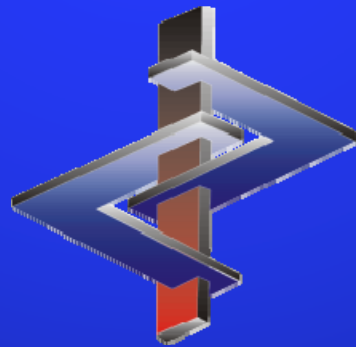


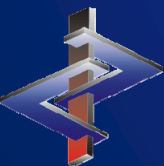
Creating a Preparation



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.

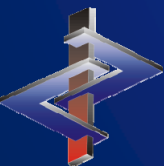
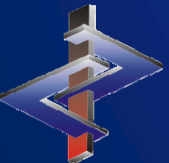


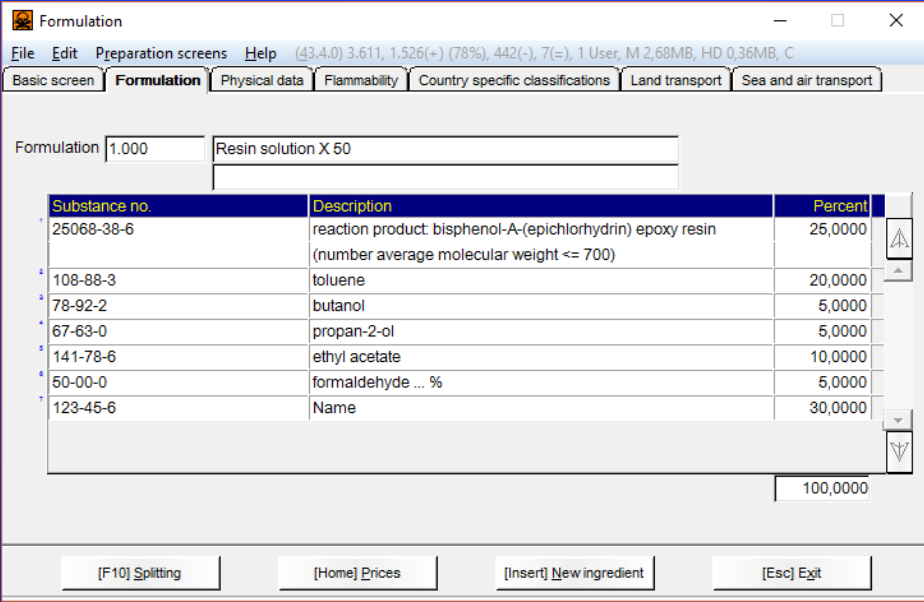
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2. Entering Additional Data
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1. Entering the Formula

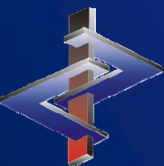
- Ingredients can be entered by their CAS Number, their name, a partial search string or an internal Product Code.
- For each ingredient, enter the percentage at which it is contained in the preparation.
- Even though non-hazardous ingredients do not have to appear on your SDS, it is recommended to input all ingredients when generating the formulation, as this way calculations performed by ChemGes can be more exact.



The screenshot shows the 'Formulation' software window. The title bar reads 'Formulation' and the menu bar includes 'File', 'Edit', 'Preparation screens', and 'Help'. Below the menu bar are several tabs: 'Basic screen', 'Formulation', 'Physical data', 'Flammability', 'Country specific classifications', 'Land transport', and 'Sea and air transport'. The 'Formulation' tab is active. In the 'Formulation' section, there are two input fields: 'Formulation' with the value '1.000' and a text field containing 'Resin solution X 50'. Below these fields is a table with three columns: 'Substance no.', 'Description', and 'Percent'. The table contains the following data:

Substance no.	Description	Percent
25068-38-6	reaction product: bisphenol-A-(epichlorhydrin) epoxy resin (number average molecular weight <= 700)	25,0000
108-88-3	toluene	20,0000
78-92-2	butanol	5,0000
67-63-0	propan-2-ol	5,0000
141-78-6	ethyl acetate	10,0000
50-00-0	formaldehyde ... %	5,0000
123-45-6	Name	30,0000

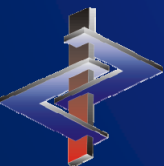
At the bottom right of the table area, there is a total percentage value of '100,0000'. At the bottom of the window, there are four buttons: '[F10] Splitting', '[Home] Prices', '[Insert] New ingredient', and '[Esc] Exit'.



2. Entering Additional Data

The image shows two overlapping software windows from ChemGes. The background window is titled 'Physical values and general information' and has tabs for 'Basic screen', 'Formulation', 'Physical data', 'Flammability', 'Country specific classifications', and 'Land transport'. The 'Physical data' tab is active, showing fields for 'Flash point' (n.a.), 'Boiling point' (-21 °C), 'Density' (0,662 g/cm³), and 'Solids' (30 %). The foreground window is titled 'Fire and explosion risks' and has tabs for 'Country specific classifications', 'Land transport', 'Sea and air transport', and 'Flammability'. The 'Flammability' tab is active, displaying a list of 14 checkboxes for hazard assessment, with several checked (e.g., 'The product is flammable or explosive', 'The product is explosive', 'The product promotes burning'). A red warning message at the top of this window reads 'Please check the system made proposal'. At the bottom, there are buttons for '[F9] Creation proposal' and '[←], [Esc] Basic screen'.

- 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](#))

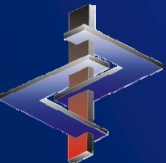
On this screen, you can also find **WHMIS 1988** and **NFPA/HMIS**.

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 main window shows the preparation name 'Resin solution X 50' and its product code '1234567890'. The interface is divided into several sections for classification details:

- GHS classification:** Lists hazard categories such as 'Danger' (3.10/1; Asp. Tox. 1 - H304), 'Warning' (2.6/3; Flam. Liq. 3 - H226), and 'Warning' (3.2/2; Skin Irrit. 2 - H315).
- DPD classification:** Shows hazard codes like 'Xn', 'N', and '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'.
- Transport:** Details transport codes including 'ADR: 3', 'DOT: 3', 'IMDG: 3', and 'IATA: 3'.
- WHMIS 1988 and NFPA/HMIS:** Displays hazard diamonds with values 1, 3, and 0.

The bottom of the screen features a toolbar with various function keys and a 'Quotients' button.



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.

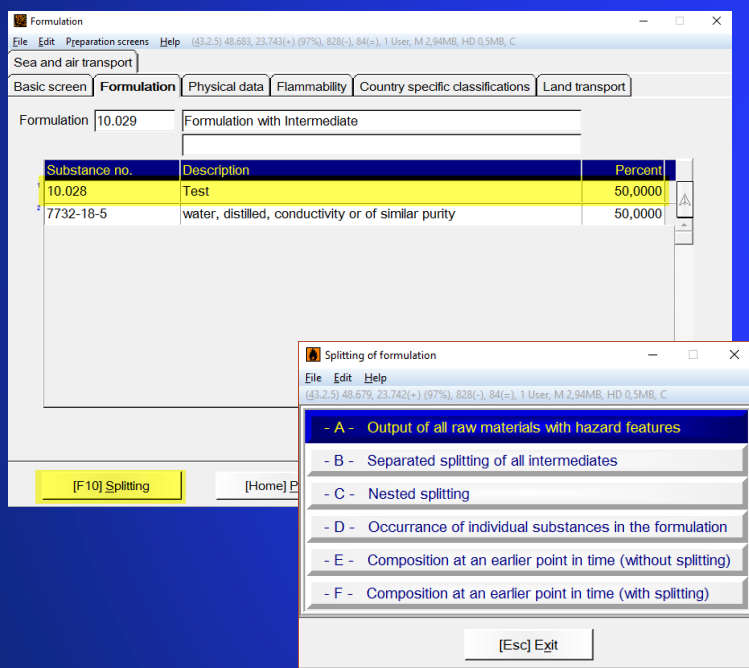
Country specific classification: This screen allows for the input and viewing of country specific data, such as VOCs or Water Hazard Class.

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)

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' software interface. The main window displays a table with the following data:

Substance no.	Description	Percent
10.028	Test	50,0000
7732-18-5	water, distilled, conductivity or of similar purity	50,0000

Below the table, there is a button labeled '[F10] Splitting'. A dialog box titled 'Splitting of formulation' is open, showing the following options:

- A - Output of all raw materials with hazard features
- B - Separated splitting of all intermediates
- C - Nested splitting
- D - Occurrence of individual substances in the formulation
- E - Composition at an earlier point in time (without splitting)
- F - Composition at an earlier point in time (with splitting)

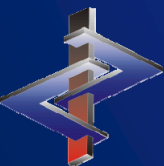
The dialog box also has an '[Esc] Exit' button at the bottom.

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 **Splitting 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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