

IUCLID 5

Guidance and Support

Installation Guide for IUCLID 5
Stand-alone Application

Installer for Microsoft[®] Windows[®]



February 2013

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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>.

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Chapter 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® Windows® (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.

If you encounter any problems during the installation that cannot be solved using information in this manual, or the documentation of third party softwares; before contacting the ECHA Helpdesk, please try the IUCLID FAQ located at the IUCLID web site <http://iuclid.eu>.

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®)
- 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 and the IUCLID plugins that are in use. For example, using the Query Tool plugin will increase the resources required to obtain a reasonable running speed; especially on a large database.

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 SE Runtime Environment 6 (Java 7 is not compatible)
- Database - PostgreSQL 8.2, 8.3, 8.4 (recommended) or 9.
- The latest version of the Windows installer for IUCLID 5. It 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.



Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set*, a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

Chapter 2. Making a fresh installation of IUCLID 5

If Java and PostgreSQL are already installed as required, go straight to Installation of IUCLID 5.

2.1. Installation of software required by IUCLID 5

The installation of third party software is described by the respective publishers. Please refer to their web sites for full instructions.

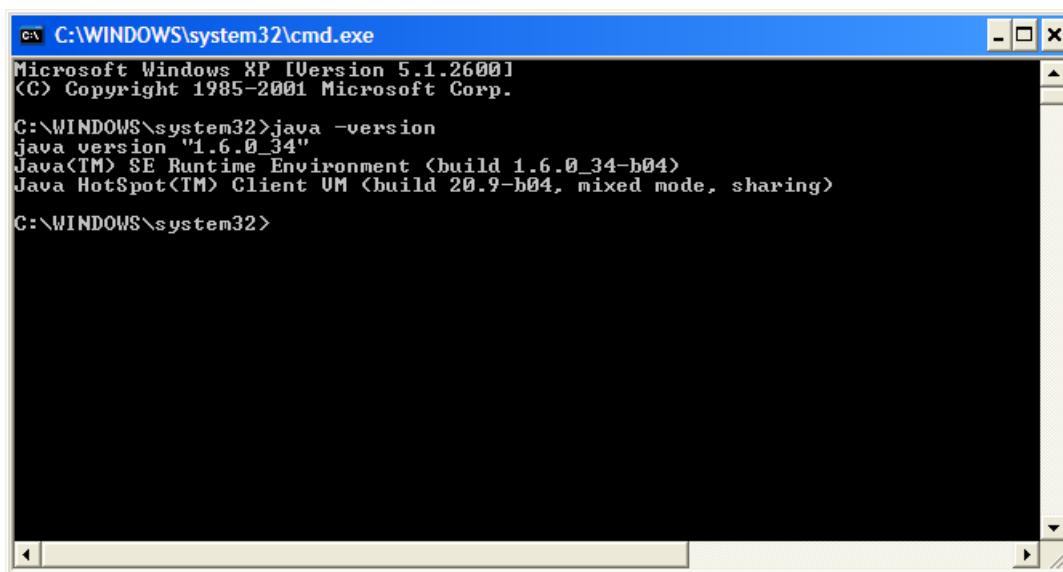
2.1.1. Installation of Java

1. Verify whether Java (JRE) of the correct version is installed on the computer to which IUCLID 5 will be installed:

Open a command prompt (Start -> Run... -> Open: cmd). At the command prompt, enter the following:

```
java -version
```

Figure 2.1. Check version of Java



```
C:\WINDOWS\system32\cmd.exe
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.

C:\WINDOWS\system32>java -version
java version "1.6.0_34"
Java(TM) SE Runtime Environment (build 1.6.0_34-b04)
Java HotSpot(TM) Client VM (build 20.9-b04, mixed mode, sharing)

C:\WINDOWS\system32>
```

2. If a message similar to the one shown in the screen shot above is **not** shown, or the version of Java is **not** 1.6x, IUCLID 5.3.2 cannot be run. Note that IUCLID 5.3.2 does not work with Java 1.7. To use Java 1.6, the providers of Java recommend that all other versions of Java are removed from the computer, and only the most recent update of Java 1.6 is installed. All the available versions of Java, and the latest recommendations as to how they can be used, are available from the web site www.java.com.

Figure 2.2. Select either the default, or a custom destination for the installation



Figure 2.3. Installation is under way



Figure 2.4. Installation of Java is complete

2.1.2. Installation of PostgreSQL

If either version 8.2, 8.3 or 8.4 of PostgreSQL is already installed and running as a service with a user `postgres`, the existing installation can be used. There is no need to upgrade to 9, although 9 is supported. If PostgreSQL is not already installed on the computer, or you would like to upgrade to 9, download PostgreSQL 9 from the site www.postgresql.org/download and install it. The web site of PostgreSQL offers a range of alternative ways to download and install the PostgreSQL software. The screen shots shown below show the use of the *one click installer* available from the PostgreSQL web site. An example of the file name of the installer is *postgresql-9.0.4-1-windows.exe*.

The default fresh installation of PostgreSQL, made using the *one click installer*, 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 manage databases. If the installer creates the superuser `postgres`, you will have to enter a password for it into step 4 of the *one click installer*, as shown in the sequence of figures below. Remember this password because it will be required later, during the configuration of IUCLID 5. If you are unsure of what values to enter into the *one click installer*, use the pre-filled defaults.

Figure 2.5. Installer for PostgreSQL



Figure 2.6. Installation directory for PostgreSQL

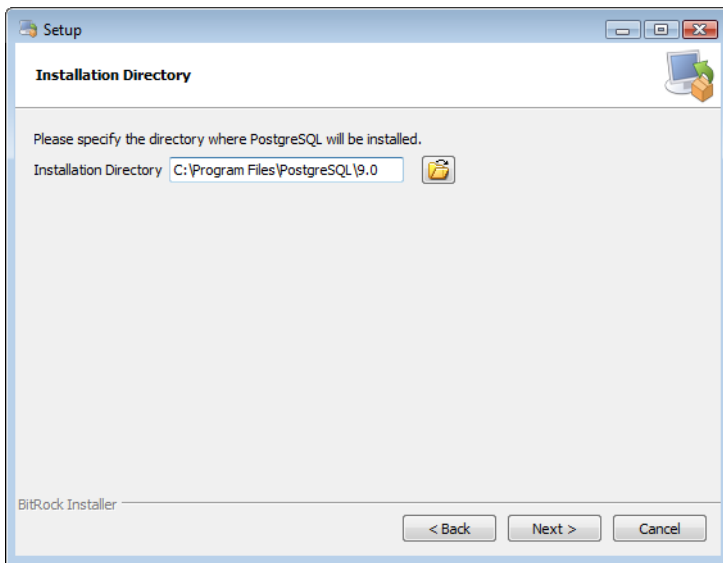


Figure 2.7. Data directory for PostgreSQL

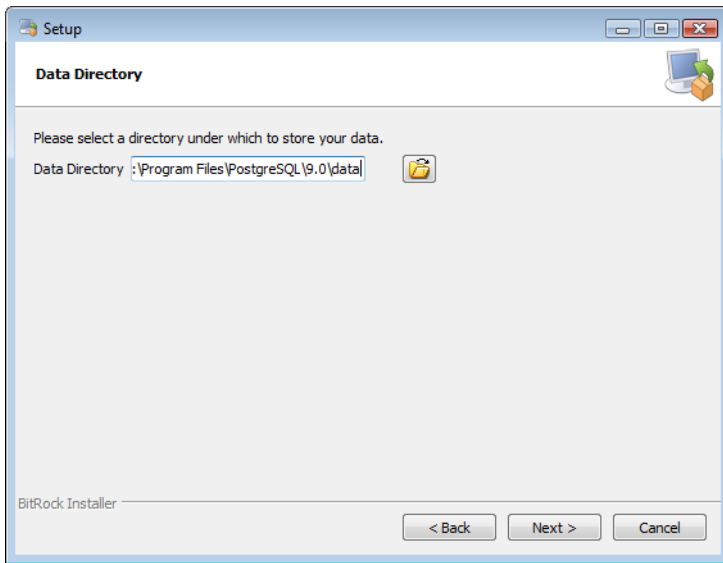


Figure 2.8. Password for the database superuser (postgres) and the Windows service account (postgres)

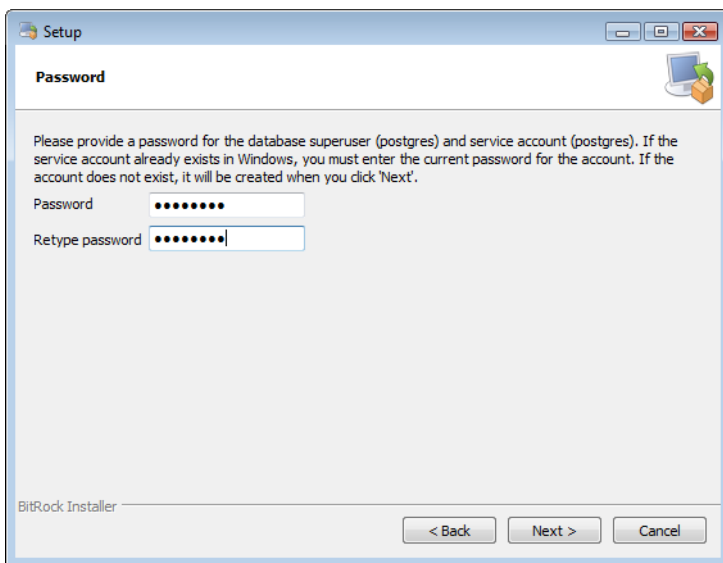


Figure 2.9. Port number for PostgreSQL

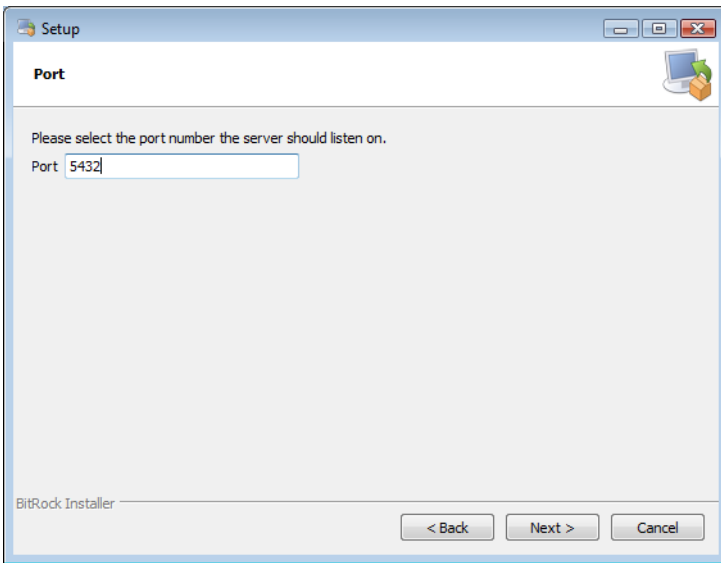


Figure 2.10. Set the default locale for PostgreSQL

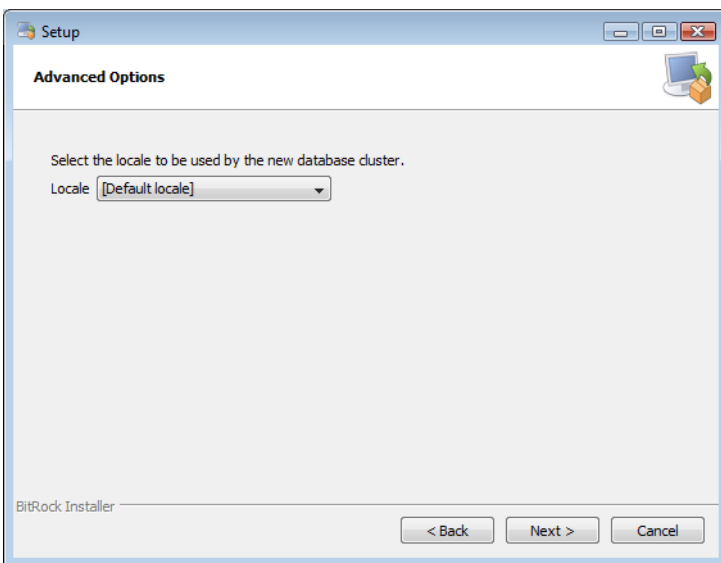


Figure 2.11. Confirm installation of PostgreSQL

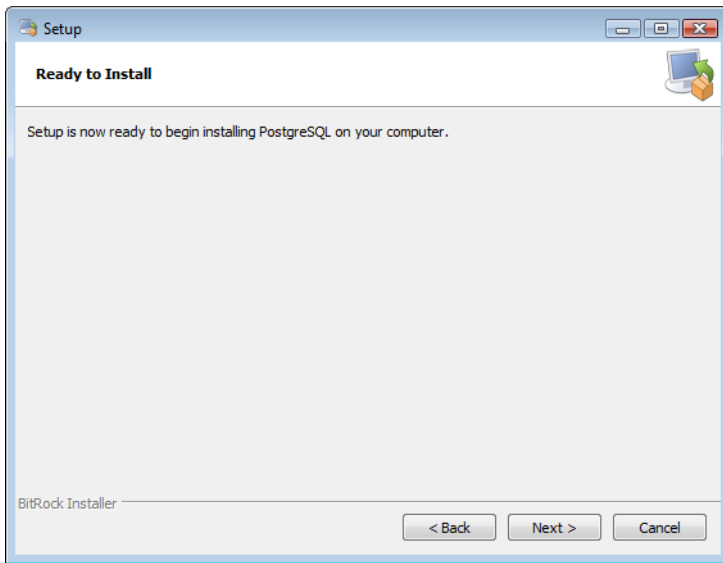


Figure 2.12. Installation of PostgreSQL in progress

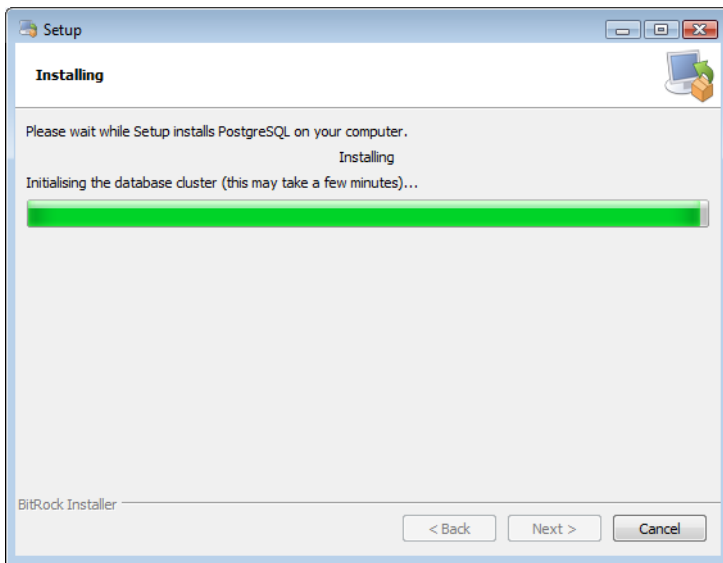


Figure 2.13. Installation of PostgreSQL complete

Unless you particularly want to run the Stack Builder, untick the box in the screen shown above. To finish the installation, click on the button Finish.

2.2. Installation of IUCLID 5

After downloading the Windows installer installation package for IUCLID 5, unzip its content to a convenient folder.

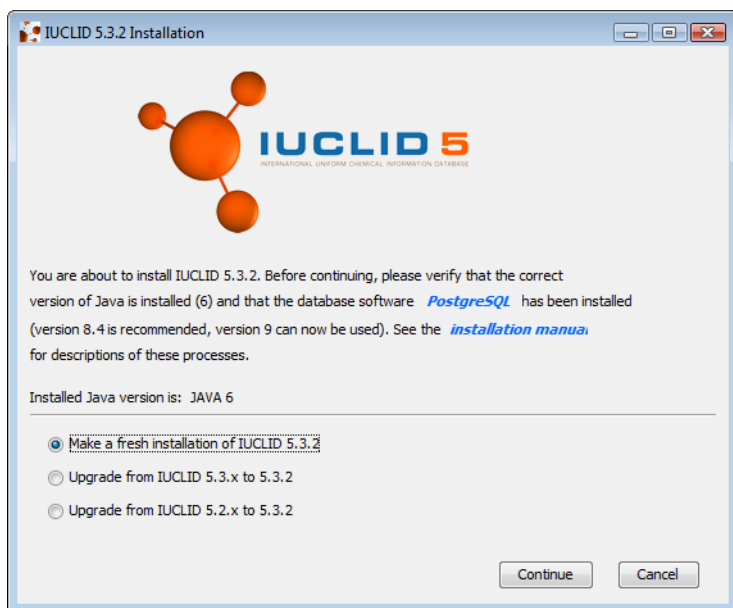
The installer is supplied as an executable Java file named `iuclid5_install.jar`. It can be launched either by double-clicking on the file, or by running it from the command line, as you would a script. Bear in mind that the user account under which the installer is run, must have permission to write to the folder in which IUCLID 5 will be installed.

If you experience problems in running the installer, for a possible solution, see Appendix A, *Tips on launching the installer and access rights* later in this document.

The first screen of the installer offers the choice between a fresh installation of IUCLID 5, or an upgrade to the most recent version. To upgrade, please refer to Upgrade later in this document. An example of the first screen is shown below. The texts in blue are links to the web site of PostgreSQL and the installation manuals on the IUCLID web site.

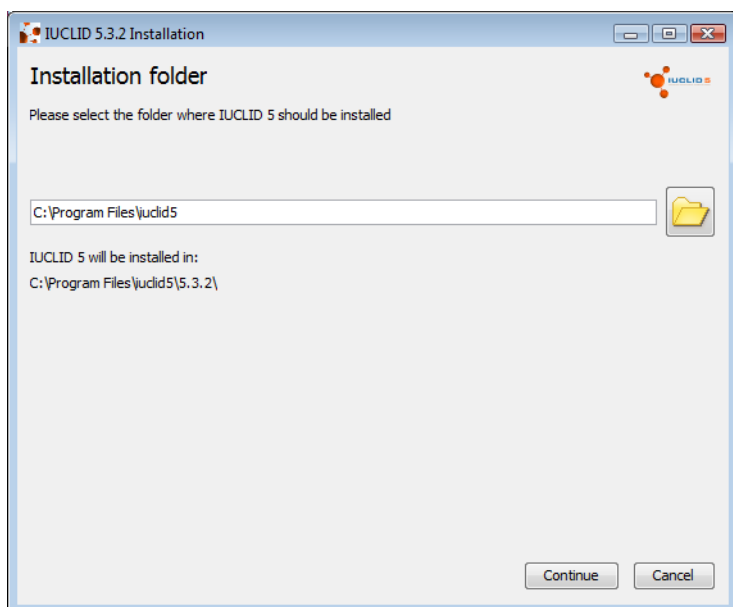
For a fresh installation of IUCLID 5 with an empty database, select the first option. In the example shown below, the option is Make a fresh installation of IUCLID 5.3.2. For a fresh installation, the procedure is independent of the version being installed. Click on the button Continue.

Figure 2.14. Install a fresh installation of IUCLID 5



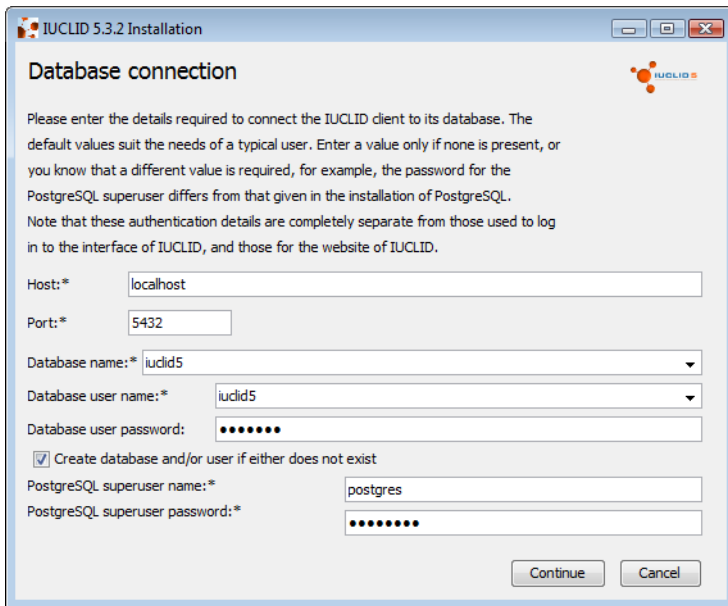
The next page of the installer allows you to define the destination of the installation. The installer automatically creates a new folder into which it installs IUCLID 5. The folder has the same name as the full version number and name of IUCLID 5. This page of the installer allows you to define the location of that folder. The default value is shown on the screen. To change it, click on the folder icon, then browse to the different location. For example, in the screen shot shown below, a new folder named IUCLID 5.3.2 will be created in the folder C:\Program Files\iuclid5. Ensure that the user account in Windows used to run the installer has the permission to write to the destination folder, then click on the button Continue.

Figure 2.15. Destination folder



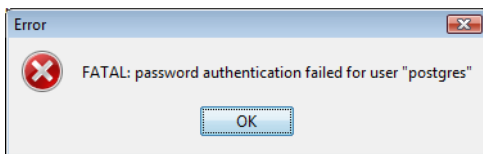
On the third screen of the installer, details are entered that define how IUCLID 5 connects to the PostgreSQL database. The default values suit the needs of a typical user, so unless values are missing, or you know that different values are required, leave the default values in place. You can use whatever value you like for **database user password**. The value of **PostgreSQL superuser password** must be the same as that entered during the installation of PostgreSQL. After entering the values, the screen should look like the example shown below. Click on the button Continue.

Figure 2.16. Database connection



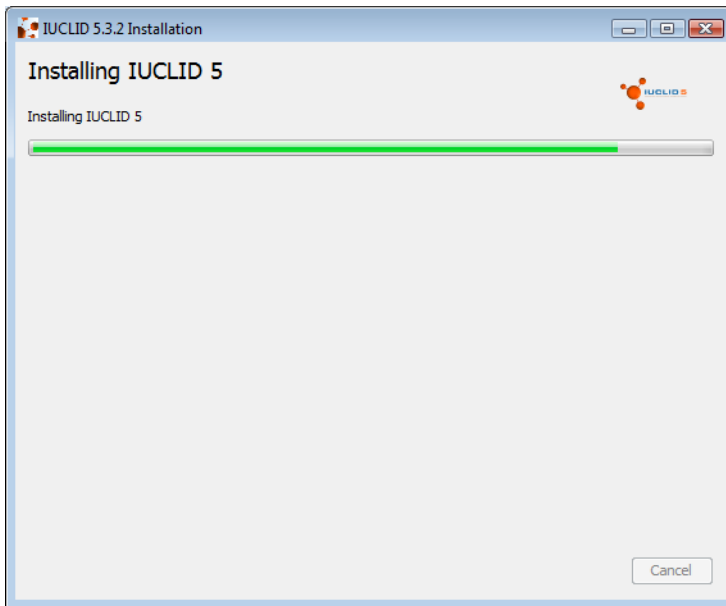
If the following error message is displayed *password authentication failed for user postgres*, try again after entering the password of the superuser for PostgreSQL that was entered during the installation of PostgreSQL.

Figure 2.17. Wrong password

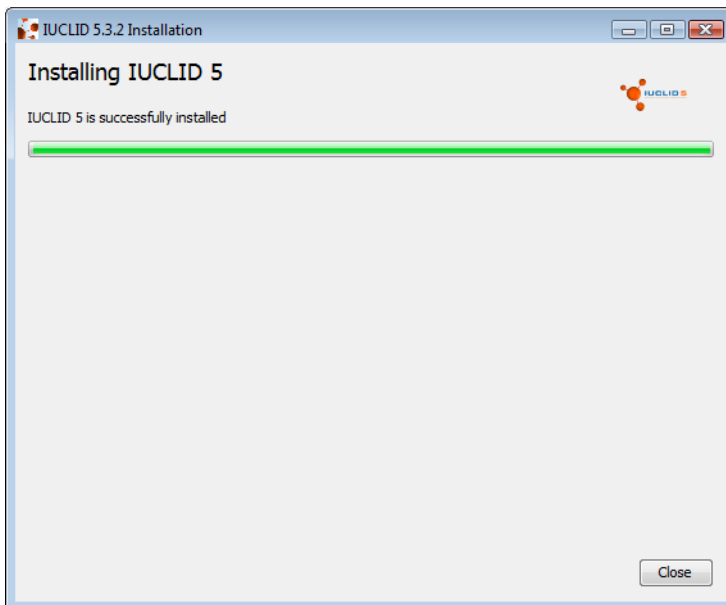


If either of the two error messages *Cannot create destination folder*, or *Access denied* are given, for a possible solution see Appendix A, *Tips on launching the installer and access rights*, later in this document.

The actual installation process will take a few seconds.

Figure 2.18. Installing IUCLID 5

When the installer has finished installing the application, the wizard can be closed by clicking on the button Close.

Figure 2.19. Successful installation

A new shortcut is created automatically on the Windows Desktop. The shortcut points to the file `iuclid5.cmd` that is included in the installation directory. If no shortcut is created, see Appendix A, *Tips on launching the installer and access rights* for possible reasons. It is possible to create a shortcut manually. The next step is to initialise the installation, as described in Chapter 4, *Initialisation of an installation of IUCLID 5* of this document. After that, if you have data that was exported from IUCLID using its built-in back-up/restore functionality, it can be imported into the fresh installation of IUCLID 5.

Figure 2.20. Example of a shortcut to IUCLID 5



2.3. Security settings for user accounts

IUCLID 5 has features designed to control the level of security of authentication of user accounts. The level of security can be tailored to that required for the particular installation of IUCLID 5. For example, when setting passwords for their user accounts, users can be forced to enter values that have a minimum strength. The values of the parameters that determine the level of security are defined in the settings file, `workstation.properties`, that is located in a folder named `conf` within the installation folder. Changes to values take effect on restarting IUCLID 5. The security features are described below.

The settings are shown below as they appear in the settings file that is supplied with the installation of IUCLID 5. The values are shown set to the hard-coded defaults and commented out. If a line is commented out, the hard-coded default value is used. A value of zero (0) disables a feature.

```
# The minimum length for a new password
# password.min.length=6
# The minimum number of character sets used in the password
# password.min.charsets=2
# If a secure question system is enabled
# password.use.secure.question=true
```

In the example shown below, the security features have been disabled.

```
# The minimum length for a new password
password.min.length=0
# The minimum number of character sets used in the password
password.min.charsets=0
# If a secure question system is enabled
password.use.secure.question=0
```

2.3.1. Minimum password length

This feature is used to prevent the use of overly weak passwords for user accounts. The password of a user account must contain at least this number of characters. If an attempt is made to create a password with fewer characters, an informative error message is given and the user is presented with an opportunity to try again.

The security policy is applied to passwords only when they are created. Therefore, if the minimum length of passwords is increased, users can still log in using existing passwords, even if they are now considered to be too short. The user-manager can force a user to create a new password by ticking a box for the account in the IUCLID 5 client. The user is then required to create a new password when they next log in.

2.3.2. Minimum number of character sets in passwords

This feature is used to prevent the use of overly weak passwords for user accounts. The password of a user account must contain at least one character from all the character sets. The value is an integer from 1 to 4. A value of 1 means only character set 1, a value of 2 means both character sets 1 and 2, etc. The four character sets are: 1 = a lowercase letter [a-z], 2 = an uppercase letter [A-Z], 3 = a digit [0-9], 4 = a non-alphanumeric symbol [!@#%&*_=-+].

For example, if the value is 3, a password of "AdkbScfw" is rejected for being too weak, but "AdkbSc37" is accepted because it contains at least one character from sets 1, 2 and 3.

If an attempt is made to create a password that does not comply, an informative error message is given, and the user is presented with an opportunity to try again.

The security policy is applied to passwords only when they are created. Therefore, if the minimum number of character sets allowed within passwords is increased, users can still log in using existing passwords, even if they are now considered to contain too few character sets. The user-manager can force a user to create a new password by ticking a box for the account in the IUCLID 5 client. The user is then required to create a new password when they next log in.

2.3.3. Security question

This feature is designed to allow an alternative method of user authentication to the user name/password combination. It can help to reduce the resources required for user management by preventing account blocking due to forgotten passwords. Each user can define their own security question and a secret answer. This is done from the graphical user interface of the client, after the user has logged in. A user can log in by answering their question correctly, instead of supplying the password. The question is answered via a link on the log in page, [Forgot your password?](#). The feature is turned on or off for the whole instance of IUCLID 5 using a value of `true` or `false`.

Chapter 3. Upgrade

Before starting the upgrade, it is important to back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up functionality of the database. Making only a copy of the file system on which IUCLID is installed is not recommended as a means of backing-up.

This chapter describes how to upgrade a previous version of IUCLID 5. In the full version number of IUCLID 5, the 5 five is followed by a major and then a minor version number, separated by full stops. For example, in IUCLID 5.3.2, the major version number is 3 and the minor version number is 2. Dependent upon the version of IUCLID 5 that is being upgraded, there are three main scenarios in the upgrade process. These are each described in a dedicated sub-section of this chapter. The scenarios are:

1. An increase in only the minor version number. For example, upgrade from IUCLID 5.3.1 to IUCLID 5.3.2.

The installer automatically transfers all the data from the previous database to the new one.

2. An increase in the major version number. For example, upgrade from IUCLID 5.2.1 to IUCLID 5.3.2.

Changes in the database must be made using a migration step. The installer can perform the migration of data for you.

3. An upgrade from either IUCLID 5.0 or IUCLID 5.1.

The Windows installer cannot be used to perform the upgrade.

Identify the scenario that applies to your upgrade, then continue reading from its dedicated section below. If you are unsure which version you are currently using, you can read it from within the interface of IUCLID 5. Start IUCLID 5, log-in, then click 'Help' and select 'About'.

3.1. Upgrade with an increase in only the minor version number of IUCLID 5 (except IUCLID 5.0/1)

The installer provides a simple way of performing the upgrade, as described in the sections that follow. On starting the new version of IUCLID 5, it can connect to the previous database without any need for a migration step.

1. Back-up the database. Use the built-in back-up functionality of IUCLID 5, and/or the back-up function of PostgreSQL.
2. Run the installer, select the upgrade option that is appropriate for your system, and then proceed with the installation.



Important

The upgrade functionality of the Windows installer can be used only if IUCLID 5 was installed using the Windows installer.

For instructions on how to upgrade IUCLID 5 without the Windows installer, please refer to the specific installation manual for your computer set-up.

3.1.1. Launching the installer

After downloading the Windows installer installation package, unzip its content to a convenient folder.

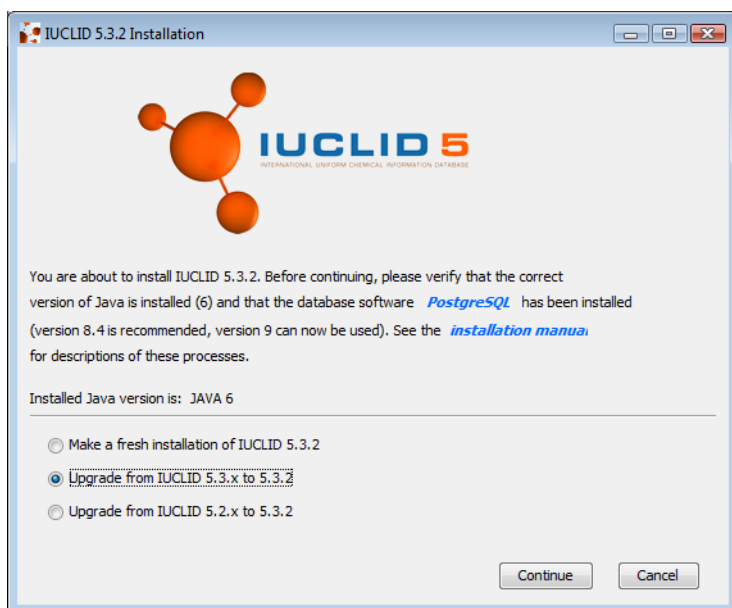
The installer is supplied as an executable Java file named `iuclid5_install.jar`. It can be launched either by double-clicking on the file, or by running it from the command line, as you would a script. Bear in mind, that the user account under which the installer is run, must have permission to write to the folder in which IUCLID will be installed.

If you experience problems in running the installer, for a possible solution, see Appendix A, *Tips on launching the installer and access rights* in the Appendix of this document.

3.1.2. Selecting the upgrade scenario

On the first screen of the installer, select the second option. In the example below, and for the subsequent screen shots in this section, the option is Upgrade from IUCLID 5.3.x to 5.3.2.

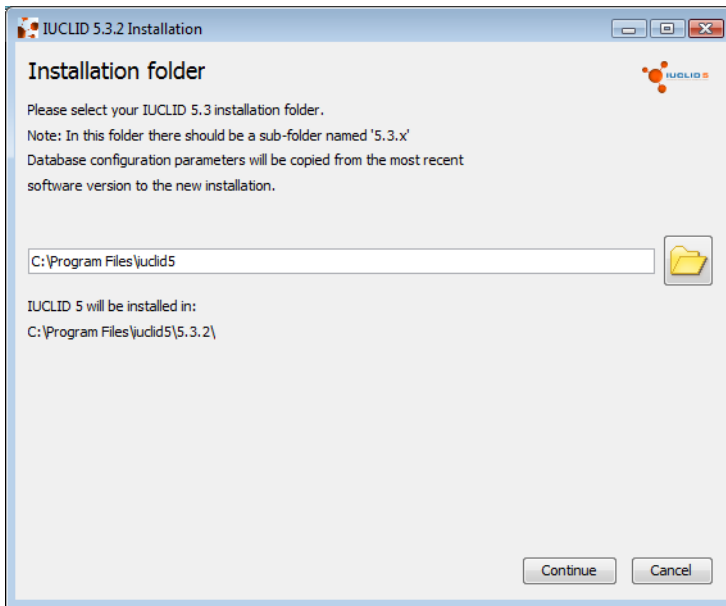
Figure 3.1. Upgrade IUCLID 5 with an increase in only the minor version number



Click the button Continue.

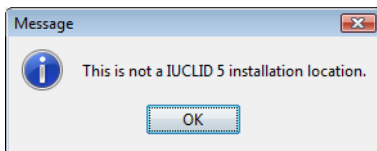
3.1.3. Locations of the installation to be upgraded and the new installation

The installer creates a folder into which it will install the new version of IUCLID 5. This folder will be in the same higher level folder as the installation being upgraded. The higher level folder is set on the second page of the installer. It can have either the default value of C:\Program Files\iuclid5, as shown in the screen shot below, or you can enter a different value. However, the folder selected must contain the installation that is being upgraded. The installer reads the configuration parameters from the installation folder of the highest previous version of IUCLID 5 it can find, and then copies them to the new installation. The installer does not modify the installation being upgraded. In the example shown below, the destination folder for the upgraded installation is named IUCLID 5.3.2.

Figure 3.2. Installation folder

When you are sure that the values are correct, click Continue.

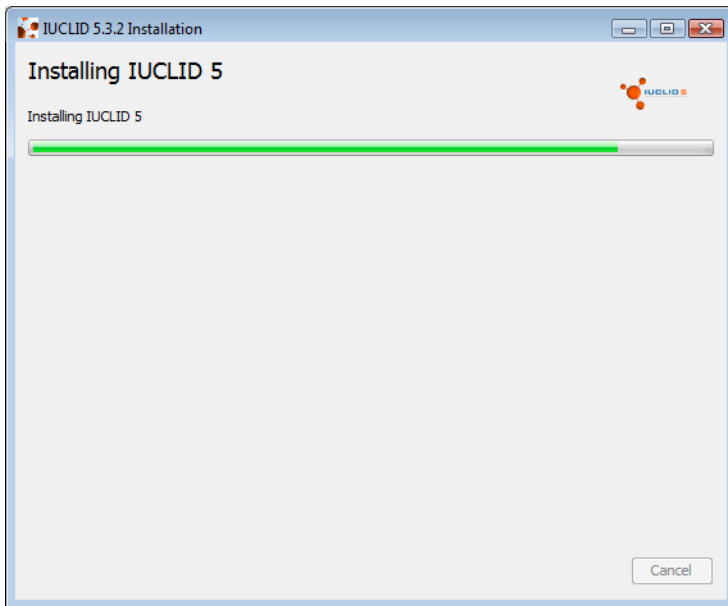
The following error message is displayed if the Windows installer cannot find a version of IUCLID 5 that it can upgrade with the options you have entered.

Figure 3.3. Installer cannot find suitable previous installation

There are also two other types of error message that can be displayed: *Cannot create destination folder* and *Access denied*. If either of these are given, for a possible solution see Appendix A, *Tips on launching the installer and access rights* later in this document.

3.1.4. Installation of IUCLID 5 application files

The creation of the new folder and the copying of data to it take a few seconds, as shown in the example below.

Figure 3.4. Installing IUCLID 5

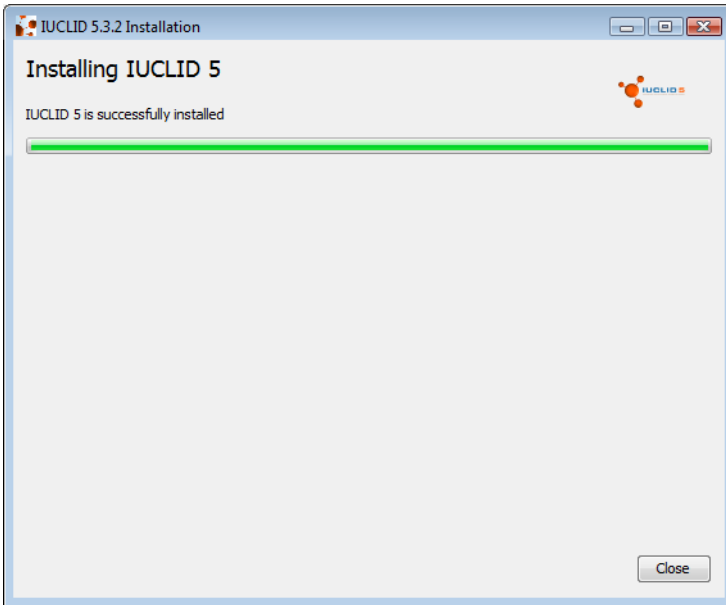
During the installation process, the following operations are performed:

- The new versions of the application files are copied to the installation folder of the new version.
- Plugins that had been installed in the previous version of IUCLID 5, are copied over to the new version of IUCLID 5, but only if they are compatible with the new version. The installer automatically detects whether a plugin is compatible. If a plugin is no longer visible in the user interface of IUCLID 5 after upgrading, visit the IUCLID web site at <http://iuclid.eu> to see whether a compatible version is available.
- The configuration files for the previous installation are copied to the new installation.
- A shortcut to IUCLID 5 is created on the desktop of the Windows account under which the installation is performed, as shown below.

Figure 3.5. Shortcut to IUCLID 5

After a successful upgrade, the following screen is shown.

Figure 3.6. IUCLID 5 is upgraded successfully



Click Close.

3.1.5. Starting IUCLID 5

You can now launch the upgraded IUCLID 5 by double-clicking the icon that the installer created on your Desktop, as shown below. It is also possible to launch IUCLID 5 by running the file `iuclid5.cmd` that is included in the installation directory. The initialisation process is not required. All of the data that was present in the upgraded system should be present in the new system. Therefore, it should be possible to log in to any of the user accounts from the previous system.

Figure 3.7. Shortcut to IUCLID 5



3.2. Upgrade with an increase in the major version number of IUCLID 5 (except IUCLID 5.0/1)

In this scenario, the Windows installer provides a simple way of upgrading an existing installation of IUCLID 5, as described in the sections that follow. The upgrade process consists of the following three parts:

1. Back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up function of PostgreSQL.
2. Run the installer, select the upgrade option and proceed with the installation.
3. Run the migration tool. This is a script that is supplied along with the installer. It migrates existing IUCLID 5 data. IUCLID 5 cannot be started until the migration tool has been successfully run.



Important

The upgrade functionality of the Windows installer can be used only if IUCLID 5 was installed using the Windows installer.

For instructions on how to carry out the installation of IUCLID 5 without the Windows installer, please refer to the specific installation manual for your computer set-up.

3.2.1. Launching the installer

After downloading the Windows installer installation package, unzip its content to a convenient folder.

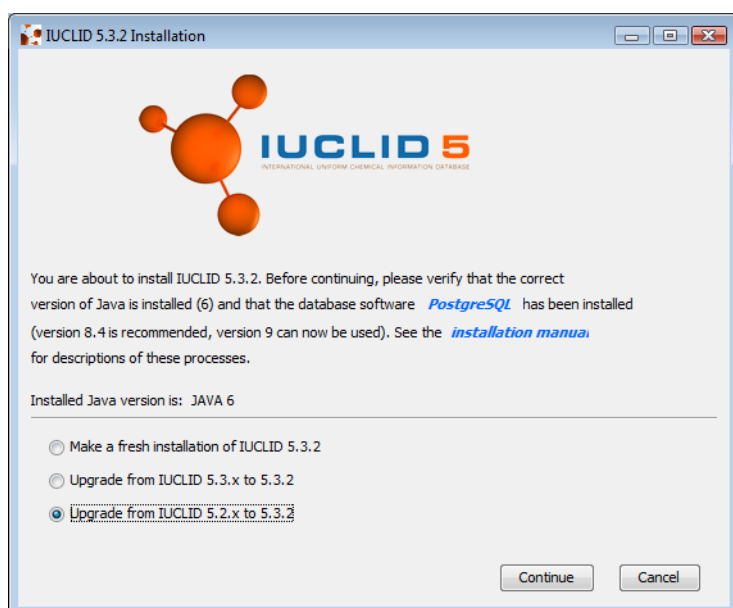
The installer is supplied as an executable Java file named `iuclid5_install.jar`. It can be launched either by double-clicking on the file, or by running it from the command line, as you would a script. Bear in mind, that the user account under which the installer is run, must have permission to write to the folder in which IUCLID will be installed.

If you experience problems in running the installer, for a possible solution, see Appendix A, *Tips on launching the installer and access rights* in the Appendix of this document.

3.2.2. Selecting the upgrade scenario

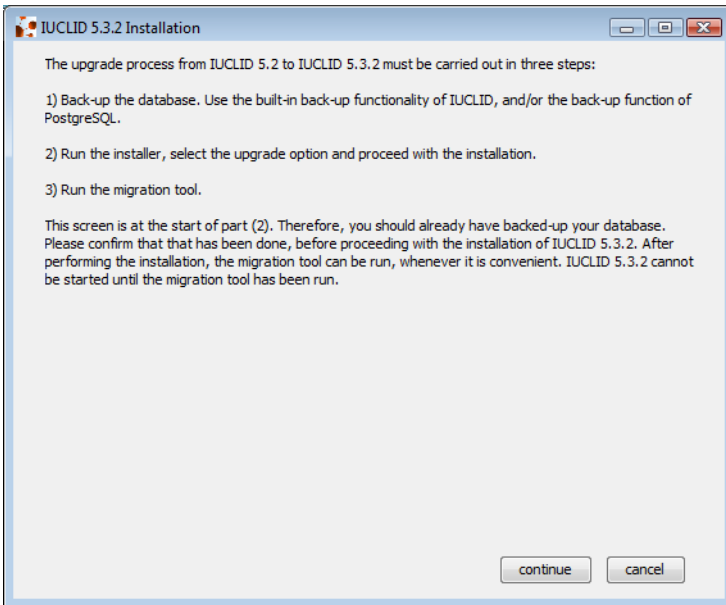
On the first screen of the installer, select the second option. In the example below, and for the subsequent screen shots in this section, the option is Upgrade from IUCLID 5.2.x to 5.3.2. Click the button Continue.

Figure 3.8. Upgrade IUCLID 5 with an increase in the major version number



The next screen provides some reminders about the overall process of this type of upgrade, as shown in the example below.

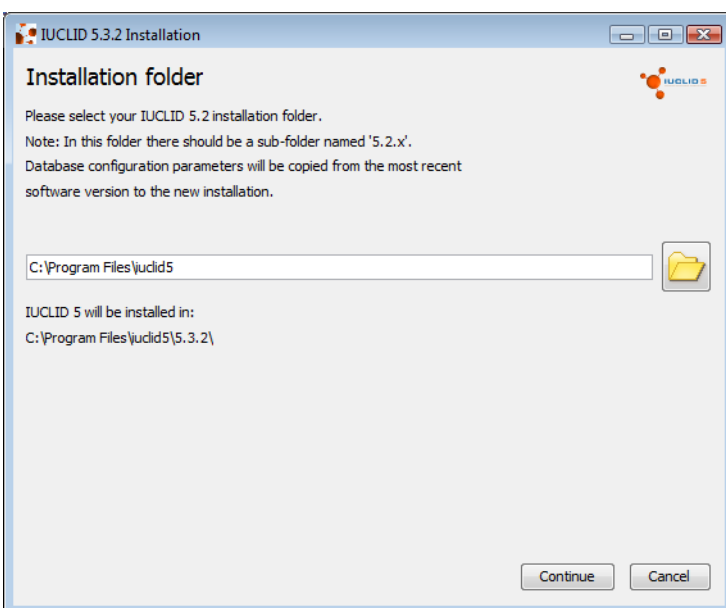
Figure 3.9. Summary of the upgrade process



3.2.3. Locations of the installation to be upgraded and the new installation

The installer creates a folder into which it will install the new version of IUCLID 5. This folder will be in the same higher level folder as the installation being upgraded. The higher level folder is set on the second page of the installer. It can have either the default value of C:\Program Files\iuclid5, as shown in the screen shot below, or you can enter a different value. However, the folder selected must contain the installation that is being upgraded. The installer reads the configuration parameters from the installation folder of the highest previous version of IUCLID 5 it can find, and then copies them to the new installation. The installer does not modify the installation being upgraded. In the example shown below, the destination folder for the upgraded installation is named IUCLID 5.3.2.

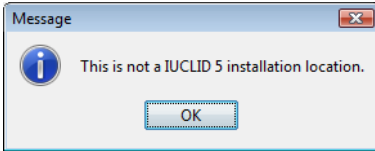
Figure 3.10. Installation folder



When you are sure that the values are correct, click Continue.

The following error message is displayed if the Windows installer cannot find a version of IUCLID 5 that it can upgrade with the options you have entered.

Figure 3.11. Installer cannot find suitable previous installation

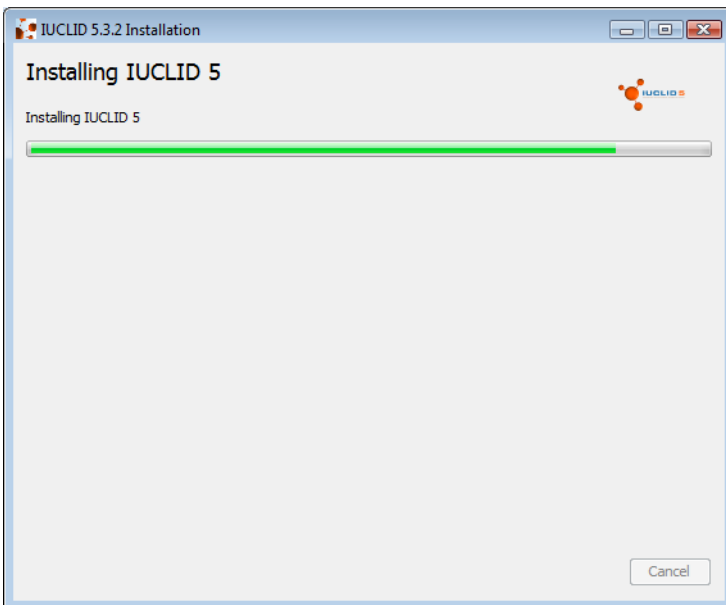


There are also two other types of error message that can be displayed: *Cannot create destination folder* and *Access denied*. If either of these are given, for a possible solution see Appendix A, *Tips on launching the installer and access rights* later in this document.

3.2.4. Installation of IUCLID 5 application files

The creation of the new folder and the copying of data to it take a few seconds, as shown in the example below.

Figure 3.12. Installing IUCLID 5

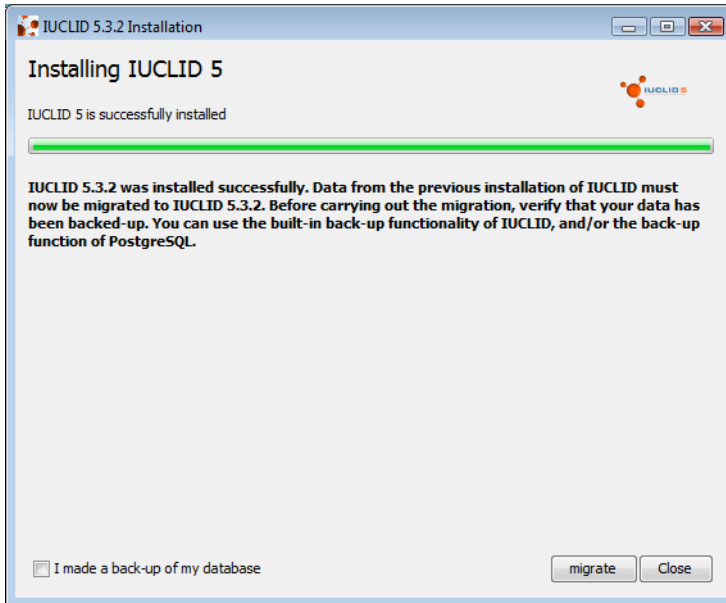


During the installation process, the following operations are performed:

- The new versions of the application files are copied to the installation folder of the new version.
- Plugins that had been installed in the previous version of IUCLID 5, are copied over to the new version of IUCLID 5, but only if they are compatible with the new version. The installer automatically detects whether a plugin is compatible. If a plugin is no longer visible in the user interface of IUCLID 5 after upgrading, visit the IUCLID web site at <http://iuclid.eu> to see whether a compatible version is available.
- The configuration files for the previous installation are copied to the new installation.
- A shortcut to IUCLID 5 is created on the desktop of the Windows account under which the installation is performed, as shown below.

Figure 3.13. Shortcut to IUCLID 5

After a successful installation of the new version of the software, the following screen is shown.

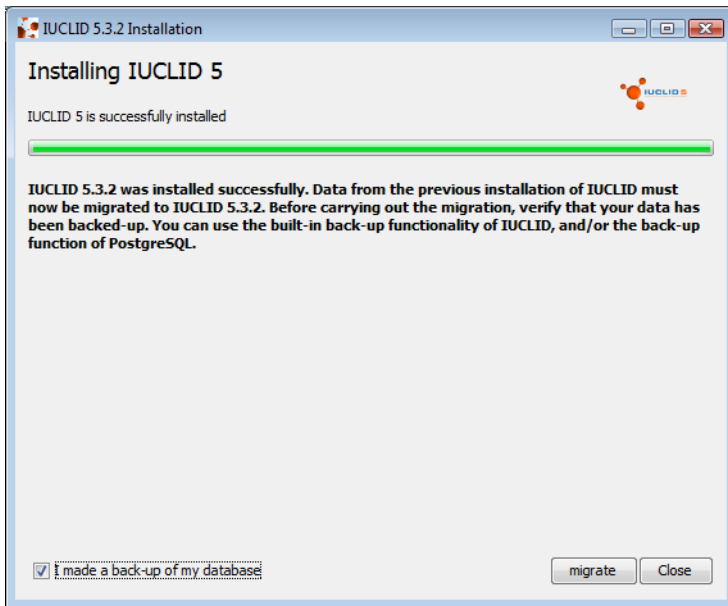
Figure 3.14. IUCLID 5 is installed successfully

This page contains advice about backing up your database and a button that starts the migration process. At this point you can choose to either begin the migration process now by clicking the button migrate, or to do it later. If you will definitely not use this screen to start the migration, you can now close the installer by clicking on the button Close. There is more information about the migration process in the next section of this manual.

3.2.5. The migration tool

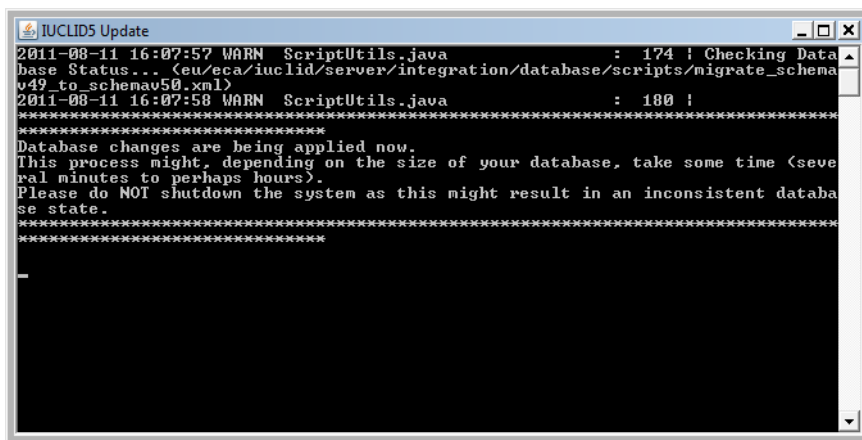
The migration tool can be run in two ways. One is to run the script named `update.bat` that was installed along with the new version of IUCLID 5 into the installation folder. The other is to start migration from the last page of the installer. This is done by first ticking the box I made a back-up of my database, then clicking the button migrate as shown below.

Figure 3.15. IUCLID 5 software installed successfully - run migration tool



Whilst the migration tool is running, a window is shown for the program *cmd* that contains a terminal to the command line of Windows. A typical example is shown in the screen shot below:

Figure 3.16. Migration tool is running



Do not allow anything to happen that might interrupt this process. Do not close the window. When the process has finished, the message *Database update successfully finished* is displayed in the window briefly, before the window closes automatically. If the process is interrupted, try starting again from the beginning. If that does not work, restore the original database from a back-up, and try again.

3.2.6. Starting IUCLID 5

After a successful migration, you can launch the upgraded IUCLID 5 by double-clicking the icon that the installer created on your Desktop, as shown below. It is also possible to launch IUCLID 5 by running the file *iuclid5.cmd* that is included in the installation directory. The initialisation process is not required. All of the data that was present in the previous version of IUCLID 5 should be present in the new version. Therefore, it should be possible to log in to any of the user accounts from the previous version.

Figure 3.17. Shortcut to IUCLID 5



3.3. Upgrading from IUCLID 5.0/1 to IUCLID 5.2 or higher



Important

There is no automatic upgrade of the database from IUCLID 5.0 / 5.1 to IUCLID 5.2 or higher versions. 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. There can be more than one database within a single instance of the database software.

3.3.1. Migration of data to the new version of IUCLID 5

Before starting to install the new version of IUCLID 5, all the data must be exported from the old IUCLID 5 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 the new version of IUCLID 5. 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. An exception is the account *SuperUser* which has a default password of *root*. To import the exported data into the new version of IUCLID 5, use the built-in Restore feature of IUCLID 5 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 the old version of IUCLID 5.

3.3.2. Database configuration for running the new and old versions of IUCLID 5 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. When upgrading from IUCLID 5.0/1 to IUCLID 5.2 or higher, a new database must be created for IUCLID 5 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 the new version of IUCLID 5 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 is run for the first time on an empty database, it will automatically create all the correct tables and the initialisation wizard will start.

3.3.3. IUCLID 5.0/1 was installed using the setup-kit

The IUCLID 5 set-up kit included the database software PostgreSQL. The set-up kit installed the PostgreSQL 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 PostgreSQL on a non-standard port (5433). Therefore, if an installation of IUCLID 5 is made with an independent installation of PostgreSQL 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 the new version of IUCLID 5 is installed exactly as described in this manual using the installer 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. In this case, the two versions of IUCLID 5 would each be running on its own independent instance of the database software, one at port 5432 and the other at port 5433.

3.3.4. IUCLID 5.0/1 was installed manually

In this case, you already have an installation of PostgreSQL that is independent of IUCLID 5, and a database for use with IUCLID 5.0/1. There is no need to install PostgreSQL again, although you might want to take this opportunity to upgrade to PostgreSQL 9. There can be more than one database running on a single instance of the database software. Therefore, to be able to run a newer version of IUCLID 5 and a previous version at the same time, create an empty database for the new version of IUCLID 5. The name of the new database must be unique within that instance of the database software.

Chapter 4. Initialisation of an installation of IUCLID 5

This chapter describes the configuration that is required to create a working IUCLID 5 system from an installation of IUCLID 5 that has an empty database. There are two scenarios: either to create a working installation from scratch, or to load data from a back-up that was made using the built-in back-up function of IUCLID 5. During initialisation from scratch, reference substance data and a legal entity are uploaded into the database, and the required user accounts can be created. For initialisation from back-up, make sure that the back-up files are accessible from the system on which IUCLID 5 will be initialised. What to do in each scenario is described in the rest of this chapter.

4.1. Starting IUCLID 5

Launch IUCLID 5 by double-clicking the icon that the installer created on your Desktop, as shown below. It is also possible to launch IUCLID 5 by running the file `iuclid5.cmd` that is included in the installation directory.

Figure 4.1. Shortcut to IUCLID 5



4.2. 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 End-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 End-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 End-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 End-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



Note

Do not click on the link **Forgot your password?** if the *First steps* wizard is being run for the first time on this database. This feature can work only after the wizard has been completed. The use of the feature **Forgot your password?** is explained later in this wizard, at step 3.



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

Figure 4.2. 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.

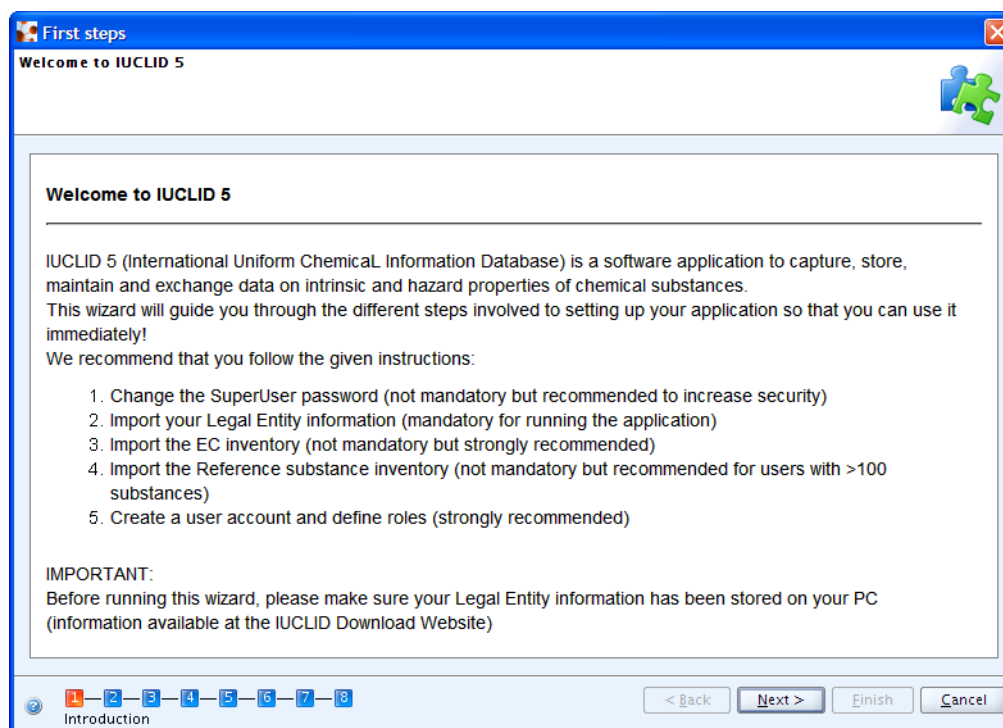


Figure 4.3. Step 2 of the First steps wizard - Init mode - New installation

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

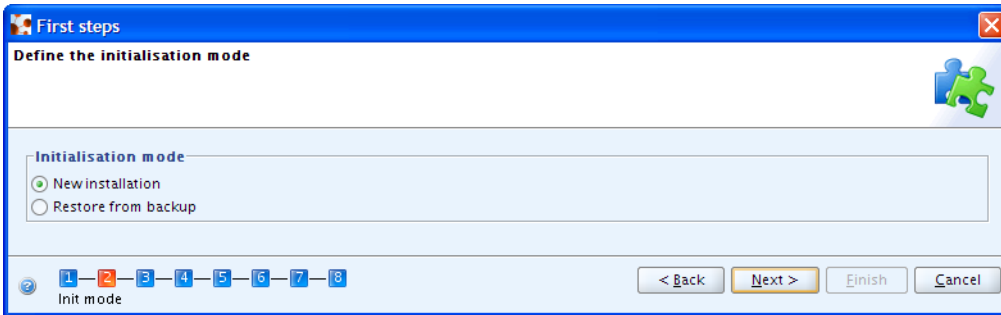
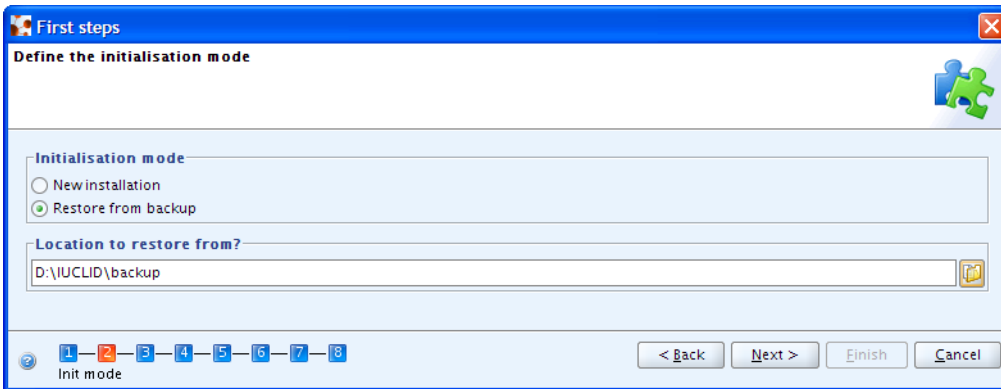


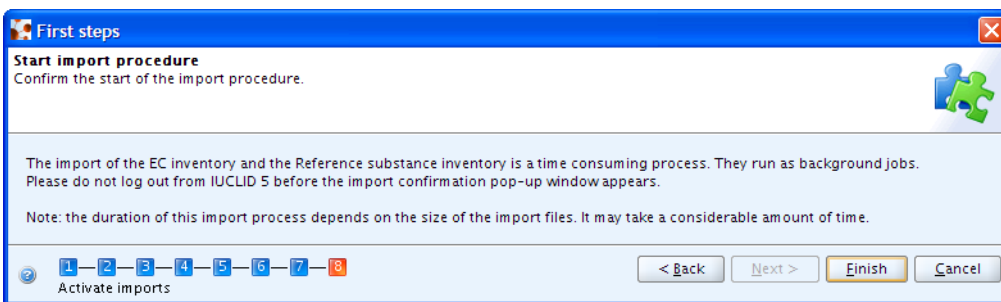
Figure 4.4. Step 2 of the First steps wizard - Init mode - Restore from backup

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.



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

Figure 4.5. Restoration from a back-up - Step 8 - Activate imports



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

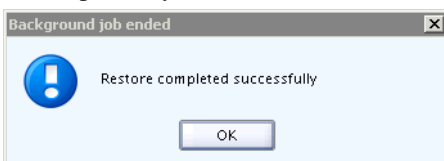
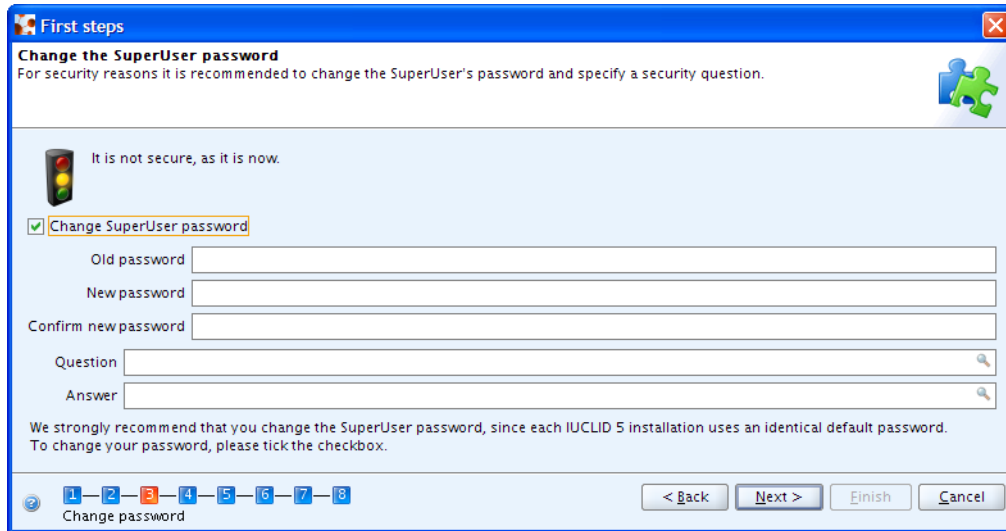


Figure 4.6. Step 3 of the First steps wizard - Change password

If the password for *SuperUser* has never been changed from its default value of *root*, the traffic light in the wizard screen will be yellow. To change the password, check the box *Change SuperUser password*, enter the current password, and then the new password, and then the new password again.

To proceed, click the button **Next**.



Tip

IUCLID 5 has a feature that can check the strength of passwords. If the feature is turned on, and the password you enter is considered to be too weak, an error message is displayed that explains what a password must contain. If that happens, read the error message carefully then create a password that satisfies the criteria. For example, the default settings require the password to be at least 6 characters in length, and to contain at least one uppercase letter, and one lowercase letter. The policy for the SuperUser is the same as that for all users. The password policy is set by editing a settings file within the installation files of IUCLID 5. This is documented in the relevant installation manual for your instance of IUCLID 5. Existing passwords can still be used to log in, even if they do not conform to the current policy. When a password is created, it must conform to the current password policy.

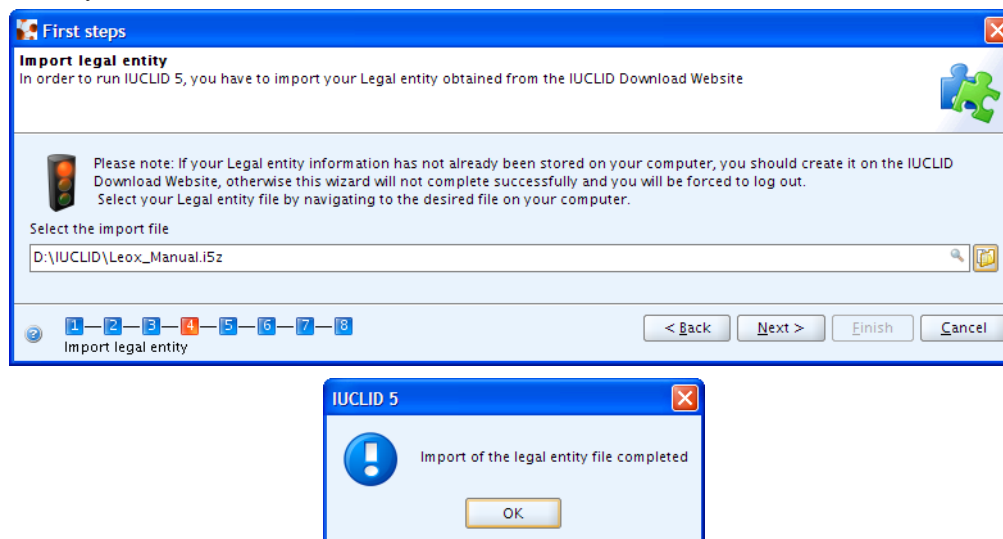


Tip

IUCLID 5 has a feature that allows a user to log in by answering a security question, instead of providing the password for the account. Users define their own questions and answers from within their own accounts. However, the SuperUser is a special case, because the question and answer can be defined before logging in for the first time. The question and answer are entered into the fields shown above in step 3 of the wizard. To use the feature to log in, a user clicks on the link **Forgot your password?** which is situated at the bottom right of the login page.

Figure 4.7. Step 4 of the First steps wizard - Import Legal Entity

To import a Legal entity (see the IUCLID 5 End-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.



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 4.8. 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 End-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.

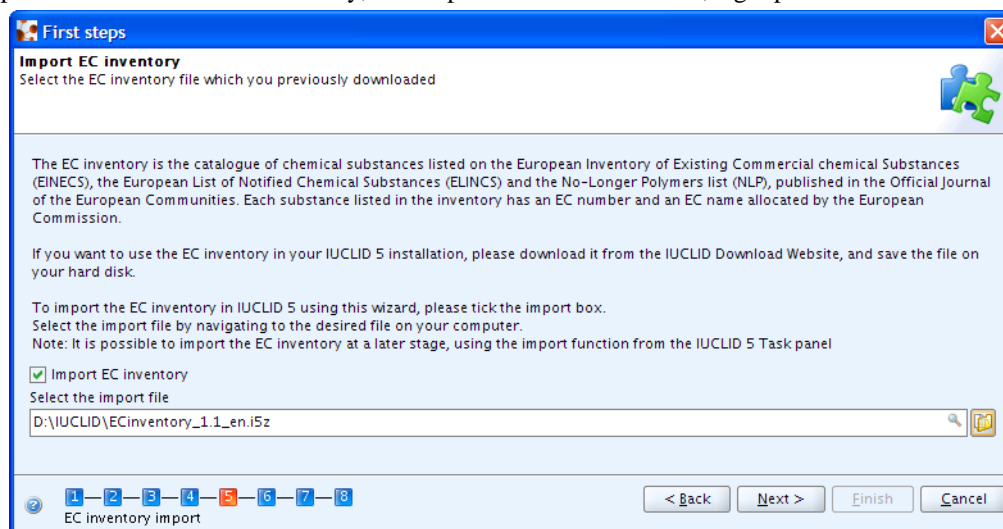
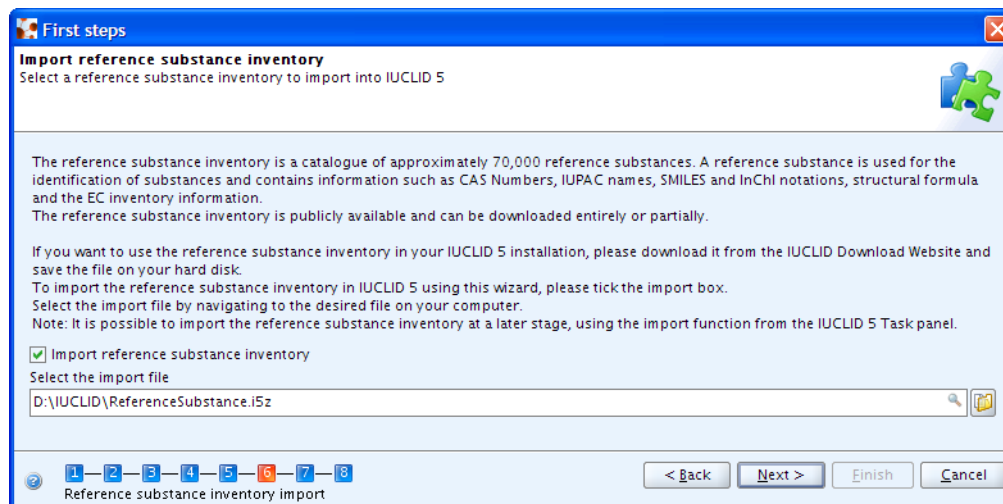


Figure 4.9. Step 6 of the First steps wizard - Import reference substance inventory

Reference substance inventory import - Select the file for the Reference substance inventory (see the IUCLID 5 End-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 long time. The import of the Reference substance inventory itself can take **up to several hours**.

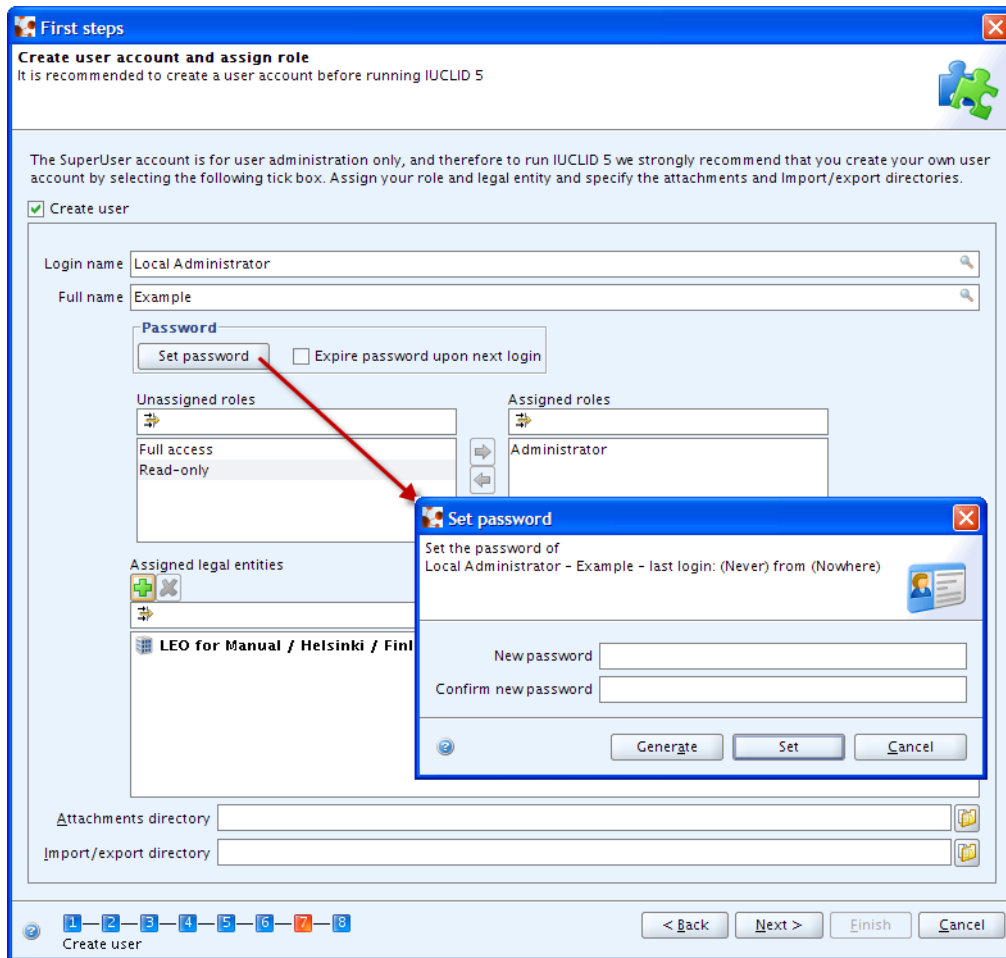


Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set*, a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

Figure 4.10. Step 7 of the First steps wizard - Create user account and assign role

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.



- 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.
- Click `Set password` to define a password.



Tip

IUCLID 5 has a feature that can check the strength of passwords. If the feature is turned on, and the password you enter is considered to be too weak, an error message is displayed that explains what a password must contain. If that happens, read the error message carefully then create a password that satisfies the criteria. For example, the default settings require the password to be at least 6 characters in length, and to contain at least one uppercase letter, and one lowercase letter. The policy for the SuperUser is the same as that for all users. The password policy is set by editing a settings file within the installation files of IUCLID 5. This is documented in the relevant installation manual for your instance of IUCLID 5. Existing passwords can still be used to log in, even if they do not conform to the current policy. When a password is created, it must conform to the current password policy.



Tip

If you want a use-once password that is reasonably hard to guess and that definitely conforms to the password policy, you can let IUCLID 5 make one for you, by clicking on the button *Generate*. It will be displayed in a new window for you to make a record of it. On closing that window it will be automatically entered into the fields *New password* and *Confirm new password*.

- Ticking the box *Expire password upon next login* forces whoever logs in to the account first to set their own 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 provided by default).



Tip

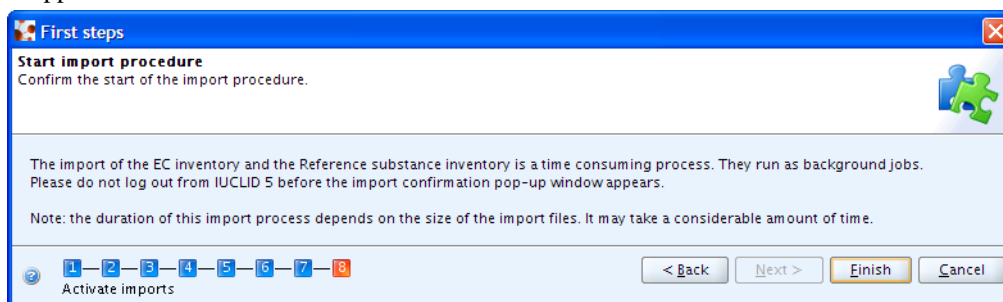
It is recommended to create a user with the *Administrator* Role regardless of whether a stand alone or a distributed version of IUCLID 5 is set up. Once a user has been created, the IUCLID 5 administrator (in case of a distributed version) can define different other user(s) and assign different role(s)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

Figure 4.11. 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.



4.3. 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 End-user Manual.

Chapter 5. Un-installation of IUCLID 5

The un-installation of IUCLID 5 is a manual process. IUCLID 5 can be un-installed by deleting the files that were copied to the destination machine, and reversing any changes made during the installation process. For more details about the actions that might be required, see the IUCLID FAQ located at the IUCLID web site <http://iuclid.eu>.

Appendix A. Tips on launching the installer and access rights

If the installer does not launch on double clicking it, one reason could be that Windows associates the file extension jar, with some application other than Java. To get around this, launch the installer with an explicit instruction to use Java, as described in below. If required, there are more detailed step by step instructions given later in this Appendix.

Force installer to be opened by Java

1. Open a terminal in Windows that gives access to the command line.
2. Change to the directory in which the installer file is located.
3. Enter the command `java -jar iuclid5_install.jar`

If during the installation, Windows displays error messages of the types shown below, and/or the desktop shortcut is not created, the installer had insufficient access rights.

Error message: **Cannot create the destination folder**

Error message: **C:\Program Files\iuclid\5.2.x\iuclid5.ico (Access is denied)**

If the shortcut was not created automatically, but the installation was a success, it is recommended to create the shortcut manually, rather than re-install with different access rights. The manual creation is described below.

Three ways to obtain the correct access rights

1. Run the installer from the command line. This is described in a dedicated section below.
2. Select a destination folder to which the installer has write access, i.e. replace the default value `C:\Program Files\iuclid5` with something suitable on your system.
3. If you have access to a user account of type *built-in user*, log in to it and start the installer by double-clicking on the file `iuclid5_install.jar`.

To run from the command line

1. Log on as a user that has administrator rights.
2. Open the application *Command Prompt* using the option *Run as administrator*.
3. Enter the administrator password when prompted.
4. In the *Command Prompt* window, move to the folder that contains the installer Java file.
5. Enter the name of the Java file then press the key *Enter*.

Extra detail about the command line

1. Getting the command line

- a. Click on the *Start* icon at the bottom left of the Windows Desktop
- b. Select from the menu *All Programs / Accessories*

c. Right-click on the application *Command Prompt* then select *Run as administrator*

2. Moving to the correct directory

a. to view the content of the current directory, enter the command *dir*

b. to change to a particular drive, enter its drive letter followed by a colon, e.g. *G:*

c. to enter a folder, enter the command *cd* followed by the directory name, e.g. *cd Documents*

d. to go one level up in the file system, enter the command *cd ..*

Manual creation of the shortcut

1. Right-click on the Windows desktop and select the menu item *New Shortcut*.

2. Enter the location or *Browse* to the file named *iuclid5.cmd* that is included in the installation directory.

3. Enter a name for the shortcut then click *Finish*.

4. To attach a IUCLID 5 icon to the shortcut, right-click the shortcut and select *Properties*.

5. Select *Change Icon* then *Browse* to the installation directory and select the file *iuclid5.ico*. Click *Apply* and *OK* where appropriate.

If you are still having problems with the installation, before contacting the IUCLID Helpdesk, please try the FAQ located on the IUCLID web site <http://iuclid.eu>.