or skin sensitiser to concentrations of 0.1% wt/wt.

Category of pure substance	% wt/wt in solution	Category of solution
Category 1 (1A or 1B)	100 – 0.1 <0.1	Category 1 not classified

Germ cell mutagenicity

Germ cell mutagenicity has three categories/subcategories according to the GHS:

- Category 1A Substances known to induce heritable mutations in the germ cells of humans
- Category 1B Substances that should be regarded as if they induce heritable mutations in the germ cells of humans (on basis of animal experiments)
- Category 2 Substances that may possibly induce heritable mutations in the germ cells of humans (on basis of animal experiments)

For solutions of chemicals for which experimental data are not available, the following rules are provided by GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1 (1A or 1B)	100 - 0.1 <0.1	Category 1 not classified
Category 2	100 - 1 <1	Category 2 not classified

Carcinogenicity

Carcinogenicity has three categories/subcategories according to the GHS:

- Category 1A Known to have carcinogenic potential for humans,
largely based on human evidence
- Category 1B Presumed to have carcinogenic potential for humans,
largely based on animal evidence
- Category 2 Suspected human carcinogen,
based on human and animal evidence

For solutions of chemicals for which experimental data are not available, the following rules are provided by GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1 (1A or 1B)	100 – 0.1 <0.1	Category 1 not classified
Category 2	100 – 0.1 <0.1	Category 2 not classified

Reproductive toxicity

Reproductive toxicity has three categories/subcategories according to the GHS:

- Category 1A Known human reproductive toxicant,
largely based on data from humans
- Category 1B Presumed human reproductive toxicant,
largely based on data from animals
- Category 2 Suspected human reproductive toxicant,
based on data from either animals or humans

For solutions of chemicals for which experimental data are not available, the following rules are provided by GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1 (1A or 1B)	100 – 0.1 <0.1	Category 1 not classified
Category 2	100 – 0.1 <0.1	Category 2 not classified

Some authorities allow a cutoff of 0.3% wt/wt in some circumstances, but RiskAssess has adopted the more cautious values shown above.

Specific target organ toxicity – single exposure

Specific target organ toxicity – single exposure has three categories according to the GHS:

- Category 1 Significant toxicity, after single exposure based on data from human or animal studies
- Category 2 Presumed toxicity, after single exposure based on data from human or animal studies
- Category 3 Transient target organ effects, based on data from human or animal studies

For solutions of chemicals for which experimental data are not available, the following rules are provided by GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1 (1A or 1B)	100 – 1 <1	Category 1 not classified
Category 2	100 – 1 <1	Category 2 not classified
Category 3	100 – 20 <20	Category 3 not classified

Some authorities allow a cutoff of 10% wt/wt on a label, but RiskAssess has adopted the more cautious values shown above. Category 3 is rarely used and the 20% cutoff is recommended in the GHS.

Specific target organ toxicity – repeated exposure

Specific target organ toxicity – repeated exposure has two categories according to the GHS:

- Category 1 Potential to produce significant toxicity, after repeated exposure based on data from human or animal studies
- Category 2 Presumed potential to harm health, after repeated exposure based on data from human or animal studies

For solutions of chemicals for which experimental data are not available, the following rules are provided by GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1 (1A or 1B)	100 – 1 <1	Category 1 not classified
Category 2	100 – 1 <1	Category 2 not classified

Some authorities allow a cutoff of 10% wt/wt on a label, but RiskAssess has adopted the more cautious values shown above.

Aspiration hazard

Aspiration hazard has two categories according to the GHS:

- Category 1 Cause, or may be regarded as if they cause, human aspiration toxicity
- Category 2 Cause concern due to a presumption that they cause human aspiration toxicity

For solutions of chemicals for which experimental data are not available, the following rules are provided by GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1	100 – 10 <10	Category 1 not classified
Category 2	100 – 10 <10	Category 2 not classified

Viscosity must be considered for classification of solutions.

In practice, chemicals posing an aspiration hazard are usually non-aqueous and have low solubility in water. Aqueous solutions of such chemicals would rarely be used in schools.

Hazardous to the aquatic environment

Acute toxicity

Acute toxicity to the aquatic environment has three categories according to the GHS:

- Category 1 LD 50 <1 mg/L for a variety of animals
- Category 2 LD 50 1 - 10 mg/L for a variety of animals
- Category 3 LD 50 10 - 100 mg/L for a variety of animals

Chronic toxicity

Chronic toxicity to the aquatic environment has three categories according to the GHS, for rapidly degradable substances with adequate experimental data:

- Category 1 No observable effect <0.01 mg/L for a variety of animals and plants
- Category 2 No observable effect <0.1 mg/L for a variety of animals and plants
- Category 3 No observable effect <1 mg/L for a variety of animals and plants

Different concentrations apply for substances that degrade slowly and have adequate data. Substances without adequate experimental data are assessed on the basis of short-term toxic effects. Consult the GHS [1] for details.

Acute and chronic toxicity

In general, the different categories involve a 10-fold difference in toxic effects. For solutions of chemicals for which experimental data are not available, RiskAssess uses the following rules based on the GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1	100 – 10	Category 1
	10 - 1	Category 2
	1 – 0.1	Category 3
	<0.1	not classified
Category 2	100 – 10	Category 2
	10 - 1	Category 3
	1 – 0.1	not classified
Category 3	100 – 10	Category 3
	<10	not classified

Information on toxicity to the aquatic environment is often not provided by manufacturers, since many jurisdictions do not require it. Often, there is inconsistency in the data presented for chemically similar substances; in these cases, RiskAssess applies the most reliable data to all the chemically similar substances.

Hazardous to the ozone layer

Hazardous to the ozone layer has one category according to the GHS:

Category 1 Any substance listed in the Annexes of the Montreal Protocol

For solutions of chemicals for which experimental data are not available, the following rules are provided by GHS:

Category of pure substance	% wt/wt in solution	Category of solution
Category 1	100 – 0.1 <0.1	Category 1 not classified

Chemicals posing a hazard to the ozone layer are organic compounds containing chlorine and bromine. There is relatively little use of such chemicals in schools and most of them do not dissolve in water at concentrations higher than 0.1% wt/wt.

[1] United Nations "Globally Harmonized System of Classification and Labelling of Chemicals (GHS)" 6th ed., New York and Geneva, 2015. Free download from http://www.unece.org/trans/danger/publi/ghs/ghs_rev06/06files_e.html

[2] Safe Work Australia "Hazardous Substances Information System"
<http://www.safeworkaustralia.gov.au/sites/swa/whs-information/hazardous-chemicals/hsis/pages/hsis>

[3] European Chemicals Agency "Classification and Labelling Inventory"
<http://echa.europa.eu/information-on-chemicals/cl-inventory-database>