# IUCLID 5 Guidance and Support

Installation Guide for IUCLID 5 Version 5.2 Stand-alone Application

Installer for Microsoft<sup>®</sup> Windows<sup>®</sup>



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A wealth of additional information on the European Union is available on the Internet. It can be accessed at the addresses: http://iuclid.echa.europa.eu. http://echa.europa.eu. http://europa.eu.

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# **Chapter 1. Introduction**

# **1.1. Introduction**

IUCLID 5 can be installed either as a stand-alone application, or in a multi-user environment that uses client-server architecture. This document describes how to use a dedicated installer to install IUCLID 5 as a stand-alone application on a computer running Microsoft<sup>®</sup> Windows<sup>®</sup> (hereafter referred to as Windows). The installer can be downloaded from the IUCLID 5 web site. The installation is performed by ensuring that the prerequisite software is installed, then running the installer; typically by double clicking on it. If the instructions in this document are followed with care, no prior specialist knowledge is required of either the IUCLID 5 software, or the software components required to run it.

### 1.1.1. Hardware requirements

The following requirements are provided as only a guide.

- At least 1 GB of mother board RAM (2 GB for Windows Vista<sup>®</sup>)
- Pentium Core 2 duo or equivalent

An installation of IUCLID 5 will most likely run on a lower specified machine but the performance might not be satisfactory. The requirements depend in part on the version of Windows.

# 1.2. Software requirements

The software prerequisites for the installation are as follows:

- Windows with access to a user account that can run the installer and create the required directories.
- Java J2SE Runtime Environment v6
- Database PostgreSQL 8.2 or higher.
- The Windows installer for IUCLID 5.2 that can be downloaded without charge from the IUCLID 5 web site.
- Once you have completed the installation of IUCLID 5, you should test it by starting and configuring it. The configuration requires access to at least a legal entity file (LEOX). The creation of a LEOX is described on the IUCLID 5 web site where the installation software is published. In addition, it is recommended to upload a set of reference substances and the EC inventory. These are also available from the web site at which the IUCLID 5 software is published.

# **Chapter 2. Installation**

# 2.1. Important technical information about existing IUCLID 5.0 / 5.1 stand-alone installations



#### Important

There is no automatic upgrade of the database from IUCLID 5.0 / 5.1 to IUCLID 5.2. The data must be transferred manually from the old to the new database as described in the sub-section below.

Each installation of IUCLID 5 must have its own database.

## 2.1.1. Migration of data to IUCLID 5.2 from a previous version

Before starting to install IUCLID 5.2, all the data must be exported from IUCLID 5.1.x using the Back-up plugin that is available on the IUCLID web site. The export process is essential because the exported data will later be imported into IUCLID 5.2. When it is run, the Back-up plugin asks the user to create and enter a single password. This will become the password for all the user accounts in the new installation, with the exception of the account "SuperUser" which has a default password of "root". To import the exported data into IUCLID 5.2, use the built-in Restore feature of IUCLID 5.2 that can be found from the menu File / Administrative tools. This feature allows the upload of data that was exported using the Back-up plugin on 5.1.x.

# 2.1.2. Database configuration for running IUCLID 5.2 and a previous version at the same time

If you already have a previous version of IUCLID 5, it is recommended to keep it for the time being. It can be deleted in the future when you are absolutely sure that it is no longer needed. What follows is some information and advice as to how you can manage more than one version of IUCLID 5. As stated above, each installation of IUCLID 5 must have its own database. A new database must be created for IUCLID 5.2 because the structure of the database differs from that of previous versions. This requirement can be met in a variety of different ways. The following sub-sections describe two common sets of circumstances. The database for IUCLID 5.2 can be run on the same instance of the database software as a previous version of IUCLID 5, however, it must have a unique name within that instance of the database software. When IUCLID 5.2 is run for the first time on an empty database, it will automatically create all the correct tables.

#### 2.1.2.1. IUCLID 5.0 / 5.1 was installed using the setup-kit

The IUCLID 5 set-up kit included the database software Postgres. The set-up kit installed the Postgres database software, the IUCLID 5 software, and stored the database data, all under the same folder named IUCLID. The set-up kit created installations of IUCLID 5 that run Postgres on a non-standard port (5433). Therefore, if an installation of IUCLID 5.2 is made with an independent installation of Postgres running on the standard port (5432), it is possible to run it at the same time as an installation that was made with the set-up kit. For example, if IUCLID 5.2 is installed using the installer according to its instructions and with default settings, the new installation can be run at the same time as a previous installation that was made with the set-up kit.

#### 2.1.2.2. IUCLID 5.0 / 5.1 was installed manually

In this case, you will already have an installation of PostgreSQL that is independent of IUCLID, and a database for use with IUCLID 5.0 / 5.1. There is no need to install Postgres again, although you might want to take this opportunity to upgrade to the latest version. There can be more than one database running on a single instance of the database software. Therefore, to be able to run IUCLID 5.2 and a previous version at the same time, create a new empty database for IUCLID 5.2. The name of the new database must be unique within that instance of the database software.

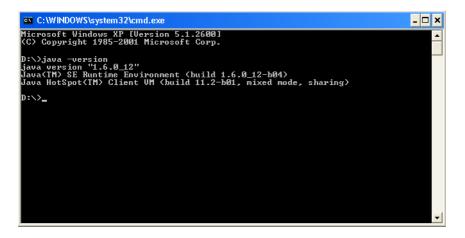
# 2.2. Installation of Java

1. Verify if a JRE has already been installed on your computer:

Open a command prompt (Start # Run... # Open: cmd) and at the command prompt: type:

java -version

#### Figure 2.1. Check Java version



2. If Java (JRE) 1.6 is not already installed on the computer, download the latest version from the Sun site at www.java.com and install it.

#### Figure 2.2. Java Installation Wizard

🛃 Java Se	tup		- 🗙
Sil) Java	Change Current Destination Folder Browse to the destination folder.		Sun Sun
Look in:		×	E 💣
Eolder n	ame: \jre1.6.0_18		
JD: Dava	We1.0.0_10		
		ОК	Cancel

#### Figure 2.3. Choose Java Installation Directory



#### Figure 2.4. Java Installation Complete



# 2.3. Installation PostgreSQL

If PostgreSQL 8.2 or higher is not already installed on the computer, download the latest version from the site www.postgresql.org/download and install it. If version 8.2 or higher of PostgreSQL is already running as a service with a user "postgres", this step is not necessary. The default fresh installation of PostgreSQL 8.4 automatically starts PostgreSQL as a service, creates the user "postgres" if necessary and supplies administration tools (e.g. pgAdmin III) that can be used to create the database. If the installer creates the user "postgres", you will have to create a password for it, as shown in the figure below, and enter it later into the configuration file for IUCLID 5.

Figure 2.5. PostgreSQL version 8.4 installer

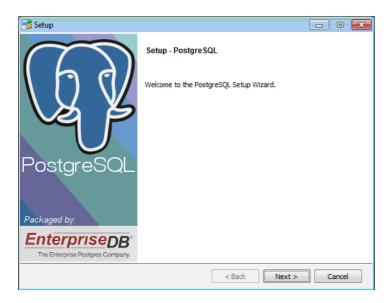
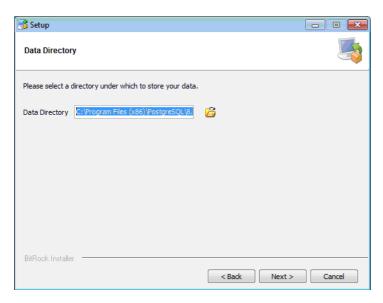


Figure 2.6. Postgres Installation directory

📑 Setup			- • •
Installation Directory			<b>S</b>
Please specify the directory where PostgreSQL will be installed.			
Installation Directory C:\Program Files (x86)\PostgreSQL\8.	6		
BitRock Installer			
	< Back	Next >	Cancel

#### Figure 2.7. Postgres data directory



#### Figure 2.8. 'postgres' user password

📑 Setup		- • ×
Password		<b>E</b>
service account alre	assword for the database superuser (postgres) and service accoun eady exists in Windows, you must enter the current password for t xist, it will be created when you click 'Next'.	t (postgres). If the he account. If the
Password	******	
Retype password	*****	
BitRock Installer	< Back Next	> Cancel

#### Figure 2.9. Postgres port number

📑 Setup	
Port	<b></b>
Please select the port number the server should listen on.	
Port 5432	
BitRock Installer	
BICHOCK INstaller	< Back Next > Cancel

#### Figure 2.10. Set the default locale

📑 Setup			
Advanced Optior	s		
Select the locale to	be used by the new database clus	ter.	
Locale [Default	ocale]		
☑ Install pl/pgsql database?	n template1		
BitRock Installer -		< Back Next >	Cancel

#### Figure 2.11. Confirm Postgres installation

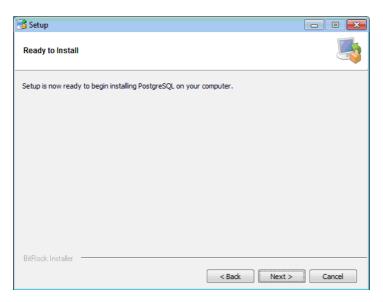


Figure 2.12. Postgres Installation in Progress

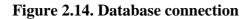
📑 Setup		-
Installing		}
Please wait while Setup installs PostgreSQL on your compu	iter.	
Installing	g	
Unpacking C:\Program Files (x86)\PostgreSQL\8.4\bin\po	gAdmin3.exe	
BitRock Installer		_
	< Back Next > Cancel	

Figure 2.13. Postgres Installation Complete



# 2.4. Installation of IUCLID 5

The installer is supplied as an executable java file named iuclid5\_install\_5.2x.jar. To launch the installer, either double click on the file in a file manager, or enter the following command into a command prompt, java -jar iuclid5\_install\_5.x.jar. The first screen of the installer helps to set-up the connection to the PostgreSQL database. The default values suit the needs of a typical user, so unless values are missing, or you know that different values are required, leave the default values in place and click on continue.



🕌 IUCLID 5.	.2.0 Installatio	วท		
Database	e connectio	n		
Host:	localhost			
Port:	5432			
Database:	iuclid5			*
User name:	iuclid5			~
Password:	•••••			
🔽 Create da	atabase/user if it d	loes not exist		
Superuser nar	ne	postgres		
SuperUser pa:	ssword	•••••		
			Continue	Cancel

If the following error message is displayed "*password authentication failed for user postgres*", enter the password of the postgres user you gave during the installation of postgreSQL.

#### Figure 2.15.

Error	
8	FATAL: password authentication failed for user "postgres"
	OK

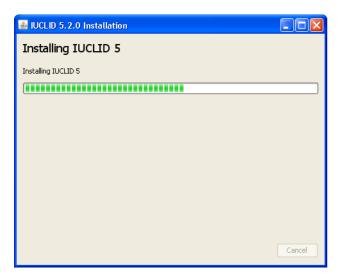
The second step of the installer allows you to change the destination folder of IUCLID 5.

#### Figure 2.16.

▲ IUCLID 5.2.0 Installation	
Destination folder	
C:\Program Files\uclid5 The application will be installed in: C:\Program Files\uclid5\5.2.0\	
	Continue Cancel

The actual installation process will take a few seconds.

#### **Figure 2.17.**



When the installer has finished installing the application, you can close the installer.

#### Figure 2.18.

IUCLID 5.2.0 Installation	
Installing IUCLID 5	
IUCLID 5 is successfully installed	
a	ose

A new shortcut has been created on your Desktop.

#### Figure 2.19.



# Chapter 3. Initialisation of an installation of IUCLID 5

This section describes the configuration that is required to create a working IUCLID 5 system from the software that has been installed. Data must be uploaded into the database, and if more than one person is to use the system, user accounts must be created, and the users must be instructed how to access the system.

# 3.1. Starting IUCLID 5

Launch IUCLID 5 by double-clicking the icon that the installer created on your Desktop, as shown below.

#### Figure 3.1. A shortcut to the IUCLID 5 application



# 3.2. First steps wizard

When you start IUCLID 5 for the first time, the "First steps" wizard is run automatically. It guides you through the steps required to make a working user account and to upload the data required to use IUCLID 5 in a practical setting. The settings that relate to user accounts can also be changed after having run the wizard, using the features described in the IUCLID 5 User Manual.



#### Important

This wizard allows a single user account to be created, per run. This user is in addition to the SuperUser account that comes with the installation. It is essential to have at least one user account in addition to SuperUser because SuperUser should be used only for the special tasks that only it can carry out. See the IUCLID 5 User Manual for more detail.

As part of the First steps wizard, a legal entity must be uploaded into the IUCLID 5 installation in the form of a LEOX file. Therefore, before running this wizard, make sure that a LEOX file for the legal entity of your company or organisation is accessible to your computer. For more information, see the IUCLID 5 User Manual.

The First steps wizard provides the option of uploading the following information to your IUCLID 5 installation. For details, see the IUCLID 5 User Manual:

- EC Inventory
- Inventory of Reference substances

Although these uploads are optional, it is strongly recommended to do them during the first run of the First steps wizard. To do so, you will need to have the data accessible to your computer whilst running this wizard.

The First steps wizard can be run at any time, but only by the "SuperUser". This is done from the file menu within IUCLID 5 Administrative tools / Initialise.

When starting the IUCLID 5 for the first time, the only user available is an administrator named "SuperUser". Log in as SuperUser by entering the following case-sensitive values into the login screen as shown below:

Username: SuperUser

#### Password: root



The First steps wizard then proceeds. Each page of the wizard is described in a figure below.

#### Figure 3.2. Step 1 of the First steps wizard - Introduction

The wizard presents some useful information. There are no actions other than to read the information. Click the Next button.

🔽 First steps
Welcome to IUCLID 5
Welcome to IUCLID 5
IUCLID 5 (International Uniform ChemicaL Information Database) is a software application to capture, store, maintain and exchange data on intrinsic and hazard properties of chemical substances. This wizard will guide you through the different steps involved to setting up your application so that you can use it immediately! We recommend that you follow the given instructions:
<ol> <li>Change the SuperUser password (not mandatory but recommended to increase security)</li> <li>Import your Legal Entity information (mandatory for running the application)</li> <li>Import the EC inventory (not mandatory but strongly recommended)</li> <li>Import the Reference substance inventory (not mandatory but recommended for users with &gt;100 substances)</li> <li>Create a user account and define roles (strongly recommended)</li> </ol>
IMPORTANT: Before running this wizard, please make sure your Legal Entity information has been stored on your PC (information available at the IUCLID Download Website)
②         □

#### Figure 3.3. Step 2 of the First steps wizard - Init mode - New installation

To initialise a new database, select the button New Installationas shown below and continue to the next step.

First steps	
Define the initialisation mode	
Initialisation mode New installation Restore from backup	
2 <b>1 - 2 - 3 - 4 - 5 - 6 - 7 - 8</b> Init mode	< <u>Back</u> <u>Next&gt;</u> Einish <u>C</u> ancel

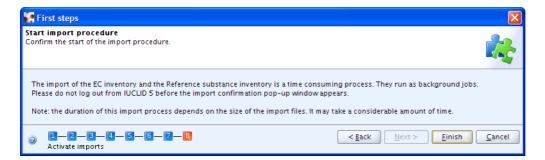
#### Figure 3.4. Step 2 of the First steps wizard - Init mode - Restore from backup

To restore from a backup of a previous version of IUCLID 5, select the button Restore from backup then enter the directory containing the backup files as shown in the example below.

First steps	
Define the initialisation mode	<b>**</b>
<ul> <li>Initialisation mode</li> <li>New installation</li> <li>              Restore from backup      </li> </ul>	
D:\IUCLID\backup	
2 1-2-3-4-5-6-7-8 Init mode	< <u>Back</u> <u>N</u> ext > <u>Einish</u> <u>Cancel</u>

Click Next. The wizard jumps to its last step, where the importation of data is started, as shown below.

#### Figure 3.5. Restoration from a back-up - Step 8 - Activate imports



The import may take some . Click Finish. When the restoration is complete, the following screen is shown.



#### Figure 3.6. Step 3 of the First steps wizard - Change password

If you have not yet changed the default password of the SuperUser to a more secure value than "root", the traffic light in the wizard screen will be yellow. To change the password, check the box Change SuperUser password, enter the old password "root" and then enter the new password. After confirming the password, click the button **Next**.

🚰 First steps		
Change the SuperUse For security reasons it is	<b>r password</b> recommended to change the SuperUser's password.	
It is not secure	;, as it is now.	
🗌 Change SuperUser p	assword	
Old password		
New password		
Confirm new password		
	d that you change the SuperUser password, since each IUCLID 5 installation uses an identical default passwoi rd, please tick the checkbox.	rd.
2 2 - B - 4 Change password	-5-6-7-8	<u>C</u> ancel

#### Figure 3.7. Step 4 of the First steps wizard - Import Legal Entity

To import a Legal entity (see the IUCLID 5 User Manual) select its LEOX file by browsing to the file. The browsing is accessed by clicking on the folder icon to the right of the field "Select the import file". Click the **Next** button. The Legal entity is imported immediately.

First steps	
Import legal entity In order to run IUCLID 5, you have to import your Legal entity obtained from tl	ne IUCLID Download Website
Please note: If your Legal entity information has not already been st Download Website, otherwise this wizard will not complete success Select your Legal entity file by navigating to the desired file on you Select the import file	ully and you will be forced to log out.
D:\IUCLID\Leox_Manual.i5z	۵ 🏳
IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	< <u>B</u> ack <u>N</u> ext > <u>Finish</u> <u>C</u> ancel
IUCLID 5 Import of the legal OK	entity file completed



#### Important

You must import at least one Legal entity in order to succeed with this wizard. If you have no Legal entity in the IUCLID 5 system, the traffic light in the wizard screen will be red. The First steps wizard will be automatically launched when you log in to IUCLID 5 until a Legal entity has been successfully imported.

#### Figure 3.8. Step 5 of the First steps wizard - Import EC Inventory

EC inventory import - To import the EC inventory, select the file for the EC inventory (see the IUCLID 5 User Manual). The EC Inventory will not be imported immediately. The import will start at the end of the First steps wizard. Depending on your machine speed and the size of the inventory, this import can take some time, e.g. up to half an hour.

First steps
Import EC inventory Select the EC inventory file which you previously downloaded
The EC inventory is the catalogue of chemical substances listed on the European Inventory of Existing Commercial chemical Substances (EINECS), the European List of Notified Chemical Substances (ELINCS) and the No-Longer Polymers list (NLP), published in the Official Journa of the European Communities. Each substance listed in the inventory has an EC number and an EC name allocated by the European Commission.
If you want to use the EC inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website, and save the file on your hard disk.
To import the EC inventory in IUCLID 5 using this wizard, please tick the import box. Select the import file by navigating to the desired file on your computer. Note: It is possible to import the EC inventory at a later stage, using the import function from the IUCLID 5 Task panel
✓ Import EC inventory
Select the import file
D:\/IUCLID\ECinventory_1.1_en.i5z
Image: Section of the section of t

#### **Figure 3.9. Step 6 of the First steps wizard - Import reference substances**

Reference substance inventory import - Select the file for the Reference substance inventory (see the IUCLID 5 User Manual). The Reference substance inventory will not be imported immediately. The import will start at the end of the first steps wizard together with the EC Inventory import. Depending on your machine speed and the size of the inventory, this bulk operation may take a very long time. The Reference substance inventory itself can take **up to several hours** to import.

🙀 First steps
Import reference substance inventory Select a reference substance inventory to import into IUCLID 5
The reference substance inventory is a catalogue of approximately 70,000 reference substances. A reference substance is used for the identification of substances and contains information such as CAS Numbers, IUPAC names, SMILES and InChI notations, structural formula and the EC inventory information. The reference substance inventory is publicly available and can be downloaded entirely or partially. If you want to use the reference substance inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website and save the file on your hard disk. To import the reference substance inventory in IUCLID 5 using this wizard, please tick the import box. Select the import file by navigating to the desired file on your computer. Note: It is possible to import the reference substance inventory at a later stage, using the import function from the IUCLID 5 Task panel. Import reference substance inventory Select the import file D:\IUCLID\ReferenceSubstance inventory
Image: Second state     Image: Second state       Reference substance inventory import     Image: Second state

#### Figure 3.10. Step 6 of the First steps wizard - Import reference substances

Create a new user account and define its user access rights by assigning it a role. It is essential to create a new user because general working within IUCLID 5 with the SuperUser is not supported. Only one user can be created per run of the First steps wizard.

First steps	×
Create user account and assign role It is recommended to create a user account before running IUCLID 5	
The SuperUser account is for user administration only, and therefore to run IUCLID 5 we strongly recommend that you create your own account by selecting the following tick box. Assign your role and legal entity and specify the attachments and Import/export directorie Create user	
Login name Local Administrator Full name Example	a,
Full halfe     Set password       Unassigned roles     Assigned roles       *     *       Full access     *       Read-only     *	
Assigned legal entities  Assigned legal entities  Set the password of Local Administrator - Example - last login: (Never) from (Nowhere)	
LEO for Manual / Helsinki / Fin     New password     Confirm new password	
Set Cancel	
Attachments directory	
Image: Sector	ancel

• Select the checkbox Create user.

Fill in all the fields. The user needs a Login name for identification during login. The Full name is used for proper user identification. The Assigned role is needed to administrate the access permissions. In a newly installed IUCLID 5 the roles "Administrator", "Full access" and "Read-only" are provided by default.

- Enter a Login name, as it should be used for identification during login, and the Full name used for proper user identification.
- Optionally, click Set password and define a password.
- Click and highlight a role in the list of unassigned roles and assign it to the user by clicking the Right arrow. Assigning a Role is needed to administrate the access permissions (in a newly installed IUCLID 5, the roles "Administrator", "Full access" and "Read-only" are available by default).



#### Tip

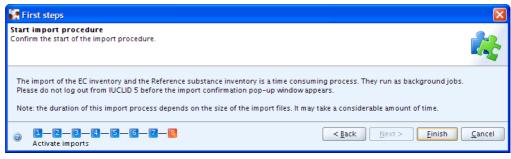
It is recommended to create a user with the "Administrator" Role regardless of whether a stand alone or a distributed version of IUCLID 5 is set up. Once a user has been created, the IUCLID 5 administrator (in case of a distributed version) can define different other user(s) and assign different role(s) to them (see the IUCLID 5 User Manual).

- Assign a Legal entity (normally the Legal entity imported in the third step of this wizard) by clicking the green plus button and performing a search for the desired Legal entity. In the Query field Legal entity name, enter the name of the desired Legal entity or an asterisk (\*) as wildcard and click the **Search** button. In the Query results list, click the desired entry and then click the **Assign** button.
- Optionally, select default attachment and import/export directories. These settings can be changed at a later stage, as described in the IUCLID 5 User Manual.
- Click the Next button

#### Figure 3.11. Step 8 of the First steps wizard - Start import procedure

If you have selected an EC Inventory and/or Reference substances inventory file(s) during the wizard steps, you can now run the imports. Click the button **Execute imports**. Note again that these imports can take up to several hours, depending on your machine speed and the amount of data you are importing.

Then click the button **Finish**. If you have launched any imports, you will now have to wait until the imports are completed. Afterwards, you should log out and then log in again as a user for the newly defined account. Remember: general working as SuperUser is not supported.



# 3.3. User management

The installation of IUCLID 5 is now ready for hand-over to whoever will be maintaining the system and whoever will be managing the user accounts. The management of user accounts and their roles is described in the IUCLID 5 User Manual.