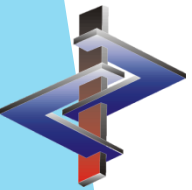


Creating a Preparation

Introduction

- **Raw Materials are those with a CAS number and Preparations are a combination of Raw Materials.**
 - Many companies have Raw Materials that are in actuality intermediate products consisting of Raw Materials (CAS Numbers).
 - It is necessary to set up these intermediates in ChemGes as preparations, so that, for calculation, as is legislatively required, they can be broken down into their Raw Materials.
 - This also means that data/classification changes need to be done at the lowest level of the breakdown, so that they carry through. (i.e. Changing the classification of an intermediate will not carry through to the final product – it is necessary to change the Raw Material Data so that it leads to the desired change).
- **ChemGes does not contain any Preparations by default.**

Please direct additional questions to our hotline
Via telephone at +1 (902) 832-3425 or +43 2628 619 00
Via email to info@dr-software.com



Introduction

- **ChemGes calculations are based on formulae from the legislation**, as far as they exist and on formulae based on the legislation, generated by our staff of experts.
 - We do not base our calculations or data on 'Guidance Documents' (ie ECHA, EPA,...). When there is a discrepancy, the legislation takes precedence.
- **Transport legislation calculation**
 - In most cases, it is possible to calculate a specific transport classification, but some classes, as well as often the UN Numbers, require human input. In such cases, ChemGes will make an educated and logical suggestion.
 - Our Programmers, Chemists and Transport experts have created a system for 'calculating' the transport classification based on the data of the preparation (classification, physical data,...) and the data, or lack thereof, of the individual raw materials, where clear formulae are not present in the legislation.
 - We recommend that you review the transport classification output by ChemGes. Feel free to make changes to the transport classification and/or to the settings for transport, if these are based on sound data from another source.
 - Further details about transport classifications in ChemGes, can be found in the manual located on the downloads page of our Website www.dr-software.com or accessible through the *Help* option in ChemGes (*General Help*) or in the **Transport** power point.

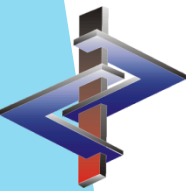
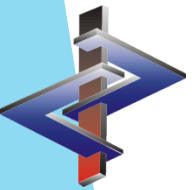


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1. Entering the Formula

- Ingredients can be entered by their CAS Number, their name, a partial search string or an internal Product Code.
- For each ingredient, enter the percentage at which it is contained in the preparation.
- Even though non-hazardous ingredients do not have to appear on your SDS, it is recommended to input all ingredients when generating the formulation, as this way calculations performed by ChemGes can be more exact.
- You can enter ranges and $<$, $>$, \leq , \geq and \sim . ChemGes then performs all calculations (classification, physical data,...) using these range values.
- By hovering your mouse over the various fields pertaining to each substance, you can view additional information.

The screenshots illustrate the 'Formulation' screen in ChemGes, showing the process of entering ingredients and their percentages. The interface includes a menu bar (File, Edit, Preparation screens, Help) and a toolbar (Basic screen, Formulation, Physical data, Flammability, Country specific classifications, Land transport, Sea and air transport). The main area displays a list of substances with columns for Substance number, Description, Symbols, and Percent. A detailed view of a substance (formaldehyde) is shown, including its CAS number, Index number, EC number, State, Flash point, Boiling point, Melting point, Density, and Miscibility/solubility. A tooltip for ethanol shows its EU list (Standard, EU list) and other properties. A hazard classification tooltip for formaldehyde shows various hazard symbols and their corresponding H and P codes, such as H301+H311+H331 (Toxic if swallowed, in contact with skin or if inhaled) and H314 (Causes severe skin burns and eye damage).

2. Entering Additional Data

The image shows two overlapping windows from the ChemGes software. The background window is titled "Physical values and general information" and has tabs for "Basic screen", "Formulation", "Physical data", "Flammability", "Country specific classifications", "Land transport", and "Sea and air transport". The "Physical data" tab is active, showing a list of properties with values entered in yellow boxes. The foreground window is titled "Fire and explosion risks" and has tabs for "Country specific classifications", "Land transport", "Sea and air transport", "Basic screen", "Formulation", "Physical data", and "Flammability". The "Flammability" tab is active, showing a list of risk assessment criteria with checkboxes and values entered in blue boxes.

Physical values and general information

1 State	liquid
2 Flash point	-4 °C
3 Boiling point	77 - 78 °C
04 Melting point	4 °C
5 Water miscible/water soluble	<input type="checkbox"/>
6 Density	> 0.66692 - < 1.29473 g/cm ³
7 Bulk density	> 666.9 - < 1294.7 kg/m ³
8 pH-value	4 - 6
9 Solids	≤ 10.0 %
10 Flammable substances	~ 42 - ≤ 60 %
11 Ignition temperature	~ 300 °C
12 Chemical heat of combustion	
13 Viscosity bei 20°C	
14 at 40°C	
15 Vapor pressure bei 20.0 °C	97 hPa
16 bei 50.0 °C	360 hPa
17 Explosion limits	1.2 - 73 Vol%
18	46 - 910 g/m ³
19 Contains ≥ 10 % nitro cellulose	<input type="checkbox"/>

Fire and explosion risks

Please check the system made proposal

1 The product is flammable or explosive	<input checked="" type="checkbox"/>
2 The product is explosive	<input checked="" type="checkbox"/>
3 Extremely explosive	<input type="checkbox"/>
4 The product is fire promotive or contains peroxides	<input type="checkbox"/>
5 The product contains organic peroxides	<input type="checkbox"/>
6 The product forms flammable gas with water or air	<input type="checkbox"/>
7 The product is dusty and has an explosive range with air	<input type="checkbox"/>
8 The product has its ignition range at 1 bar and room temperature	<input type="checkbox"/>
9 The gas is liquefied	<input type="checkbox"/>
10 The product is self igniting in the air at room temperature	<input type="checkbox"/>
11 Flash point 30 °C	<input checked="" type="checkbox"/>
12 The boiling point is under 35 °C	<input checked="" type="checkbox"/>
13 The product promotes burning	<input checked="" type="checkbox"/>
14 During usage an ignition risk exists	<input type="checkbox"/>

Black indicated fields are without significance for the calculation

- After inputting the formulation, ChemGes automatically takes you to two screens, where you are shown some initial calculations.
- Here, please input any additional data for your preparation, that you might have, and check the data provided by ChemGes.
- ChemGes has marked the data provided automatically, based on the ingredients, in yellow and blue.
- Appropriate formulae are used when applicable.
- Certain data, such as Flash Point, cannot be calculated. Therefore, the worst-case-scenario is output.

3. Understanding the Calculation Results

GHS Classification: Here you can see the details to the classification results based on the different forms of the GHS. (see [',GHS in Brief' Power Point for details](#))

If you wish to change these classifications, that is certainly possible, but be aware that any such changes must have solid reasons to back them up.

DPD Classification: These are the results based on the old system, using R and S Phrases.

Transport: The transport classification for the ADR, DOT, IMDG, and IATA are output here. (see [',Transport' Power Point for details](#))

On this screen, you can also find **WHMIS 1988** and **NFPA/HMIS**.

The **Quotients** Button, at the bottom of the screen, lets you examine the calculations that have lead to the classification of your preparation. (see [',Quotients' Power Point for details](#))

The screenshot displays the 'Maintenance of preparations' software interface. The window title is 'Maintenance of preparations'. The menu bar includes 'File', 'Edit', 'Preparation screens', 'Print programs', 'Additional functions', and 'Help'. The main window has several tabs: 'Basic screen', 'Formulation', 'Physical data', 'Flammability', 'Country specific classifications', 'Land transport', and 'Sea and air transport'. The 'Basic screen' tab is active, showing the following information:

- Preparation: 1,000
- Resin solution X 50
- Product code: 1234567890
- Article group: [] []
- Flag: Internal Storage Code: 123/456/789

The 'GHS classification' section is highlighted in yellow and contains the following details:

- Danger**
 - 3.10/1; Asp. Tox. 1 - H304 May be fatal if swallowed and enters airways.
 - 3.7/2; Repr. 2 - H361 Suspected of damaging fertility or the unborn child.
 - 3.7/2; Repr. 2 - H361d Suspected of damaging the unborn child.
 - 3.9/2; STOT RE 2 - H373 May cause damage to organs through prolonged or repeated exposure.
- Warning**
 - 2.6/3; Flam. Liq. 3 - H226 Flammable liquid and vapour.
- Warning**
 - 3.2/2; Skin Irrit. 2 - H315 Causes skin irritation.
 - 3.3/2A; Eye Irrit. 2A - H319 Causes serious eye irritation.
 - 3.3/2; Eye Irrit. 2 - H319 Causes serious eye irritation.
 - 3.4/1; Skin Sens. 1 - H317 May cause an allergic skin reaction.
 - 3.8/3; STOT SE 3 - H336 May cause drowsiness or dizziness.

The 'Transport' section is highlighted in yellow and contains the following details:

- ADR: 3
- ADR Code: F1, PG: III, UN: 1866
- DOT: 3
- PG: III, UN: 1866
- IMDG: 3
- PG: III, UN: 1866, EmS: F-E, S-E
- IATA: 3
- PG: III, UN: 1866

The 'WHMIS' and 'NFPA' sections are also highlighted in yellow. The 'WHMIS' section shows a hazard symbol (flame) and a health symbol (exclamation mark). The 'NFPA' section shows a hazard diamond with a 3 in the red section, a 1 in the blue section, and a 0 in the yellow section. The 'DPD classification' section is highlighted in yellow and contains the following details:

- Xn
- N; R10-36/38-43-48/20-51/53-63-65-67; S2-13-23-24/25-26-29/56-37-43h-46-51-52-57-60-64; Z2

The bottom of the screen shows a status bar with various keyboard shortcuts and a 'Quotients' button highlighted in yellow.

4. Further Data Entry

Tox Values: Here you can enter Toxicological Value Data for the preparation itself.

Names: In this field, you can enter/edit the names of the Preparation in various languages and with various markings for application.

Country specific classification: This screen allows for the input and viewing of country specific data, such as VOCs or Water Hazard Class.

At any time, it is possible to return to any of the screens of your formulation and add or change information/data. After changes, please ensure that these changes are actually applied, by means of recalculations and reclassification of affected areas. (see ,Updating and Updates' Power Point for details)

Maintenance of preparations

File Edit Preparation screens Print programs Additional functions Help (44.4.7) 6,236, 2,756(-) (85%), 496(-), 14(-), 1 User, M 2,76MB, HD 0,37MB, C

Basic screen Formulation Physical data Flammability **Country specific classifications** Land transport Sea and air transport

Preparation 1,000 Resin solution X 50

Product code 1234567890 Article group Flag Internal Storage Code: 123/456/789

GHS classification **Transport**

Danger
3.10/1; Asp. Tox. 1 - H304 May be fatal if swallowed and enters airways.
3.7/2; Repr. 2 - H361 Suspected of damaging fertility or the unborn child.
3.7/2; Repr. 2 - H361d Suspected of damaging the unborn child.
3.9/2; STOT RE 2 - H373 May cause damage to organs through prolonged or repeated exposure.

Warning
2.6/3; Flam. Liq. 3 - H226 Flammable liquid and vapour.
3.2/2; Skin Irrit. 2 - H315 Causes skin irritation.
3.3/2A; Eye Irrit. 2A - H319 Causes serious eye irritation.
3.3/2; Eye Irrit. 2 - H319 Causes serious eye irritation.
3.4/1; Skin Sens. 1 - H317 May cause an allergic skin reaction.
3.8/3; STOT SE 3 - H336 May cause drowsiness or dizziness.

ADR: 3
ADR Code: F1, PG: III, UN: 1866
DOT: 3
PG: III, UN: 1866
IMDG: 3
PG: III, UN: 1866, EmS: F-E,S-E
IATA: 3
PG: III, UN: 1866

WHMIS **NFPA**
B2, D2A

DPD classification Xn N; R10-36/38-43-48/20-51/53-63-66-67; S2-13-23-24/25-26-29/56-37-43h-46-51-52-57-60-64; Z2
Creation Last alteration 05/09/2017 Last classification 05/09/2017

[Ctrl G] GHS-Ableitung [Alt F8] PDF files (-) [F10] Classification [Ctrl N] NFPA+HMIS [F9] Texts [Alt F3] Variants (4) [Page J] Quotients [F5] IPI [F6] Label [F8] SDS [F7] Tremcard [U] Next page [Ctrl T] Tox values [Ctrl X] Lock [Alt F11] Memo [Ctrl K] Copy [F1] Names [Ctrl F8] SDS versions [Esc] End [Ctrl F6] Delete [Home] Price

Country specific classifications

File Edit Preparation screens Help (47.0.9)

Basic screen Formulation Physical data Flammability **Country specific classifications** Land transport Sea and air transport

Seveso III: Qualified quantities: 5000 t, 50000 t, Category: P3b

Annex XVII REACH (Restrictions) 3, 28, 40

Waste # 08 01 11* Relevant waste hazards HP 3, HP 5, HP 6, HP 7, HP 8, HP 11, HP 13

Detergent Regulation: Fragrance Essential oil Dye

Cosmetic product according to Regulation 1223/2009/EC Leave-on Product

Biocidal Products Regulation

UFI code: Company DR Software GmbH Code 0J10-00EH-S009-RGPK

ECHA notification ABM (Z(1))

Chemical Safety Assessment available MAL-Code 5-6

WHC (Water hazard class) 3

Storage class (LGK) acc. to TRGS510 2 B

VbF BetrSichV

The product is subject to annex 2 of the ChemVerbotsV

GISCode (BG BAU)

Coating VOC value: Wood preservative

[Esc] End [F4] Printout of documentation for WHC [Ctrl W] Water hazardous contents [Ctrl A] ABM (NL) contents [Ctrl S] Solvents [Ctrl M] MAL code contents [Ctrl X] Ingredients Annex XVII [Ctrl R] REACH registry numbers [Ctrl T] Turkish registry numbers

5. Using a Preparation as an Intermediate

In order to use a preparation as an intermediate, simply create the preparation first and then enter it in the formulation screen of a new preparation, with the percentage at which it is contained.

The screenshot shows the 'Formulation' window with a table of substances and a dropdown menu open. The table lists substances with their numbers, descriptions, symbols, and percentages. The dropdown menu is open, showing options for breakdown of formulation.

Substance number	Description	Symbols	Percent
12468	formaldehyde ... %	☠️ ⚠️ ⚡️	≤ 15
78-92-2	butanol	⚠️ ⚡️	5 - ≥ 10
67-63-0	propan-2-ol	☠️ ⚠️ ⚡️	~ 4
141-78-6	ethyl acetate	☠️ ⚠️ ⚡️	≥ 15 - 25
7732-18-5	water, distilled, conductivity or of similar purity		> 6 - < 10
1330-20-7/1	xylene	⚠️ ⚡️	3 - 6
122-57-6	4-Phenyl-3-buten-2-one	⚠️ ⚡️	≤ 10
64-17-5/1	ethanol	☠️ ⚠️ ⚡️	≥ 5 - ≤ 10
10,001		☠️ ⚠️ ⚡️	4

Breakdown of formulation options:

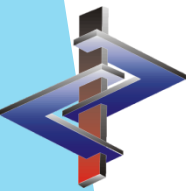
- A Output of all raw materials with hazard features
- B Output of all raw materials with the most important physical data
- C Separated breakdown of all intermediates (cumulated intermediates)
- D Breakdown of intermediates (no cumulation of same substances)
- E Nested breakdown
- F Occurrence of individual substances in the formulation
- G Composition at an earlier point in time (without breakdown)
- H Composition at an earlier point in time (with breakdown)

When such an intermediate preparation is used, the data from the raw materials (CAS Numbers) is what will be used for the calculations of the resulting preparation.

Changes made in the intermediate preparation will not carry through into the next preparation.

This is what the legislation requires.

The **Breakdown of formulation** option allows for an easy overview of the ingredients contained in the whole preparation, including the intermediate preparations.



More detailed Information can be found in the Manual to ChemGes

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