

IUCLID 5

Guidance and Support

Installation Guide for IUCLID 5.6
Client-Server Architecture

Microsoft[®] Windows[®]



March 2015

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It can be accessed at the addresses:

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Chapter 1. Introduction

IUCLID 5 can be installed either as a standalone application, or in a distributed (multi-user) environment using client-server architecture. This document describes how to install and configure the IUCLID 5 application as a server in a distributed Microsoft® Windows® environment (hereafter referred to as Windows) , and how to launch a client to connect to 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 server hosting IUCLID 5 must have at least:

- RAM: At least 2 GB on the mother board; 4 GB if PostgreSQL is run on the same machine as IUCLID 5
- Hard disk space: 200 GB
- CPU: Intel Pentium Dual @ 1.8 GHz
- Network adaptor 100 Mbps (recommended 1Gbps)

The requirements depend in part on the plug-ins that are in use. For example, using the Query Tool plug-in will increase the resources required to obtain a reasonable running speed; especially on a large database. There are no specific hardware requirements to run the IUCLID 5 client.

1.2. Software requirements

Operating system:

- The IUCLID 5 server can be hosted under Microsoft® Windows® Server 2008 or 2012. Other versions (2003) may be used, but note that the testing has been done with 2008 and 2012. The IUCLID 5 client can be run under Windows 7 or 8.

IUCLID 5 can be installed with the following open source components:

- Java SE - Runtime Environment 7 or 8. IUCLID 5.6.0.2 is compatible with Java 6, but the vendor, Oracle, recommends to uninstall Java SE 6, and then to install the latest update of Java. Various scenarios involving the use of IUCLID 5, Java 6 and Java 7 can be found in the IUCLID FAQ located at the IUCLID web site <http://iuclid.eu>. For Java, the requirement for the IUCLID 5 client is the same as that for the server.
- Tomcat 7 or 8. Installation packages can be downloaded from <http://tomcat.apache.org>.
- PostgreSQL 9.0, 9.1, 9.2 and 9.3 are supported. PostgreSQL 9.3 is recommended. Installation packages can be downloaded from <http://www.postgresql.org>

As an alternative to the free database software PostgreSQL, the commercial database software Oracle, can be used. You do not need both PostgreSQL and Oracle:

- Oracle® 11g or 12c. Oracle® 10g is not supported. Installation packages can be downloaded from <http://www.oracle.com>

The Oracle driver for Java is no longer supplied with the IUCLID installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the Oracle web site and installed in the appropriate folder. For example, for Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`. For use with Tomcat, the driver must be placed in Tomcat's library folder, e.g. `Tomcat\lib`.

The following essential components can be downloaded without charge from the IUCLID 5 web at the at <http://iuclid.eu>. Before downloading them, you must register as a user on the site.

- The IUCLID 5 distributed installation package, version 5.6.0.2.
- Once you have completed the installation of IUCLID 5, you should test it by starting and configuring it. The configuration requires access to 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, which are also available from the web site <http://iuclid.eu>.



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*.

- To start the IUCLID 5 client as described in section Section 4.1, “Starting the IUCLID 5 client”, a web browser is required. There are no specific requirements for the browser, or the computer upon which it is run.

For more information regarding system requirements, see the FAQ on the IUCLID web site located at <http://iuclid.eu>.

Chapter 2. Making a fresh installation of IUCLID 5

The following chapter contains a brief description of the actions required to make a fresh installation of IUCLID 5 that runs within a web server on Windows.

2.1. Operating System

IUCLID 5 has been tested using Windows Server 2008 and 2012. Other versions may be used as well. In that case the file locations might differ from those used in this document. For installation instructions, please refer to the documentation supplied by the manufacturer.

2.2. JAVA Development Kit

Download the JAVA Development Kit (JDK) 8 or JAVA Runtime Environment (JRE) 8 according to the architecture of the destination computer from the site <http://www.oracle.com>. [<http://www.oracle.com>] IUCLID 5.6.0.2 is compatible with Java 6, but the vendor, Oracle, recommends to uninstall Java SE 6, and then to install the latest update of Java. Various scenarios involving the use of IUCLID 5, Java 6 and Java 7 can be found in the IUCLID FAQ located at the IUCLID web site <http://iuclid.eu>.

Run the installer and follow the instructions. The default parameters are appropriate for IUCLID 5. For more information, please refer to the documentation on the site from which the software is available.

2.3. Database - PostgreSQL

PostgreSQL is an open source, object-relational database system. Installation packages, and more information about the software can be obtained from the site <http://www.postgresql.org>.

2.3.1. Installation of PostgreSQL

If either version 9.0, 9.1, 9.2 or 9.3 of PostgreSQL is already installed, the existing installation can be used. To run IUCLID 5, there is no specific need to upgrade to a higher version number of PostgreSQL. If PostgreSQL is not already installed on the computer, or you would like to upgrade it, download the new version of PostgreSQL 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-9.2.3-2-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 database 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 2.1. Installer for PostgreSQL

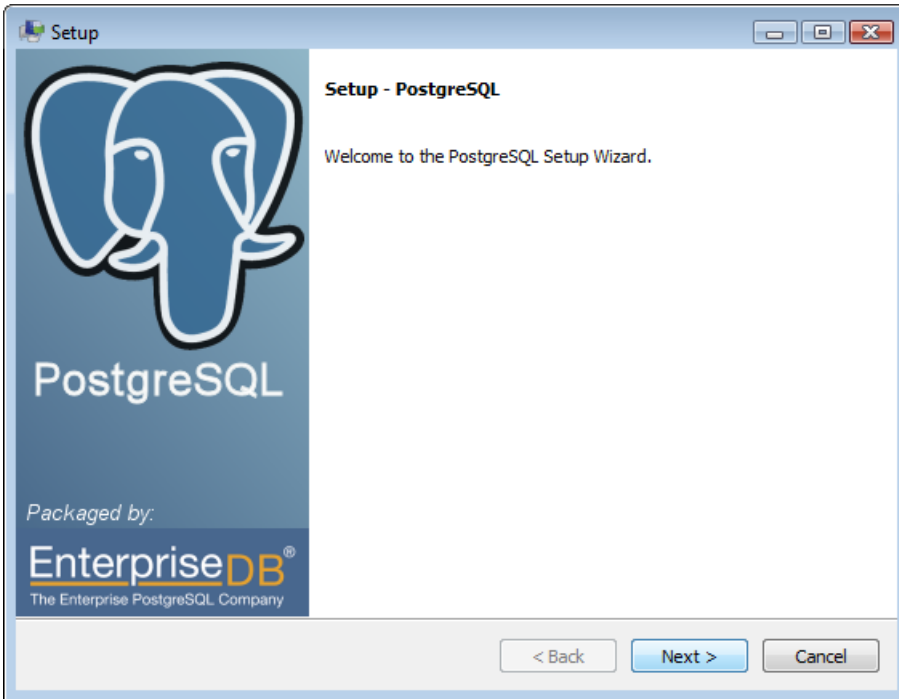


Figure 2.2. Installation directory for PostgreSQL

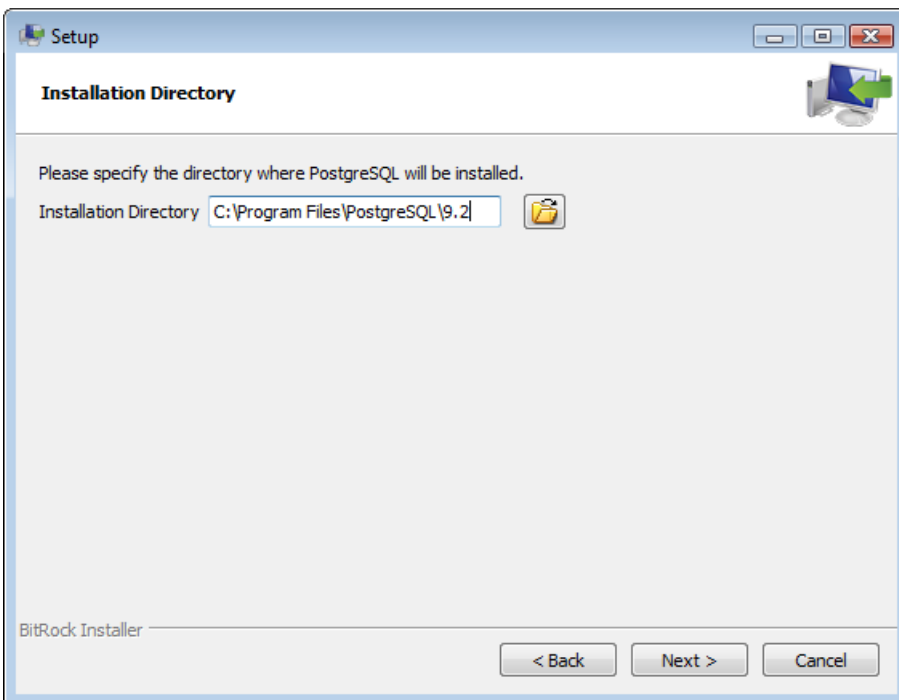


Figure 2.3. Data directory for PostgreSQL

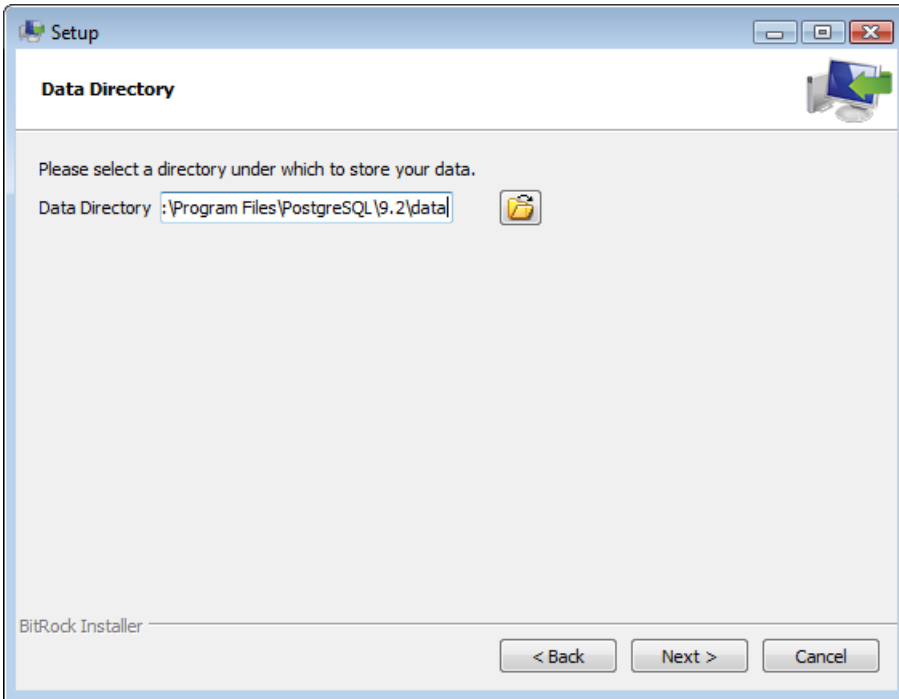


Figure 2.4. Password for the database superuser (postgres) and the Windows service account (postgres)

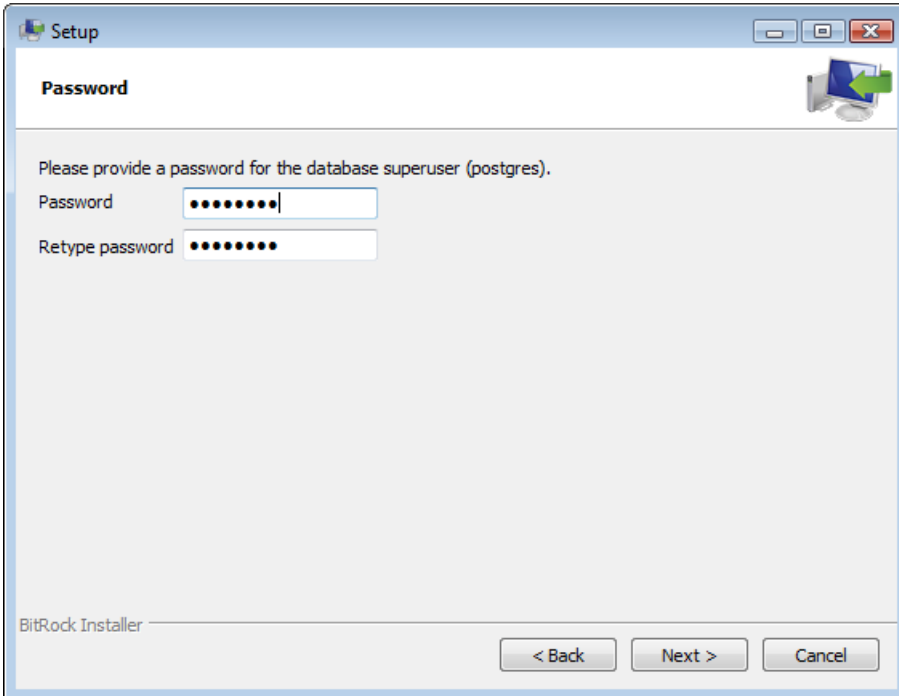


Figure 2.5. Port number for PostgreSQL

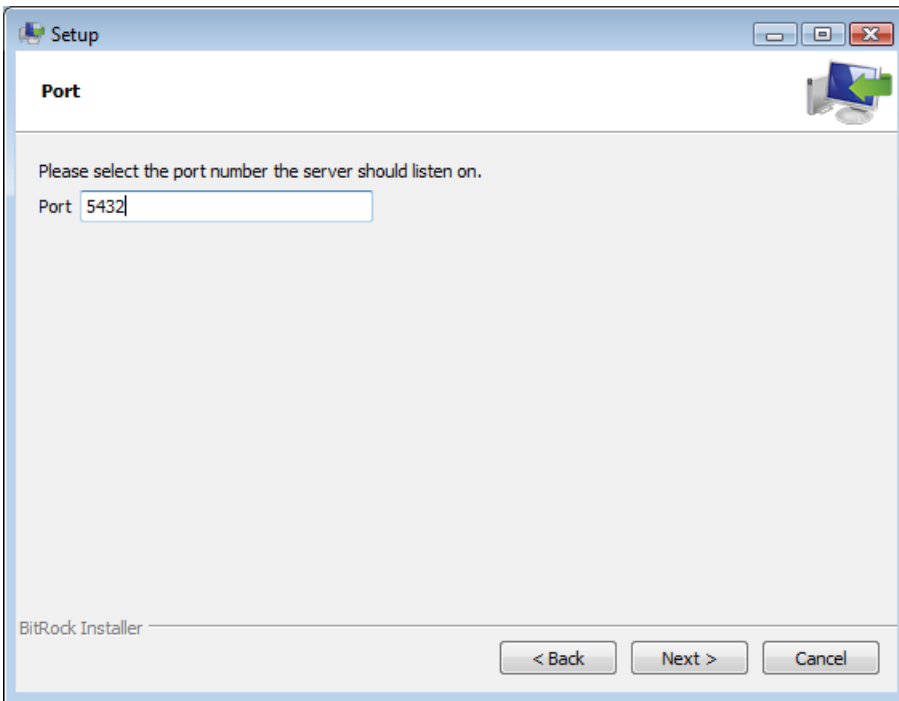


Figure 2.6. Set the default locale for PostgreSQL

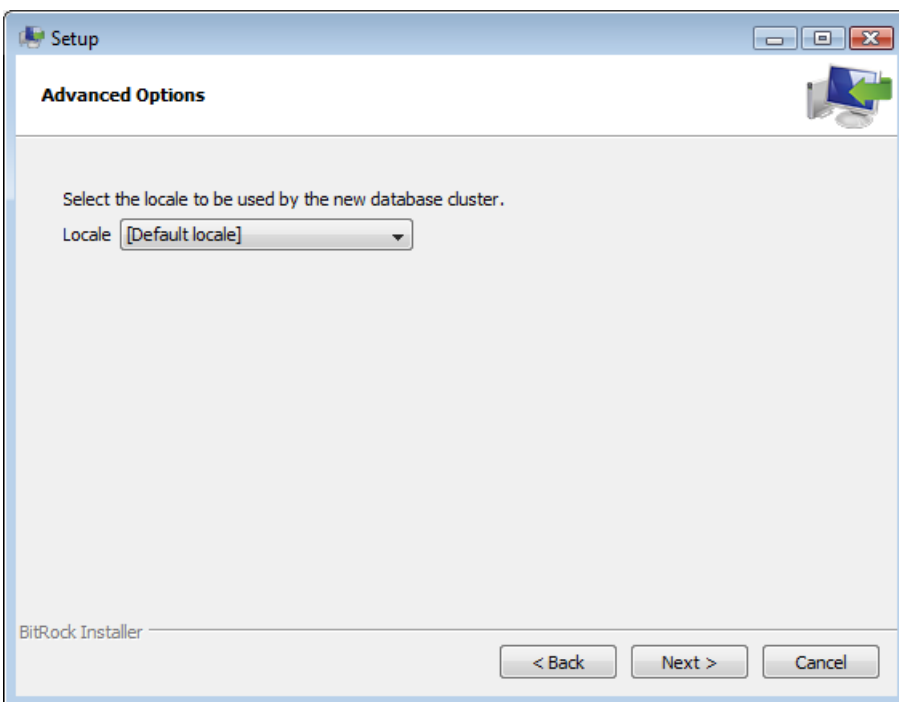


Figure 2.7. Confirm installation of PostgreSQL

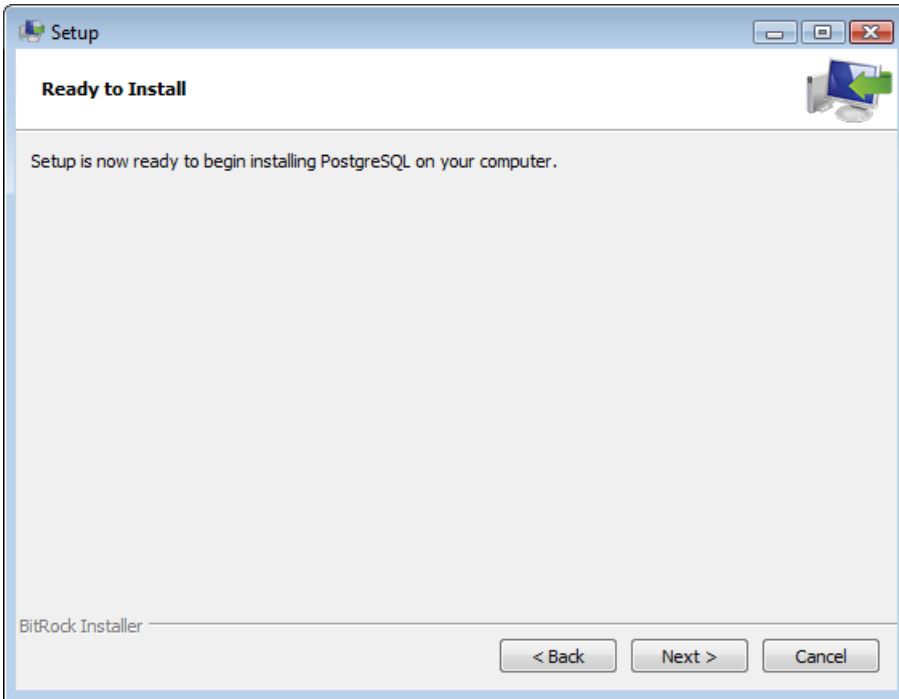


Figure 2.8. Installation of PostgreSQL in progress

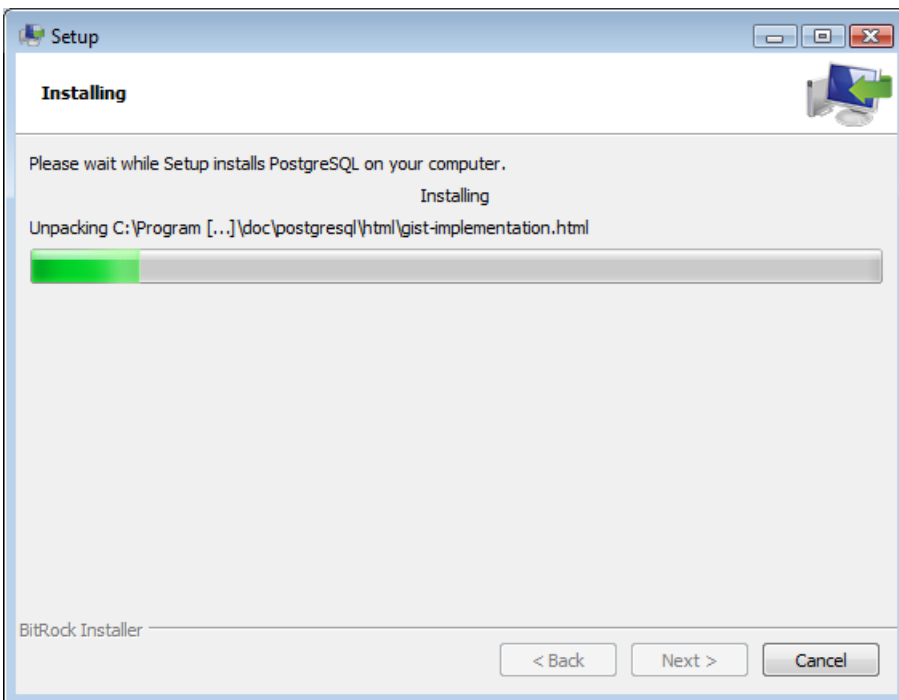


Figure 2.9. Installation of PostgreSQL complete



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.

2.3.2. Configuration of PostgreSQL

A new user and a new database need to be created.



Tip

IUCLID 5 is configured by default to connect to the database using username:*iuclid5* and password:*iuclid5*. It is convenient to specify the same password now, and change it later when the application is set up correctly.

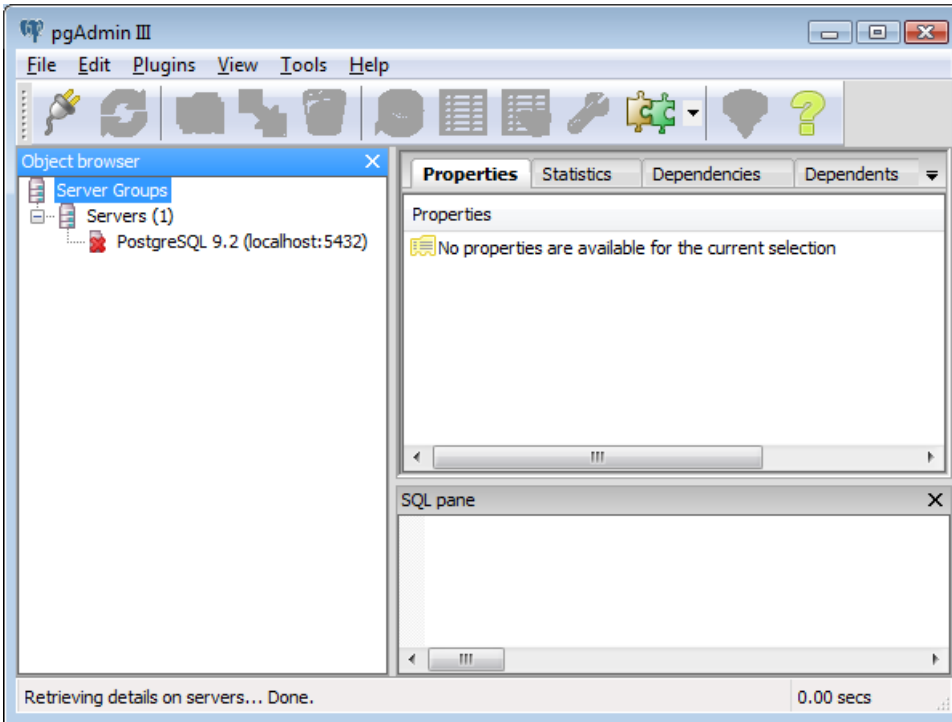


Important

Take note of the password of this user. This user name and password will be needed later to connect IUCLID 5 to the database.

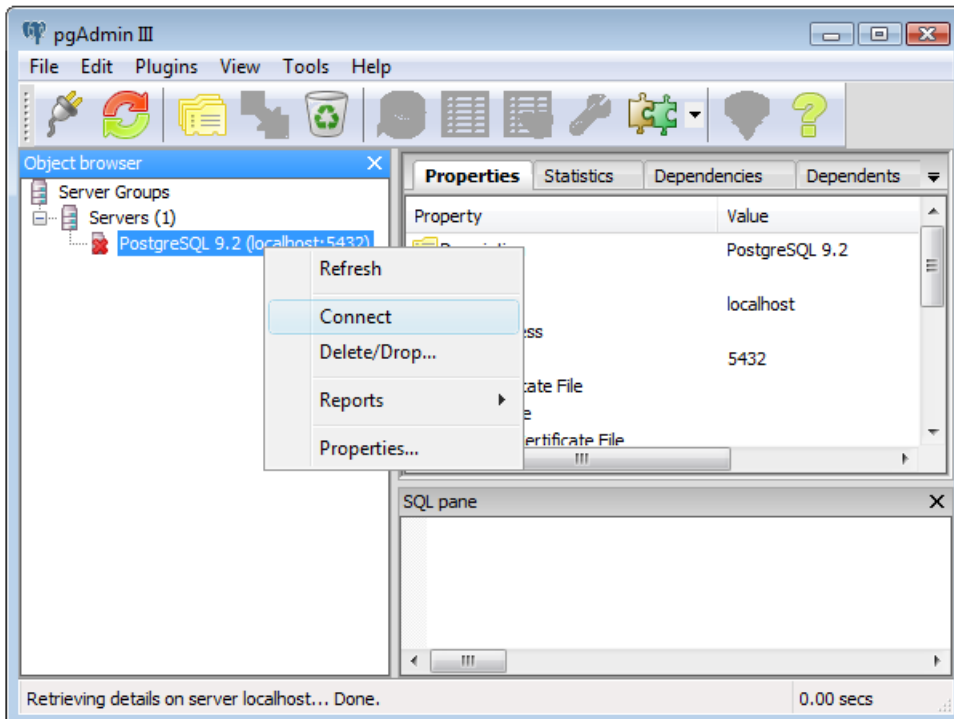
The program pgAdmin III can be used to create the database as follows. Start pgAdmin III from the menu *Start / All Programs / PostgreSQL9.2*. After the splash screen has appeared and you have closed the pop-up window that shows usage tips, the following screen is shown.

Figure 2.10. pgAdmin III interface on first opening



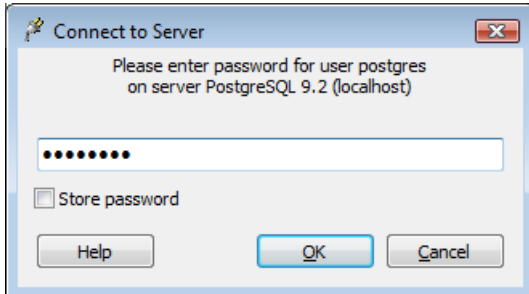
Right-click the text *PostgreSQL 9.2 (localhost:5432)* that is under the word *Servers* highlighted in blue in the figure above. Select *connect* as shown below.

Figure 2.11. Connect pgAdmin III to PostgreSQL as user postgres



Enter the password for user *postgres* as given in the postgres installer Figure 2.4, “Password for the database superuser (postgres) and the Windows service account (postgres)” then click *OK*. It is recommended to store the password to facilitate future access.

Figure 2.12. Authenticate the user postgres



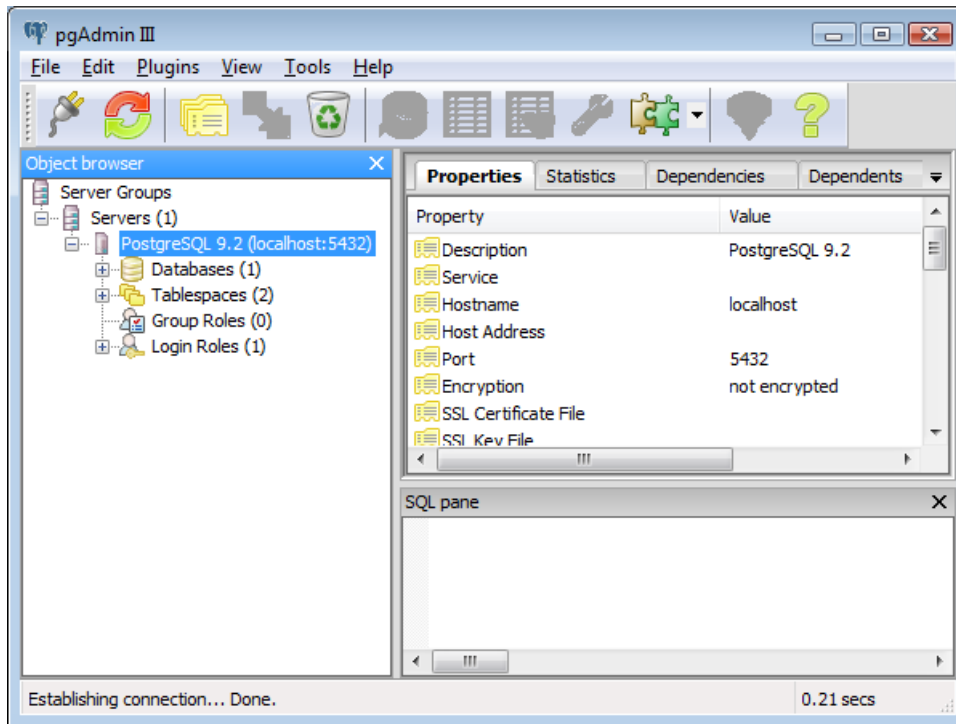
If you elect to save the password, the following warning might be displayed. Click *OK*

Figure 2.13. Saving passwords Warning



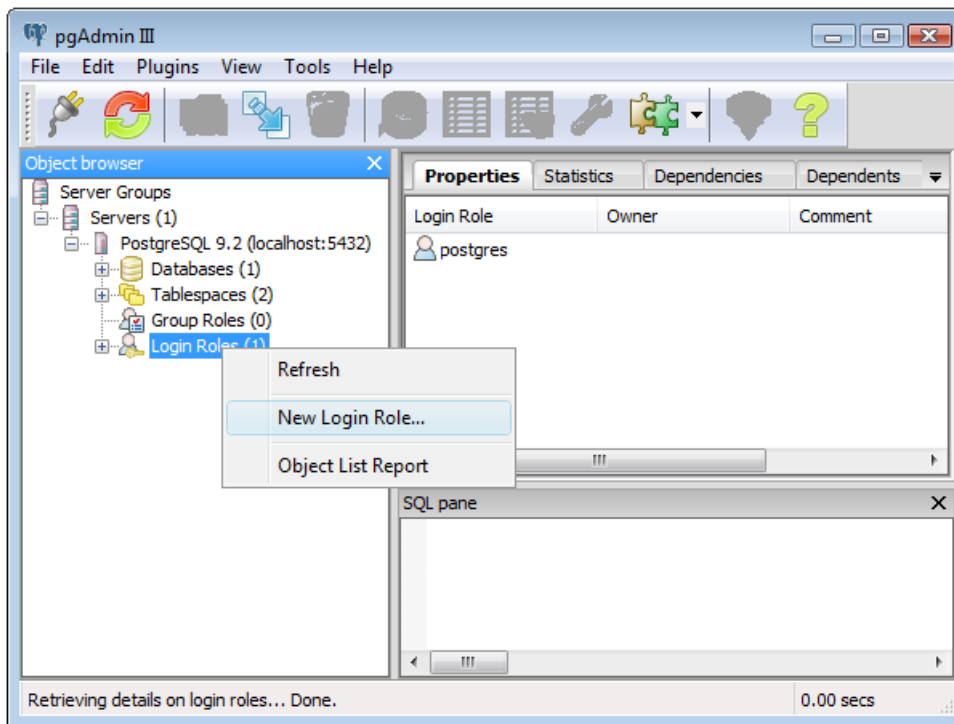
Expand the tree for *PostgreSQL 9.2 (localhost:5432)* by clicking the plus sign that has just appeared next to it, as shown in the figure below.

Figure 2.14. Initial screen in pgAdmin III



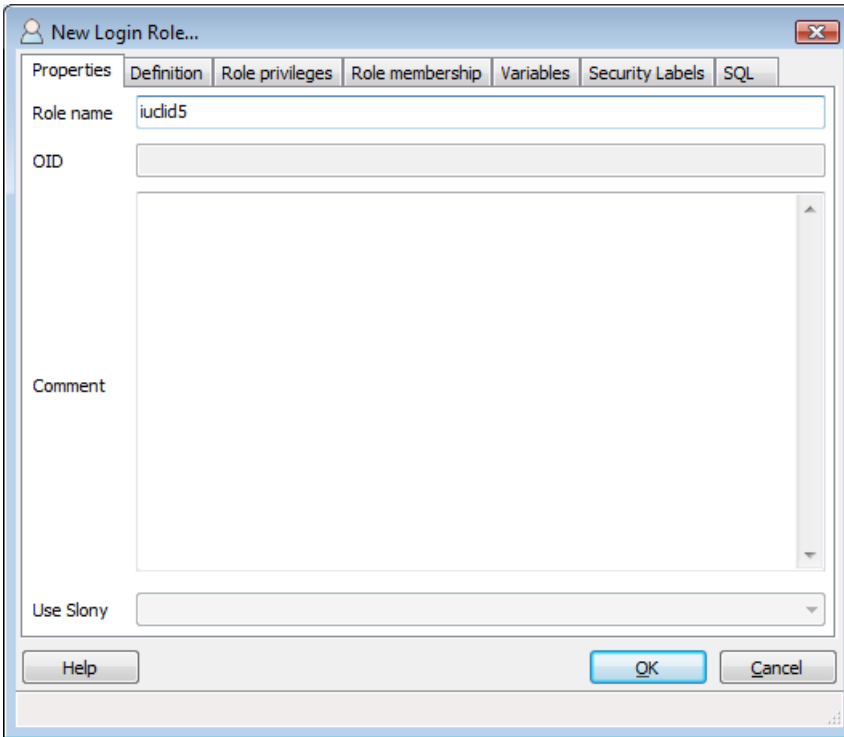
Right-click on *Login Roles* and select *New Login Role...*

Figure 2.15. Select the option New Login Role



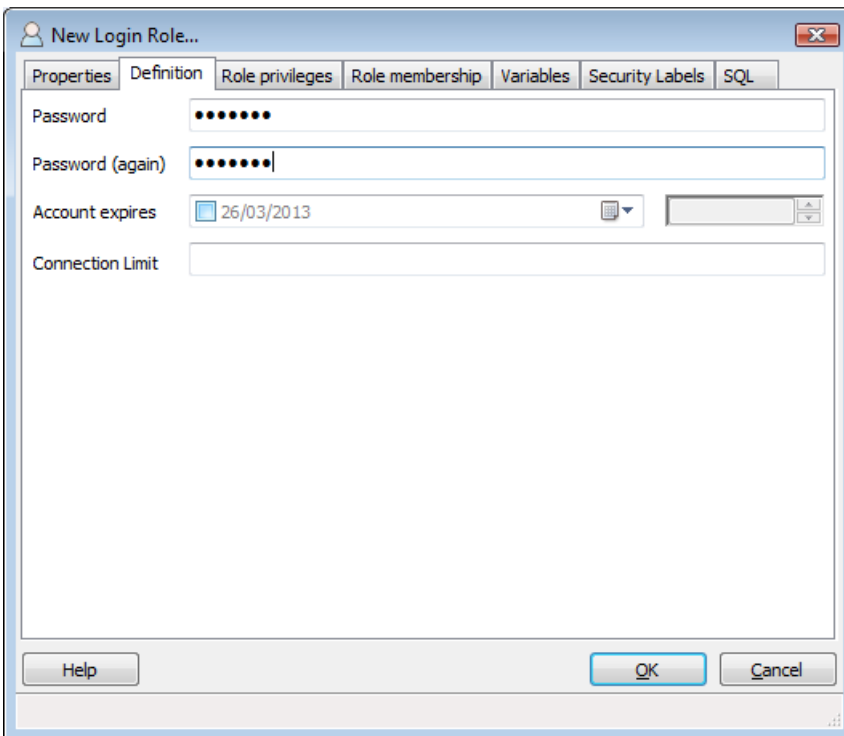
Enter the name of the login role. We recommend using a name of *iuc1id5*.

Figure 2.16. Create a new login role (i.e. a user) with the name iuclid5



The login role can have a password set, although this is optional. The password is entered under the tab Definition.

Figure 2.17. Set the password of the new login role. This step is optional.



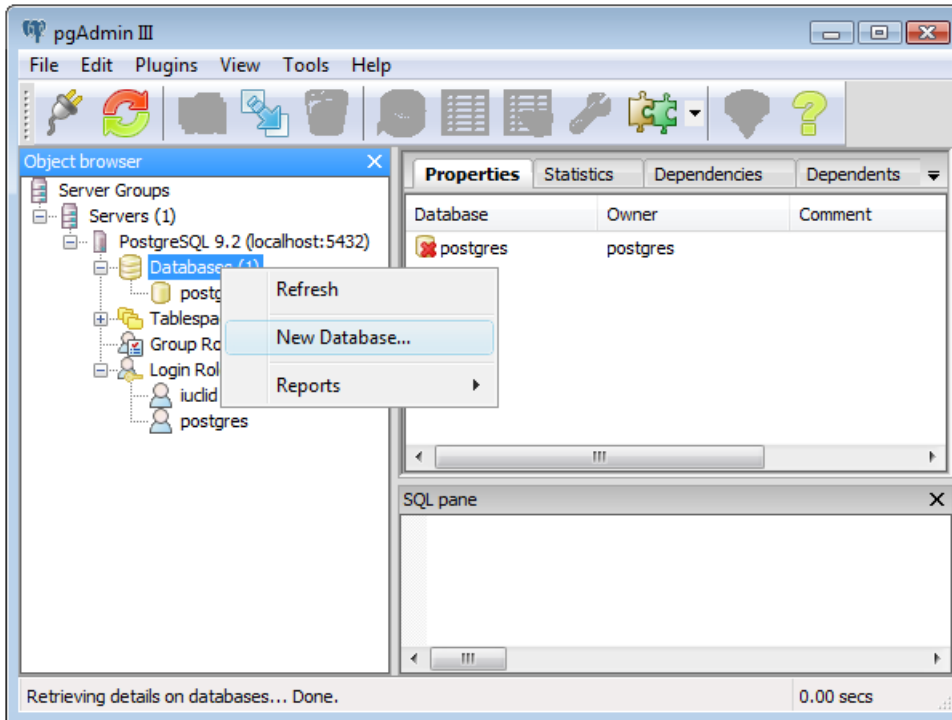


Important

Make a note of the user name and if set, the password. They are referred to later in the installation, in Section 2.6.1, “Database connection settings for PostgreSQL”. We recommend using `iuclid5` as the name of the login role, and for the password.

Request a new database by right-clicking the item *Databases*, and selecting *New Database...* as shown in the figure below.

Figure 2.18. Request a new database in pgAdmin III



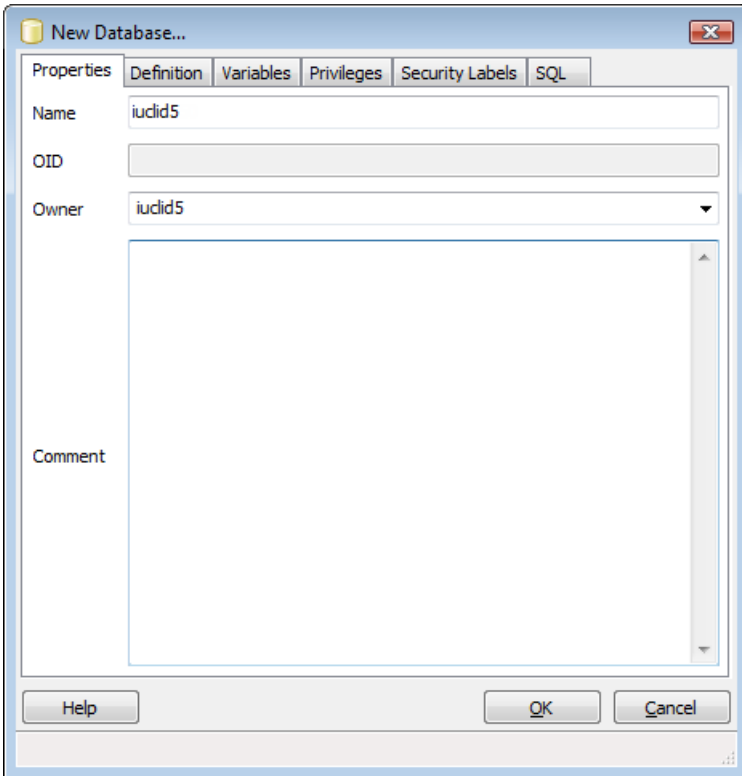
Enter the details you require. Normally these are only name=`iuclid5` and owner=`iuclid5`. The encoding, set under the tab Definition, must be left at the default value of UTF8. Click *OK*.



Important

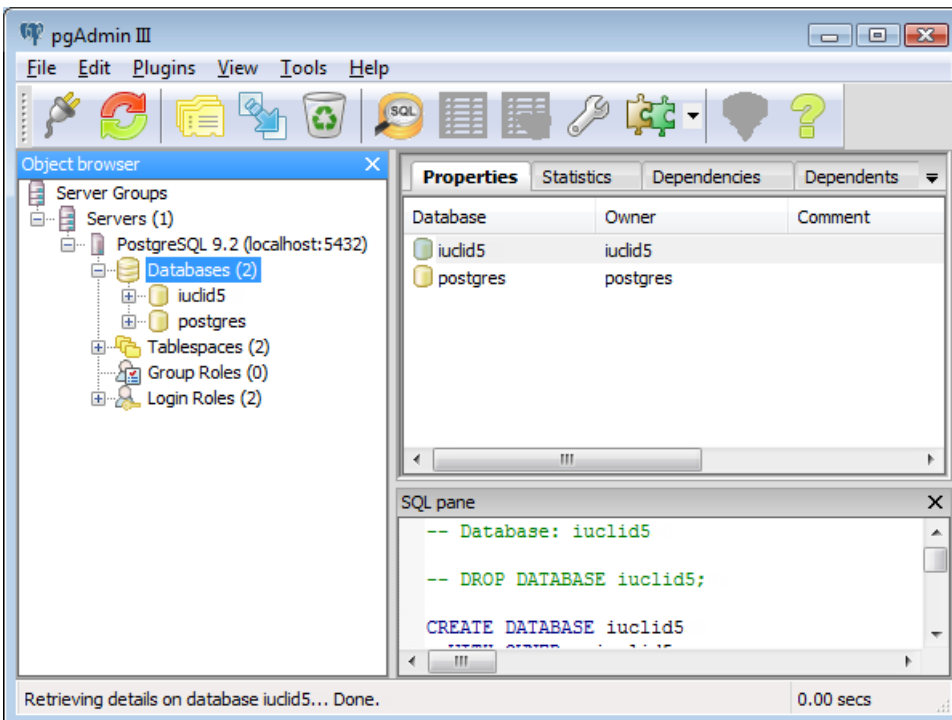
Make a note of the database name. It is referred to later in the installation, in Section 2.6.1, “Database connection settings for PostgreSQL”. We recommend using the name `iuclid5`. If there is already a database of that name, you can enter something different.

Figure 2.19. Enter the details of IUCLID 5's database into pgAdmin III



As you can see from the figure below, there is now a new database named *iuclid5*.

Figure 2.20. List of databases in pgAdmin III



You can now close *pgAdmin III* and move directly to the installation of IUCLID 5.

2.4. Database - Oracle

IUCLID 5 is published with values of settings for connection to a PostgreSQL database. Changing the configuration to use an Oracle database is described in Section 2.6.2, "Database connection settings for Oracle".

The details of the installation and configuration of Oracle database software (DBMS) are out of the scope of this document due to their complexity. Please refer to the documentation supplied by Oracle. The details of how to set up the database for IUCLID 5 are given in this section. System administrator rights for the database are required. If you have a database manager (DBA) for Oracle at your organisation, ask the DBA to carry out the actions described in the rest of this section.

Create a user account with the following system privileges:

```
CREATE SESSION
```

```
CREATE SEQUENCE
```

```
CREATE TABLE
```

```
CREATE VIEW
```

The account needs to have a default tablespace with unlimited quota and autoextend set to ON. The block size of the tablespace is recommended to be at least 16K to avoid the error *"ORA-01450 maximum key length exceeded"*. The character set must be set using NLS_CHARACTERSET=AL32UTF8.

An example of the commands required is given below.

```
CREATE tablespace iuclid5_ts
  datafile 'iuclid5_ts.dbf' /*specify absolute path*/
  size 500M
  autoextend ON
  next 500M
  maxsize 2000M;
grant CREATE session TO iuclid5 identified BY "iuclid5";
grant CREATE TABLE TO iuclid5;
grant CREATE VIEW TO iuclid5;
grant CREATE sequence TO iuclid5;
ALTER USER iuclid5 quota unlimited ON iuclid5_ts;
ALTER USER iuclid5 DEFAULT tablespace iuclid5_ts;
```

Ensure that the IUCLID 5 database user `iuclid5` has been granted only the privileges shown in the commands shown above. Do not grant the privileges of `SELECT ANY TABLE`, a role `DBA`, or direct `SELECT` to the secondary (`iuclid5`) database user tables. If the user `iuclid5` has excess privileges revoke them by, for example by using one or both of the following commands:

```
REVOKE CREATE SESSION FROM iuclid5;
```

```
REVOKE SELECT ANY TABLE FROM iuclid5;
```

The first denies access to the database whereas the second denies access to the tables.

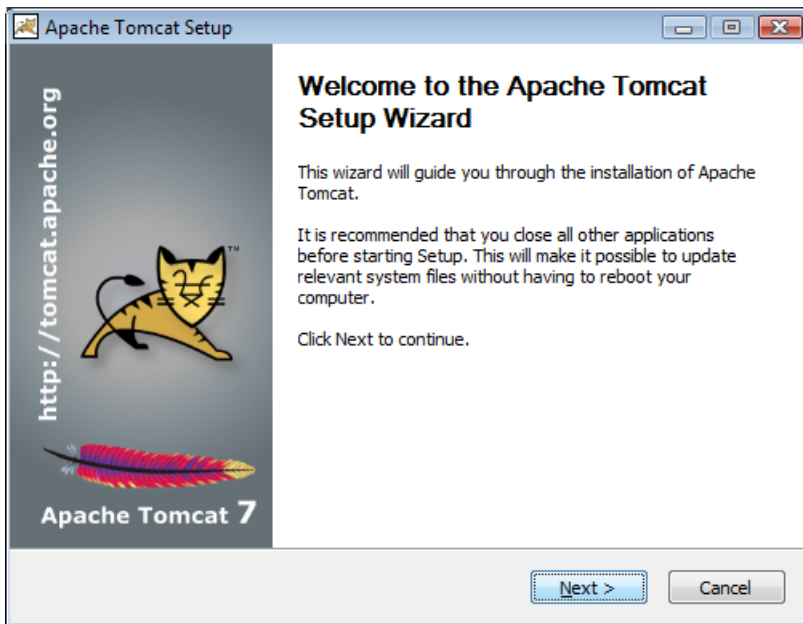
2.5. Application Server - Tomcat

Running IUCLID 5 in an application server allows multiple users to access a database at the same time over a network. Each user accesses IUCLID 5 via a client that is run on a local machine. Alternative application servers to Tomcat might work, but they are not supported.

2.5.1. Installation of Tomcat

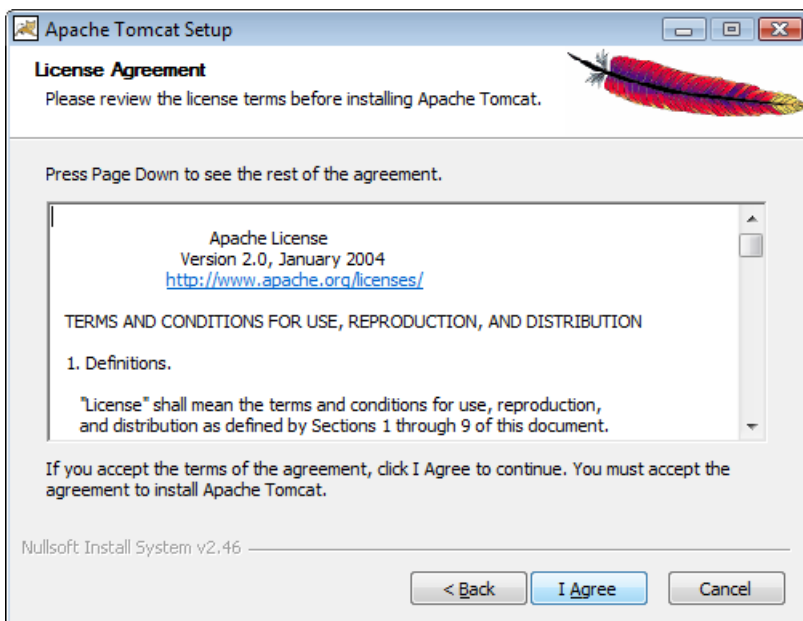
Tomcat can be installed either as an application that is controlled using a set of scripts or, as a service under Windows. The service option is convenient because it can be set up using an installer, and once installed, the software can be controlled using the service management tools in Windows. An example of the installation as a service under Windows is described below. Download and run the Windows Service Installer of Tomcat from <http://tomcat.apache.org/>. The first page of the installer is shown below:

Figure 2.21. Welcome to the Apache Tomcat Setup Wizard



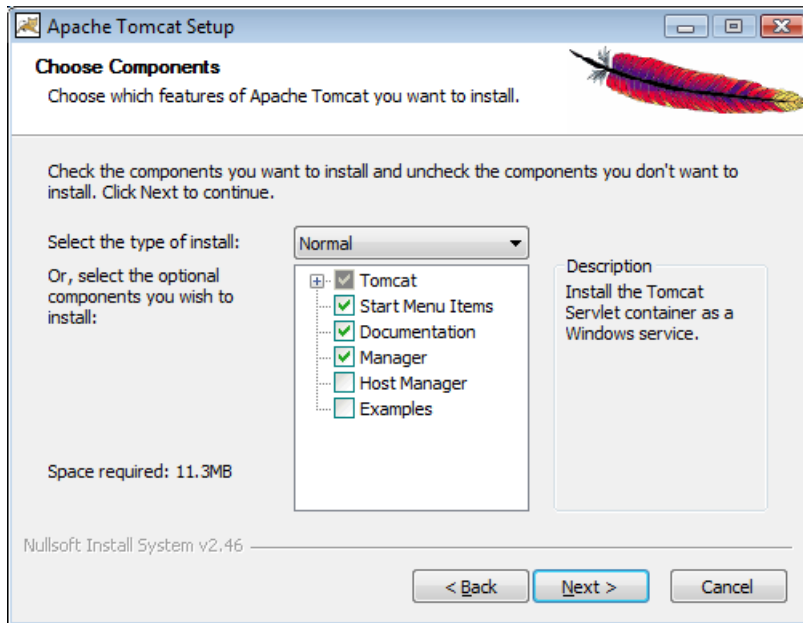
Click on the button Next.

Figure 2.22. Licence Agreement



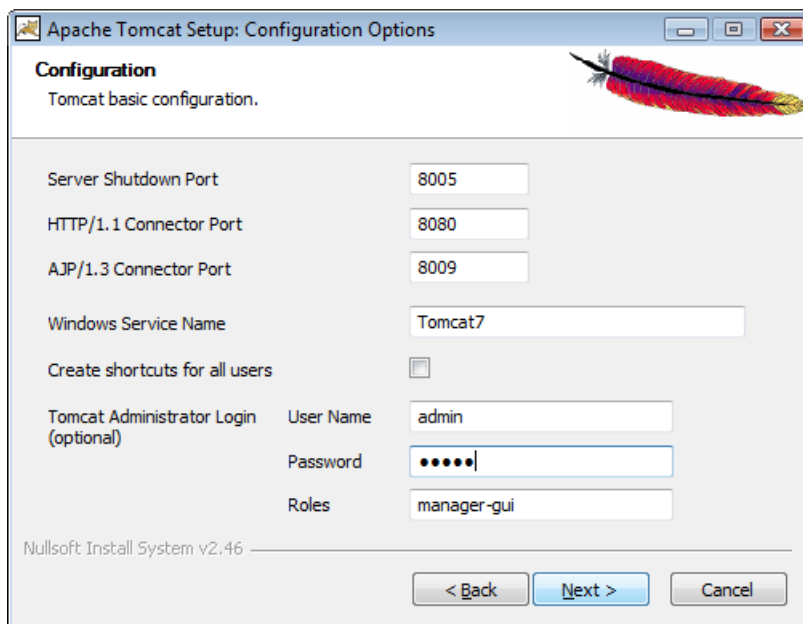
If you accept the licence, click on the button I Agree.

Figure 2.23. Choose Components



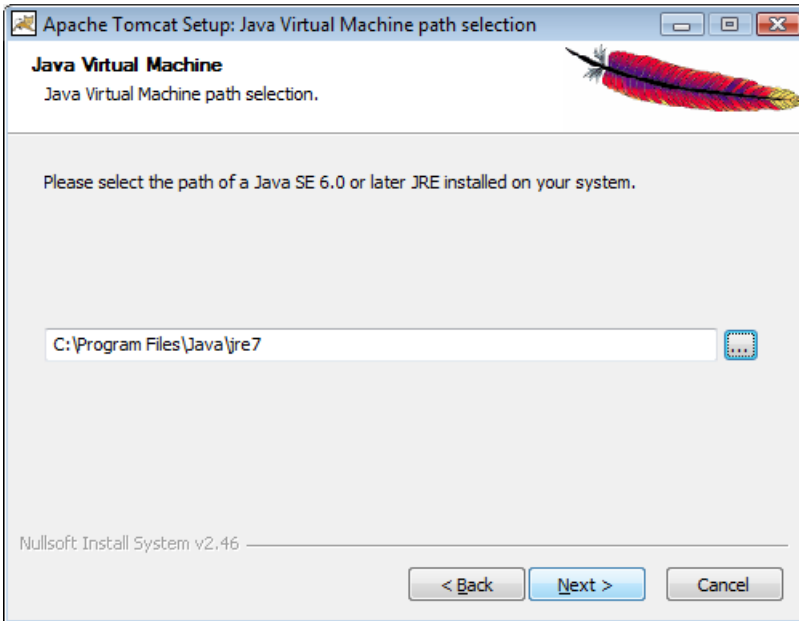
For IUCLID 5, the default values can be used. Hovering the pointer over the option Tomcat, displays a message in the field Description that states installation will be done as a service. Click on the button Next.

Figure 2.24. Configuration



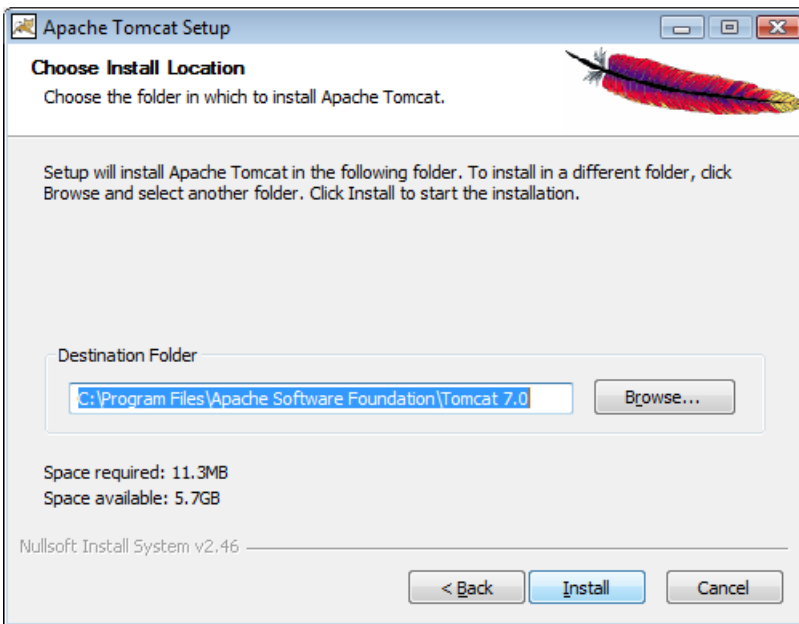
For IUCLID 5, the default values can be used. If you want control IUCLID 5 in the application server using the *Tomcat Manager*, which is recommended, enter values for the user name and password. Be careful to remember the values, because they are needed to access the *Tomcat Manager*. Click on the button Next.

Figure 2.25. Java Virtual Machine



Select the folder of the Java Virtual Machine. This is likely going to be the folder of the most up to date installation of Java, as in the example above. Click on the button Next.

Figure 2.26. Choose Install Location



Choose the installation folder. The default is shown in the screenshot above. To perform the actual installation, click on the button Install.

Figure 2.27. Installing

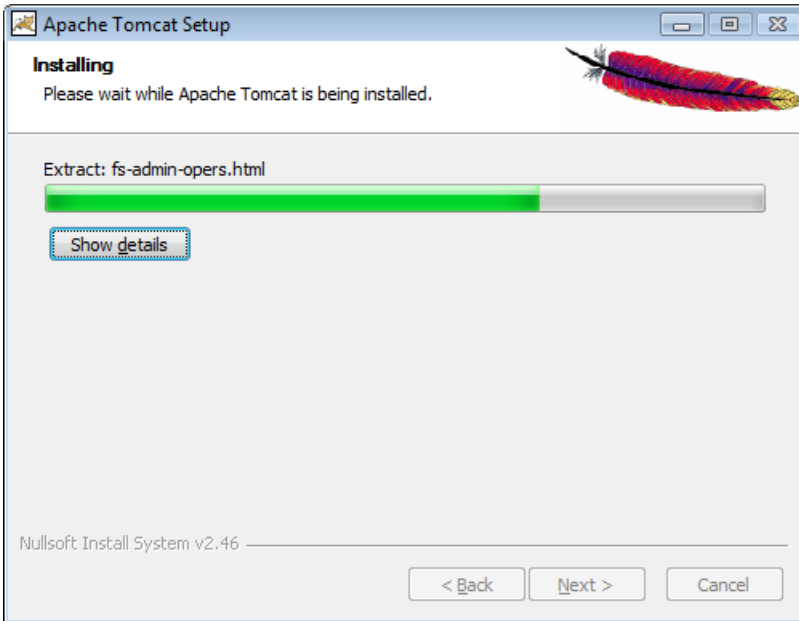
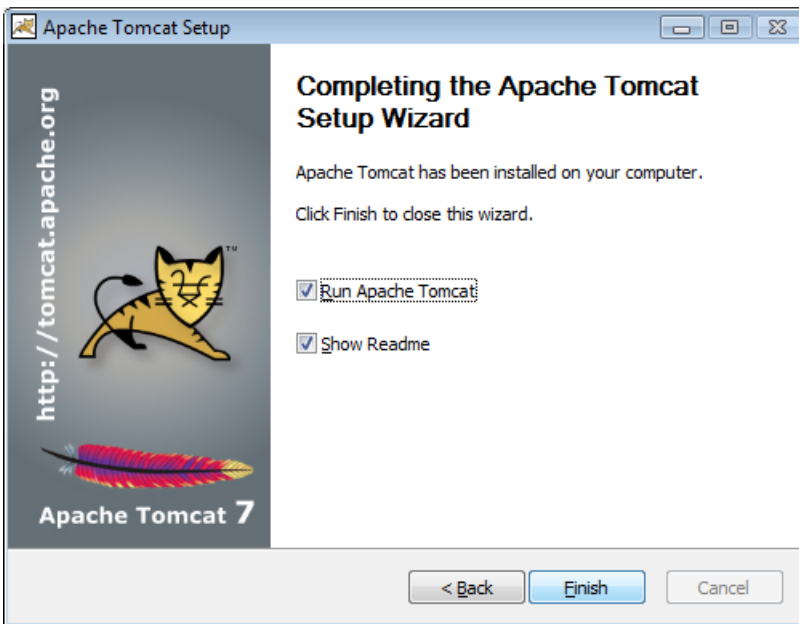


Figure 2.28. Completing the Apache Tomcat Setup Wizard



The next step is to configure Tomcat.


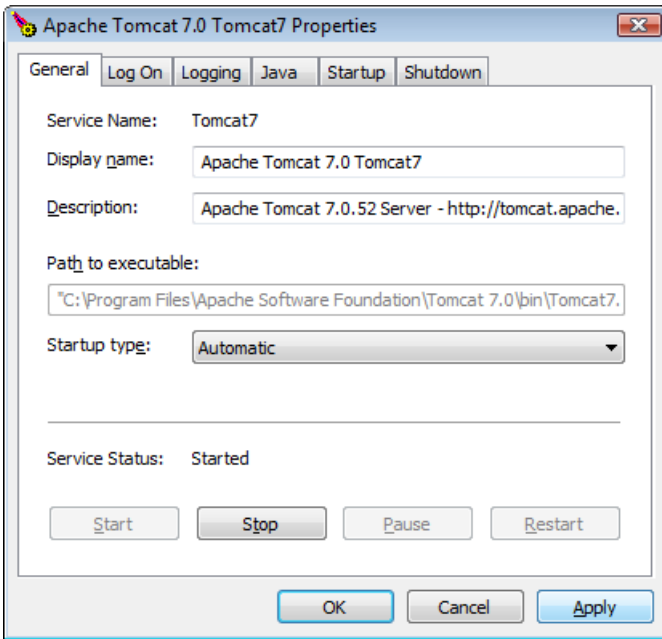
When the installation process has finished, a new icon, , appears in the Windows system tray, located at the bottom-right corner of the screen. This is Tomcat's dedicated service manager. Right-clicking on the icon displays a menu from which the Tomcat service can be started, stopped and configured, as shown in the screenshot below. Be aware that this is not the *Tomcat Manager*: that is described in the next section.

Figure 2.29. Tomcat's dedicated service manager



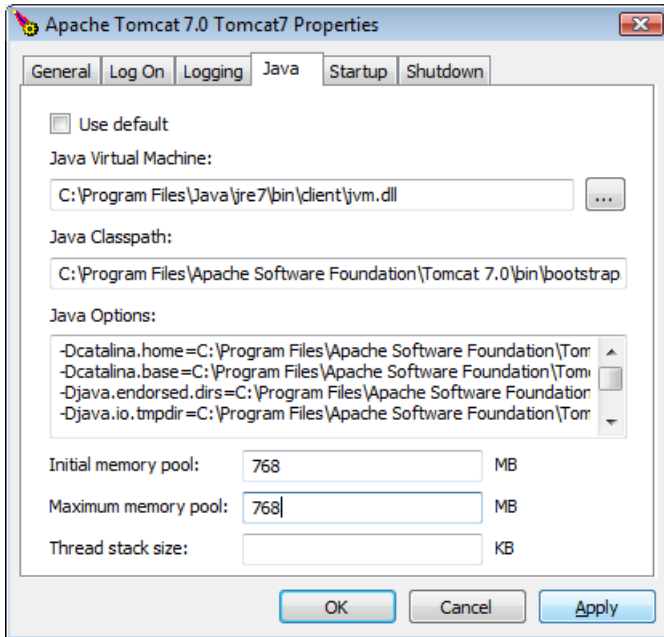
Select Configure.... Under the tab General set the startup type to Automatic.

Figure 2.30. Apache Tomcat properties - General tab



Under the tab Java enter a value of 768 MB for both Initial memory pool and Maximum memory pool, as shown below.

Figure 2.31. Apache Tomcat properties - Java tab



Note



There are two ways of manually starting and stopping the Tomcat service under Windows:

1. The service manager dedicated to Tomcat, as described above.
2. The service manager for all Windows services. This is located in Windows at Start / Computer (right click) / Manage / Computer Management / Services and Applications / Services. Select the service that has a name beginning with *Apache Tomcat*. Options are provided for Stop the Service, Restart the Service and Start the Service.

2.5.1.1. Tomcat Manager

The installation of Tomcat, by default, includes the installation of *Tomcat Manager*. Tomcat Manager is a web application supplied along with Tomcat, that provides a means of dynamically managing the running of applications within Tomcat, without having to shutdown the Tomcat application server itself. It provides a convenient way of managing the IUCLID 5 application in a distributed environment. To gain access to *Tomcat Manager*, point a web browser to the address <http://localhost:8080/manager/html/>. Log in to *Tomcat Manager* as an administrator using the username and password given during the installation of Tomcat. On logging in, the screen shown is a list of the applications currently deployed in Tomcat. Immediately after a fresh default installation of Tomcat, the following screen is shown.

Figure 2.32. IUCLID 5 Tomcat Manager default administrator screen immediately after installation

Tomcat Web Application Manager

Message: OK

Manager

[List Applications](#)
 [HTML Manager Help](#)
 [Manager Help](#)
 [Server Status](#)

Applications

Path	Version	Display Name	Running	Sessions	Commands
/	None specified	Welcome to Tomcat	true	0	Start <input type="button" value="Stop"/> <input type="button" value="Reload"/> <input type="button" value="Undeploy"/> <input type="button" value="Expire sessions"/> with idle ≥ 30 minutes
/docs	None specified	Tomcat Documentation	true	0	Start <input type="button" value="Stop"/> <input type="button" value="Reload"/> <input type="button" value="Undeploy"/> <input type="button" value="Expire sessions"/> with idle ≥ 30 minutes
/manager	None specified	Tomcat Manager Application	true	1	Start <input type="button" value="Stop"/> <input type="button" value="Reload"/> <input type="button" value="Undeploy"/> <input type="button" value="Expire sessions"/> with idle ≥ 30 minutes

Deploy

Deploy directory or WAR file located on server

Context Path (required):

XML Configuration file URL:

WAR or Directory URL:

WAR file to deploy

Select WAR file to upload

Diagnostics

Check to see if a web application has caused a memory leak on stop, reload or undeploy

This diagnostic check will trigger a full garbage collection. Use it with extreme caution on production systems.

Server Information

Tomcat Version	JVM Version	JVM Vendor	OS Name	OS Version	OS Architecture	Hostname	IP Address
Apache Tomcat/7.0.21	1.6.0_22-b04	Sun Microsystems Inc.	Windows Vista	6.0	x86	...	10.1.2.75

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Before attempting to deploy IUCLID 5, check the memory settings for Tomcat. To do that using *Tomcat Manager*, from the page shown above, click on the link *Server Status* and then check the field *JVM*. The value of *Max memory* should be at least 742 MB. Deploying IUCLID 5 in Tomcat is described in the next section.

2.5.2. Deployment in Tomcat

Deployment is the term used for the process of installing an application into an application server.

The application of IUCLID 5 is published in the form of a web archive file (WAR) which is a file with extension war. It is available from the IUCLID website [http://iuclid.eu/], packaged into a file named

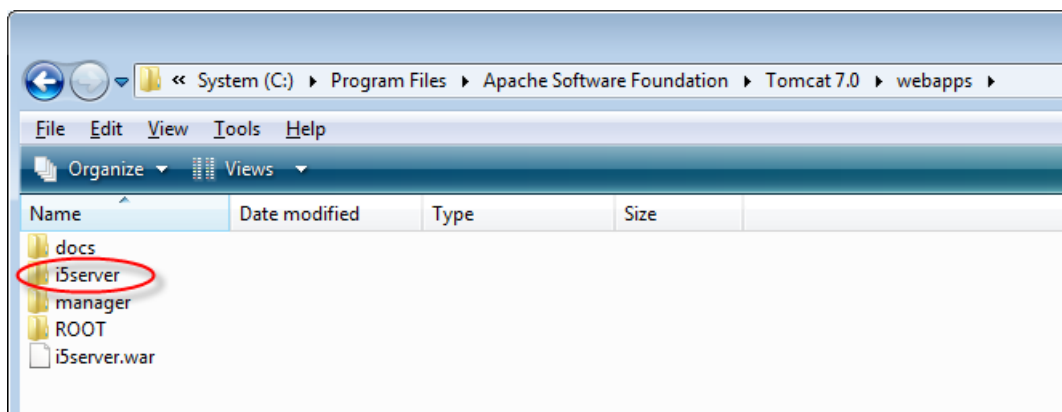
iuc1id5<version>_server_<date>.zip. Download the ZIP file from the web site. Unzip it, and then unzip an archive within it named server.zip. Inside there is a file named i5server.war. That is the file to be deployed.

Deployment of an application into Tomcat can be done in two ways:

- Statically - the application is set up whilst the application server Tomcat is not running.
- Dynamically - one or more applications can be managed whilst the application server Tomcat is still running. This allows IUCLID 5 to be installed on an instance of Tomcat without needing to have a break in service for any other applications that are running on the same instance of Tomcat.

In this installation manual, only the dynamic deployment is described. However, the static deployment may be used instead. The deployment of an application on Tomcat is described in detail on the web page Tomcat deployment [<http://tomcat.apache.org/tomcat-5.5-doc/deployer-howto.html>]. In essence, the deployment of IUCLID 5 consists of copying the archive file i5server.war into a folder within the installation of Tomcat, named webapps. If Tomcat is running whilst the copying is done, it automatically opens the archive and copies the content into the folder webapps. In addition, Tomcat automatically starts the IUCLID 5 application. An example of what the folder webapps looks like in the file browser of Windows, with IUCLID 5 deployed, is shown below:

Figure 2.33. IUCLID 5 deployed in Tomcat - file browser view



When IUCLID 5 is deployed in Tomcat, it is shown in the list of applications in Tomcat Manager, as shown below. If you are unfamiliar with *Tomcat Manager*, see Section 2.5.1.1, "Tomcat Manager".

Figure 2.34. IUCLID 5 deployed in Tomcat - application list in Tomcat Manager

Applications					
Path	Version	Display Name	Running	Sessions	Commands
/	None specified	Welcome to Tomcat	true	0	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes
/docs	None specified	Tomcat Documentation	true	0	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes
/i5server	None specified	IUCLID5 Server	true	1	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes
/manager	None specified	Tomcat Manager Application	true	1	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes

Alternatively, deployment can be done using the deploy feature of the Tomcat Manager to upload a war file into Tomcat from a file system. However, before doing that, the configuration of Tomcat Manager should be checked and possibly adjusted for the following reason.



Warning

By default, Tomcat Manager places an upper limit on the size of the war file that can be uploaded. The default value of the limit is smaller than the size of the file `i5server.war`. If the size limit is exceeded, the following error is given:

The server encountered an internal error () that prevented it from fulfilling this request. Exception `java.lang.IllegalStateException: org.apache.tomcat.util.http.fileupload.FileUploadBase$SizeLimitExceededException: the request was rejected because its size (XXX) exceeds the configured maximum (52428800)`

The solution is to increase the size of the limit, by increasing the values of the parameters `max-file-size` and `max-request-size` in the settings file `/tomcat7/webapps/manager/WEB-INF/web.xml` to values that are larger than the size of the war file. The default values are shown below:

```
<multipart-config>
<!-- 50MB max -->
<max-file-size>52428800</max-file-size>
<max-request-size>52428800</max-request-size>
<file-size-threshold>0</file-size-threshold>
</multipart-config>
```

An example of the new values required is shown below. The value is a 1 followed by 8 zeroes.

```
<max-file-size>100000000</max-file-size>
<max-request-size>100000000</max-request-size>
```

Once you are sure that the file size limit is large enough, in Tomcat Manager, click on the button Browse, that is under the lower of the two options deploy options, WAR file to deploy, as shown below:

Figure 2.35. Deploy IUCLID 5 in Tomcat - upload using Tomcat Manager

Browse to the file `i5server.war`, select it, and then click the button Open. Click on the lower of the buttons labelled Deploy. Check that IUCLID 5 appears within the list of applications.



Warning

IUCLID 5 must be stopped and started for changes to the server settings to take effect, for example, to change the settings for the connection to the database. Even though *Tomcat Manager* can be used to stop and start only the IUCLID 5 application, it is currently recommended that that is done only by stopping and starting the whole Tomcat service in Windows.

2.5.3. Undeployment in Tomcat - uninstall and upgrade

The IUCLID 5 application is undeployed if it is to be uninstalled or upgraded. Tomcat Manager is particularly useful when it comes to upgrading IUCLID 5, because it provides a reliable method of undeploying (removing) the previous version and deploying the new version, even where both archive files have the same name. In addition, this can be done without shutting down Tomcat.

To undeploy the IUCLID 5 web application using Tomcat Manager, in the application listing, click the button stop for IUCLID 5. When the value in the column Running is shown as *false*, click the button Undeploy. The IUCLID 5 web application should disappear from the application listing and its files should be deleted from the folder `webapps`.



Warning

An attempt to undeploy an application can fail if something prevents the deletion of the application files. For example, this can happen if a user with insufficient access rights is using one of the application's files. For example, a user whose account has insufficient rights might have a settings file open. Therefore, before using undeploy in Tomcat Manager, check that no other applications, and no file manager windows are open, that are currently using files or folders of the application to be undeployed.

In an upgrade, once the previous version of IUCLID 5 has been successfully undeployed, the new version can be deployed, as described above.

2.6. Configuring the connection to the database

The configuration of the connection from the IUCLID application to its database is defined in the file `server.properties` that is located in the folder `webapps/i5server/WEB-INF/classes`.

The default values are for an instance of the PostgreSQL database running on the same computer as the application server, i.e. `localhost`. The values for the database name, the database username, and its password, are all set

to the value *iuclid5*. If that configuration is used, on starting the IUCLID 5 application, it will connect to the database without the need to make any changes to the configuration file. If other values are required, they must be entered into the file `server.properties`.



Important

Make sure that there are no spaces after the username and password values in the properties file.

For any change in a configuration file to take effect, the IUCLID 5 application must pass through the start process. This can be done either individually for IUCLID 5 by (re)starting it using the *Tomcat Manager*, or by (re)starting the whole Tomcat service.

The IUCLID 5 server records its activities in log files. The configuration file for the logging is `i5server.logging.properties` which is located in the folder `WEB-INF/classes`. The default location of the logs is in the top level directory of the Tomcat installation. Consult the content of the logs if you encounter any errors that you cannot explain.

If you are following this manual to perform a fresh installation, all the software has now been installed. What remains, is some configuration, as described in Section 2.7, “Configuring the security settings for user accounts” and Section 4.1, “Starting the IUCLID 5 client”.

2.6.1. Database connection settings for PostgreSQL

The default configuration for PostgreSQL is shown below:

```
#
# Settings for using PostgreSQL
#
hibernate.connection.url=jdbc:postgresql://localhost:5432/iuclid5
hibernate.connection.username=iuclid5
hibernate.connection.password=iuclid5
hibernate.connection.driver_class=org.postgresql.Driver
hibernate.dialect=org.hibernate.dialect.PostgreSQLDialect
```

In the example configuration below, the PostgreSQL database server's name is *dbserver*, it is accepting connections on port *12345*, the database name is *chemdb*, the database user name is *joe*, and the database user password is *xxxx*:

```
hibernate.connection.url=jdbc:postgresql://dbserver:12345/chemdb
hibernate.connection.username=joe
hibernate.connection.password=xxxx
```

2.6.2. Database connection settings for Oracle

The default configuration for Oracle is shown below: Un-comment the lines as required.

```
# -----
# Settings for using ORACLE 11g
# -----
#hibernate.connection.username=<username>
#hibernate.connection.password=<password>
#hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver
#hibernate.connection.url=jdbc:oracle:thin:@localhost:1521:<database>
#hibernate.hbm2ddl.auto=validate
#hibernate.dialect=eu.eca.iuclid.server.system.persistence.ExtendedOracle9Dialect
#hibernate.jdbc.use_streams_for_binary=false
```

2.7. Configuring the 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 instance 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 two settings files, `server.properties` and `client.properties`, both of which are located in the folder `webapps/i5server/WEB-INF/classes/`. Changes to values take effect on restarting the IUCLID 5 application on the **server** side. The security features are described below, grouped together by settings file.

2.7.1. User account security settings defined in `client.properties`

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. If a line is commented out, the 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
```

2.7.1.1. 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.

2.7.1.2. 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.

2.7.1.3. 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`.

2.7.2. User account security settings defined in `server.properties`

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. If a line is commented out, the default value is used. A value of zero (0) disables a feature. A suspended account can be un-suspended by a user with user-management rights.

```
# Account expiry in days. A value of zero (0) disables the feature
account.expiry=180
# Password expiry in days. Zero (0) disables the feature.
password.expiry=90
# Max number of attempts before the account is disabled. Zero (0) disables the feature.
max.failed.login.attempts=3
# Max number of attempts to answer the reset question.
max.failed.answer.attempts=3
```

2.7.2.1. Account expiry period

This feature is used to automatically suspend an account that has not been used for a long time. If the period between two successive successful log in attempts exceeds the value, the account is suspended.

2.7.2.2. Password expiry period

This feature is used to prevent users from using the same password for long periods. It defines the life-span of a password. After the password has been in use for the period, the user is prompted to change the password when they next log in. The period is counted from the time of first logging in to the account, then after that, from the time of changing the password.

2.7.2.3. Maximum number of attempts to log in

This feature is used to prevent the combination of user name and password from being obtained by trial and error. The value is the maximum number of successive unsuccessful attempts there can be to log in to an account before it is suspended.

2.7.2.4. Maximum number of attempts to answer the security question

This feature is used to prevent the security question from being answered by trial and error. The value is the maximum number of successive unsuccessful attempts there can be to answer the security question before the account is suspended.

Chapter 3. Upgrade

This document describes the process of obtaining an installation of IUCLID 5.6.0.2 that contains all the data from a previous version. The details of how to proceed depend on the version being upgraded. There is a chapter specific to each scenario. To see the current version of IUCLID 5, log in to the application, then click *Help* and select *About*.



Tip

Bear in mind that as an alternative to the upgrade scenarios described in this chapter, no matter what version of IUCLID 5 is to be upgraded, it is possible to perform a fresh installation of IUCLID 5 using a new database name (PostgreSQL), or database schema (Oracle) , and to then transfer existing data over to it using the built-in backup/restore features of IUCLID 5.

Before starting the upgrade, it is important to backup the database. Use the built-in Backup functionality of IUCLID 5, and/or the backup functionality of the database. Making only a copy of the file system on which IUCLID 5 is installed, is not recommended as a means of backing-up.

3.1. Upgrade from IUCLID 5.6.0 or IUCLID 5.6.0.1 to IUCLID 5.6.0.2

The difference between IUCLID 5.6.0 or IUCLID 5.6.0.1 and IUCLID 5.6.0.2 is that some application files have changed, and must therefore be patched. There is no need to touch the database of 5.6.0 or 5.6.0.1. It will be used, unchanged, with IUCLID 5.6.0.2. A simple and reliable way to apply the patch is to replace the whole web application with the new version, as described in the steps below. The settings files and plug-ins can be copied from the old to the new version of IUCLID 5.

1. Back-up the database. Use the built-in Backup functionality of IUCLID 5, and/or the backup function of the database software, for example PostgreSQL. The built-in Backup feature is accessible by only the user SuperUser, from the menu File / Administrative tools / Backup.
2. Close all clients for IUCLID 5.
3. Use the application Tomcat Manager to **stop** the IUCLID 5 application on the server side, as described in Section 2.5.1.1, "Tomcat Manager".
4. Copy the configuration files, and the folders that contain the plug-ins, into a backup folder. These are indicated below, where `${tomcat_home}` is the home folder of Tomcat.

```
${tomcat_home}\webapps\i5server\WEB-INF\classes\server.properties
```

```
${tomcat_home}\webapps\i5server\WEB-INF\classes\client.properties
```

```
${tomcat_home}\webapps\i5server\WEB-INF\classes\plugins
```

```
${tomcat_home}\webapps\i5server\i5clientPlugins\remotePlugins
```

5. Use the application Tomcat Manager to **undeploy** the old version of the IUCLID 5 web application.
6. Use the application Tomcat Manager to **deploy** the new version of the IUCLID 5 web application.
7. Use the application Tomcat Manager to **stop** the newly deployed IUCLID 5 web application.
8. Copy the configuration files, and the folders that contain the plug-ins, from the backup folder into the location they were in before the upgrade, shown above in step 4.
9. Use the application Tomcat Manager to **start** the IUCLID 5 web application.
10. Run the IUCLID 5 client in the same way as before the upgrade.

11. Log in to the IUCLID 5 client as one of the users that was present before the upgrade.
12. Confirm that the version of IUCLID 5 is the new, expected version. This can be seen from the menu Help / About.
13. Confirm that the data from the previous version is accessible in the new version.

3.2. Upgrade from IUCLID 5.5.x to IUCLID 5.6.0.2



Important

There is no separate **data** migration process in upgrading from IUCLID 5.5.0 or IUCLID 5.5.1 to IUCLID 5.6.0.2. Changes required in the database are applied automatically when the upgraded application is first run. The upgrade therefore consists of copying the new software from the installation package to the destination machine, and then configuring it to connect to either the existing database, or a copy of it. If more than one version of IUCLID 5 and its database are to be maintained and made available on the same machine, run only one at a time, and use appropriate database settings to avoid conflicts. Do not run more than one instance of IUCLID 5 at the same time in the same application server.

There are various different ways to manage a Tomcat application server, as referred to in the section of this manual Deployment of IUCLID 5. The following instructions are intended to give a representative example of how the IUCLID 5 software can be upgraded to IUCLID 5.6.0.2.

1. Back-up the database. Use the built-in Backup functionality of IUCLID 5, and/or the backup function of the database software, for example PostgreSQL. The built-in Backup feature is accessible by only the user SuperUser, from the menu File / Administrative tools / Backup.
2. Close all clients for IUCLID 5.
3. Use the application Tomcat Manager to **stop** the IUCLID 5 application on the server side.
4. Make a note of the plug-ins that are present in the installation. There is no need to keep the old plug-ins, because new versions will be installed. The plug-ins reside in the following folders, where `${tomcat_home}` is the home folder of Tomcat:

client: `${tomcat_home}\webapps\i5server\i5clientPlugins\remotePlugins`

server: `${tomcat_home}\webapps\i5server\WEB-INF\classes\plugins`

5. Copy the configuration files for IUCLID 5, `server.properties` and `client.properties`, into a backup folder.

For example, where `${tomcat_home}` is the home folder of Tomcat:

```
copy ${tomcat_home}\webapps\i5server\WEB-INF\classes\server.properties
```

to

```
e:\backup\server.properties
```

6. Use the application Tomcat Manager to **undeploy** the old version of the IUCLID 5 web application.
7. Use the application Tomcat Manager to **deploy** the new version of the IUCLID 5 web application.
8. Use the application Tomcat Manager to **stop** the newly deployed IUCLID 5 web application.
9. Copy any values that are specific to your system from the previous versions of the files `server.properties` and `client.properties` to those supplied in the new version of IUCLID 5. Ensure that the new values for

the database connection are those for the database of the system to be upgraded. Remember to transfer over any settings that relate to security.

10. Note that if the Oracle database is used, the file server `.properties` must contain the following entry. Add it or edit the existing entry if required.

```
hibernate.connection.driver_class=oracle.jdbc.OracleDriver
```

11. If the database is an Oracle database, please note that the driver for Java is no longer supplied with the IUCLID 5 installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the Oracle web site and installed in the appropriate folder. For example, for Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`.
12. Install any required plug-ins using the latest versions from the IUCLID web site.
13. A separate migration process is **not** required to upgrade to IUCLID 5.6.0.2. Changes required in the database are applied automatically when the application is first run.
14. Use the application Tomcat Manager to **start** the IUCLID 5 web application.
15. Run the IUCLID 5 client in the same way as before the upgrade. The initialisation process is not required. All of the data that was present before the upgrade should be present in the new system. Therefore, it should be possible to log in to any of the user accounts that were present prior to the upgrade.
16. Log in to the IUCLID 5 client as one of the users that was present before the upgrade.
17. Confirm that the version of IUCLID 5 is the new, expected version. This can be seen from the menu Help / About.
18. Confirm that the data from the previous version is accessible in the new version.

3.3. Upgrade and migration of data from IUCLID 5.4.x to IUCLID 5.6.0.2



Important

The migration process changes the IUCLID 5 database such that it can no longer be used with previous versions of the IUCLID 5 application. Therefore, if you would like to be able to continue to use a database with the previous version of IUCLID 5, do not run the migration tool on that particular database. Either perform a fresh installation of the new version of IUCLID 5 and transfer the data across to it using Backup/Restore, or perform the upgrade and migration, on a duplicate of the old database. If more than one version of IUCLID 5 and its database are to be maintained and made available on the same machine, run only one at a time, and use appropriate database settings to avoid conflicts. Do not run more than one instance of IUCLID 5 at the same time in the same application server.

There are various different ways to manage a Tomcat web application server, as referred to in the section of this manual Deployment of IUCLID 5. The following instructions are intended to give a representative example of how the IUCLID 5 software can be upgraded and the data migrated from IUCLID 5.4.x to IUCLID 5.6.

1. Back-up the database. Use the built-in Backup functionality of IUCLID 5, and/or the backup function of the database software, for example PostgreSQL. The built-in Backup feature is accessible by only the user SuperUser, from the menu File / Administrative tools / Backup.
2. Close all clients for IUCLID 5.
3. Use the application Tomcat Manager to **stop** the IUCLID 5 web application.
4. Make a note of the plug-ins that are present in the installation. There is no need to keep the old plug-ins, because new versions will be installed. The plug-ins reside in the following folders, where `${tomcat_home}` is the home folder of Tomcat:

client: `${tomcat_home}\webapps\i5server\i5clientPlugins\remotePlugins`

server: `${tomcat_home}\webapps\i5server\WEB-INF\classes\plugins`

5. Copy the configuration files for IUCLID 5, `server.properties` and `client.properties`, into a backup folder.

For example, where `${tomcat_home}` is the home folder of Tomcat, copy the file;

`${tomcat_home}\webapps\i5server\WEB-INF\classes\server.properties`

in to your own folder such as;

`${tomcat_home}\backup`

6. Use the application Tomcat Manager to **undeploy** the old version of the IUCLID 5 web application.
7. Use the application Tomcat Manager to **deploy** the new version of the IUCLID 5 web application.
8. Stop Tomcat.
9. Copy any values that are specific to your system from the previous versions of the files `server.properties` and `client.properties` to those supplied with the new version of IUCLID 5. Ensure that the new values for the database connection are those for the database of the system to be upgraded. Remember to transfer over any settings that relate to security.
10. Note that if the Oracle database is used, the file `server.properties` must contain the following entry. Add it or edit the existing entry if required.

```
hibernate.connection.driver_class=oracle.jdbc.OracleDriver
```

11. If the database is an Oracle database, please note that the driver for Java is no longer supplied with the IUCLID 5 installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the Oracle web site and installed in the appropriate folder. For example, for Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`.
12. Install any required plug-ins using the latest versions from the IUCLID web site.
13. A migration process is required to upgrade to IUCLID 5.6.0.2. The database and all the data it contains are migrated from the previous to the new version by running IUCLID 5 in update mode, only once. IUCLID 5 is instructed to start in update mode by the line shown below in the file `server.properties`.

```
database.update.startup=true
```

The line is supplied, although commented out, in the file `server.properties` in the installation package for the new version of IUCLID 5. To run in update mode, the line must be either uncommented or added as shown above.

14. To begin the migration, start Tomcat. This automatically starts the new version of the IUCLID 5 web application.

Dependent on the quantity of data in the database, and the system resources available, the migration process can take from minutes to many hours. It is essential that the migration process is not interrupted. The progress of the migration can be monitored from the log files `i5server.log` and `iucldMT.log`. The default location of these files is on the top level directory of the Tomcat installation. The file `i5server.log` contains statements about the start and end of the migration process. The file `iucldMT.log` contains full details. If you need to know what happened during the migration process, check those files first. At the start of the process the following entry is shown:

```
integration.database.scripts.ScriptUtils - Checking Database Status...
(eu/eca/iuclid/server/integration/database/scripts
/migrate_schemav51_to_schemav55.xml)
integration.database.scripts.ScriptUtils - Upgrading table
integration.database.scripts.ScriptUtils -

*****

Database changes are being applied now.
This process might, depending on the size of your database, take some time
(several minutes to perhaps hours). Please do NOT shutdown the system as this
might result in an inconsistent database state.
```

As the migration proceeds, details of which data are being migrated are written to `iuclidMT.log`. The end of a successful migration is indicated by the following entry:

```
integration.database.scripts.ScriptUtils - Database update successfully finished.
integration.database.scripts.ScriptUtils - Checking Database Status...
(eu/eca/iuclid/server/integration/database/scripts/migrate_schemav55_patch.xml)
integration.database.scripts.ScriptUtils - Upgrading table
integration.database.scripts.ScriptUtils - Database is up to date.
```

If the migration is interrupted, or fails, for whatever reason, the database must be restored from the backup and the migration started again.



Note

The entries in the log files shown above state `schemav55` rather than `schemav56` because the migration process is only to IUCLID 5.5. There is no **data** migration process in upgrading from IUCLID 5.5.x to IUCLID 5.6.0.2. Changes required in the database to convert from IUCLID 5.5.x to IUCLID 5.6.0.2 are applied automatically when IUCLID 5.6.0.2 is first run.

15. When the migration finishes successfully, stop the new version of the IUCLID 5 web application by stopping Tomcat.
16. Set IUCLID 5 to start *not* in its update mode by commenting out the line edited previously:

```
#database.update.startup=true
```

17. Start Tomcat.
18. Run the IUCLID 5 client in the same way as before the upgrade. The initialisation process is not required. All of the data that was present before the upgrade should be present in the new system. Therefore, it should be possible to log in to any of the user accounts that were present prior to the upgrade.
19. Log in to the IUCLID 5 client as one of the users that was present before the upgrade.
20. Confirm that the version of IUCLID 5 is the new, expected version. This can be seen from the menu Help / About.
21. Confirm that the data from the previous version has been successfully migrated to the new version.

3.4. Upgrading from IUCLID 5.2.x/5.3.x to IUCLID 5.6.0.2

To upgrade from IUCLID versions 5.2.x or 5.3.x, unless the database contains a very large amount of data, it is recommended to use the Backup and Restore features of IUCLID 5 to transfer the data from the old installation to

a fresh installation of IUCLID 5.6.0.2. The Backup and Restore features are described in the IUCLID 5 End-user Manual. Making a fresh installation is described in this manual.



Warning

The built-in Backup functionality of IUCLID 5.3.1 is known to output files in which the user accounts cannot be used on restore. If you wish to use the built-in Backup functionality on data in an installation of IUCLID 5.3.1, first upgrade it to IUCLID 5.3.2. The built-in Backup functionality in IUCLID 5.3.2 does not suffer from this problem.

As an alternative to using Backup and Restore into a fresh installation, it is possible to perform step-wise upgrades in which the database is migrated from IUCLID 5.2.x/5.3.x to 5.4.x to 5.6.0.2. For example, this method might be required if the amount of data is so large that it makes use of the Backup feature impractical. If you choose the migration method, obtain the installation packages to perform the required upgrades, and then proceed as per the instructions included therein.

Note that the plug-ins for IUCLID 5.2.x/5.3.x are not compatible with IUCLID 5.6. Therefore, they must not be copied over to the new installation. Compatible versions can be downloaded from the IUCLID web site.

3.5. Upgrading from IUCLID 5.0/5.1.x to IUCLID 5.6.0.2

To upgrade from 5.0/5.1.x, no migration process is available, and so the method of using Backup then Restore into a fresh installation must be used. In IUCLID 5.0/5.1.x there is no built-in Backup function. Instead, the functionality is provided by a plug-in, *Backup Plug-in 5.0.3* that is available on the IUCLID web site under downloads for IUCLID 5.1.1.

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 the IUCLID 5 client

Connect to the application with a browser by entering the address *http://<address of your server>:8080/i5server*. An example of the page displayed is shown below.

Figure 4.1. Example default page for Java Web Start of IUCLID 5



The page shown above page contains links that use Java Web Start technology to start a Java client that connects to the IUCLID 5 server and displays IUCLID 5's graphical user interface (GUI) on the client machine. In the example shown above, the link under the text *(with 1GB RAM)* is being hovered over. Following a link downloads a file named `i5client.jnlp` that the browser should open using Java(TM) Web Start Launcher. The difference between the

links is in the values of parameters passed to the IUCLID 5 server. The options included are for varying amounts of memory to be allocated to the IUCLID 5 Java client, and for different types of data compression to be employed in the connection to the application server. If IUCLID 5 runs slower than you would like, and you have the available memory, select a link for a larger amount of RAM. The client can be run directly from a browser, or by first downloading a file `i5c1ient.jar` from one of the links, and then running that. Depending on your browser settings, when you click on one of the links above you will see either a dialogue box, or IUCLID 5 will run and you will see the login page. The browser dialogue asks whether you would like to save a file or run it straight away. The choice is yours. A convenient way to access the IUCLID 5 server without using a browser, is to download one of the files from the default page, save it to the desktop of your local machine used to access IUCLID 5, and then change its icon to the one that comes with the IUCLID 5 installation. Double clicking on the icon then launches the IUCLID 5 GUI. Once you see the login page, you are ready to go through the *First steps* wizard, as described in the next section.

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.

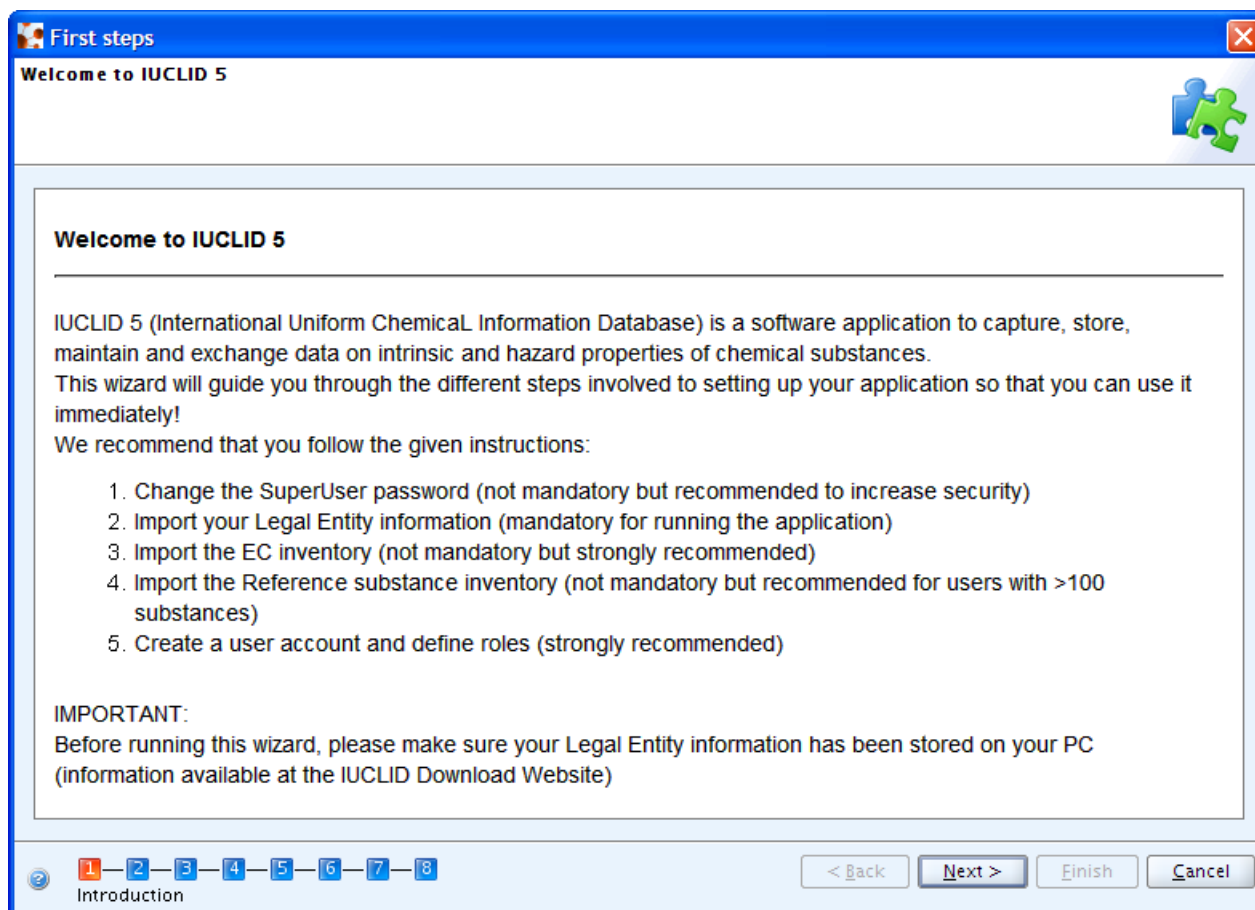


Figure 4.3. Step 2 of the First steps wizard - Init mode - New installation

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

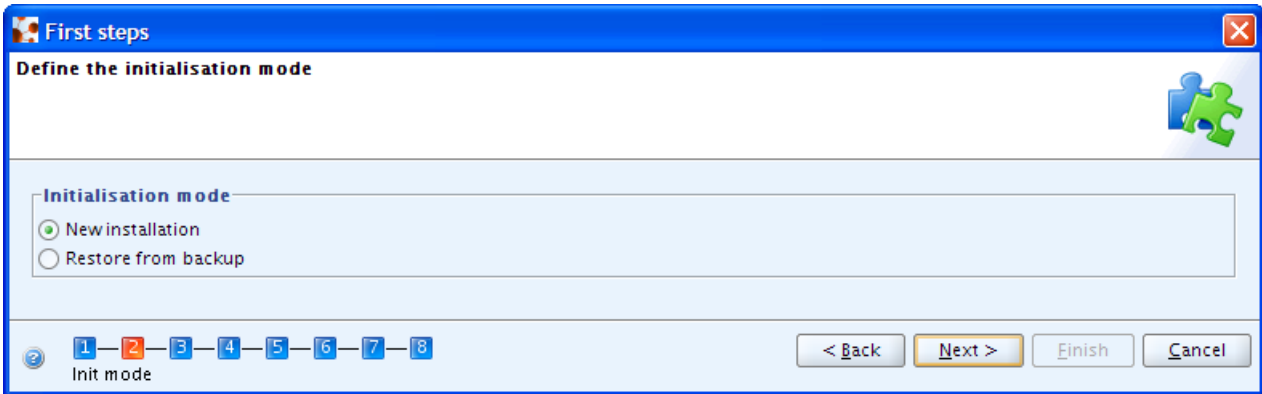
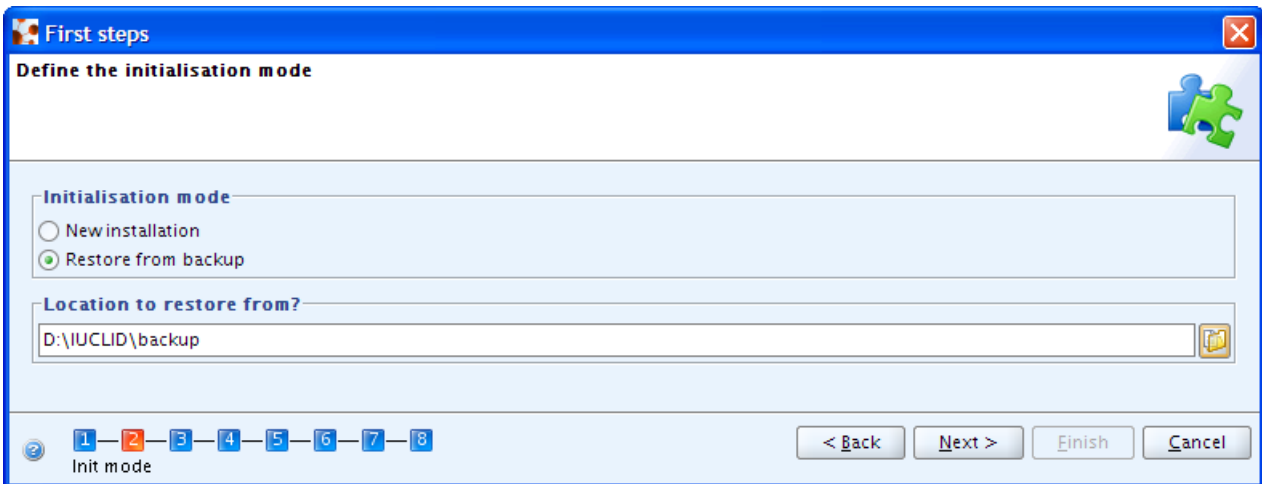


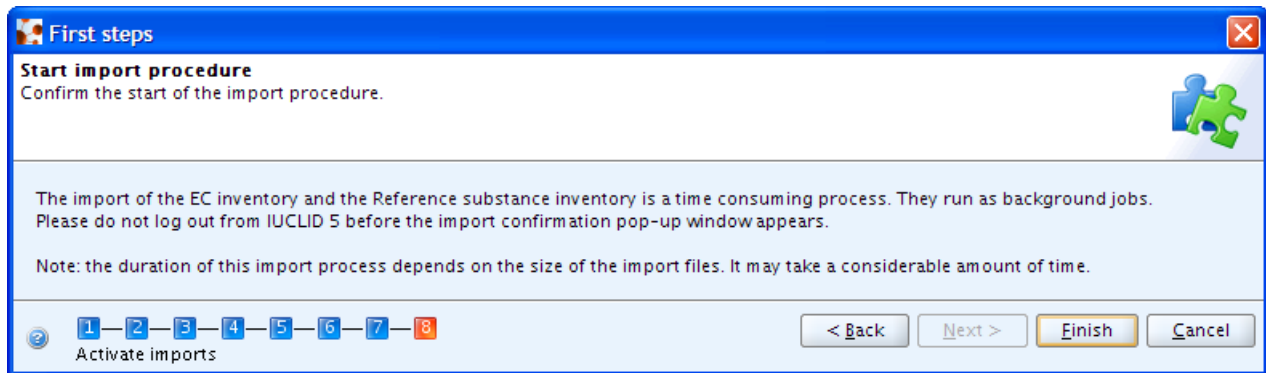
Figure 4.4. Step 2 of the First steps wizard - Init mode - Restore from backup

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 backup - Step 8 - Activate imports



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

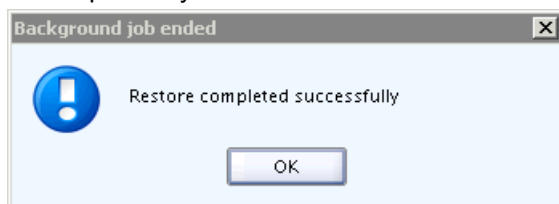
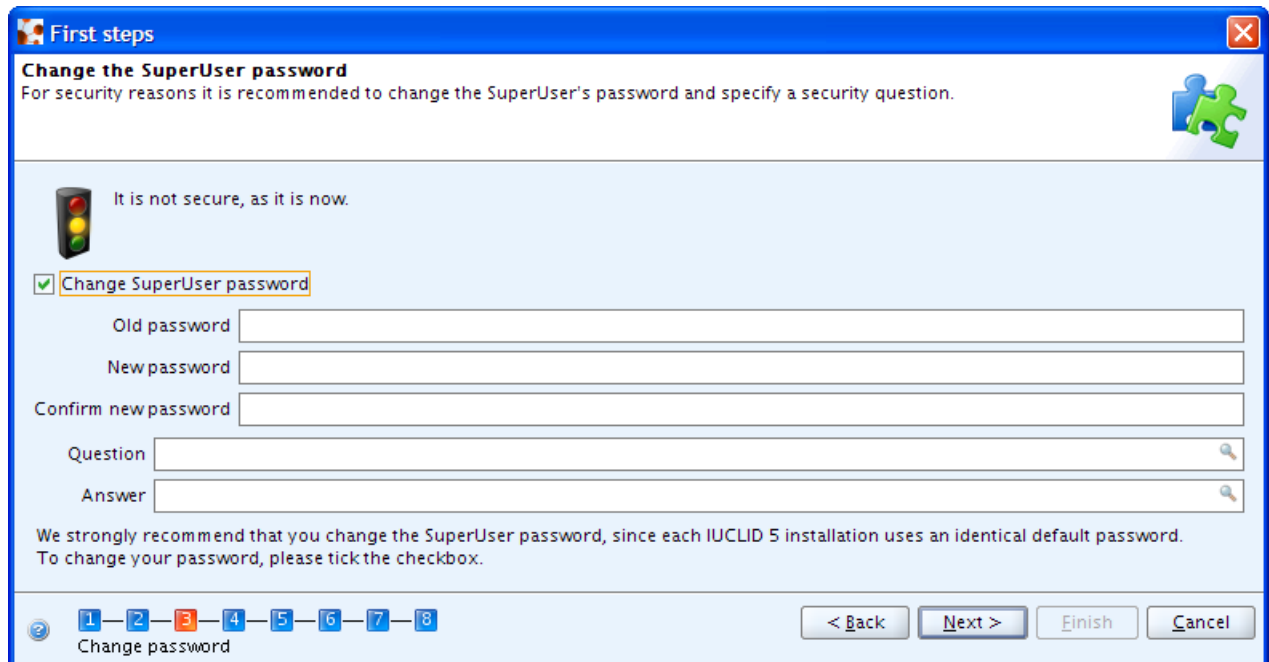


Figure 4.6. Step 3 of the First steps wizard - Change password

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.

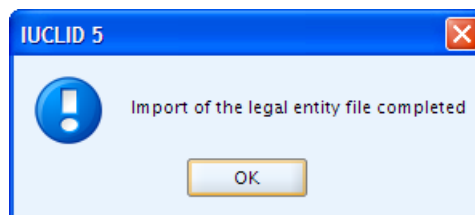
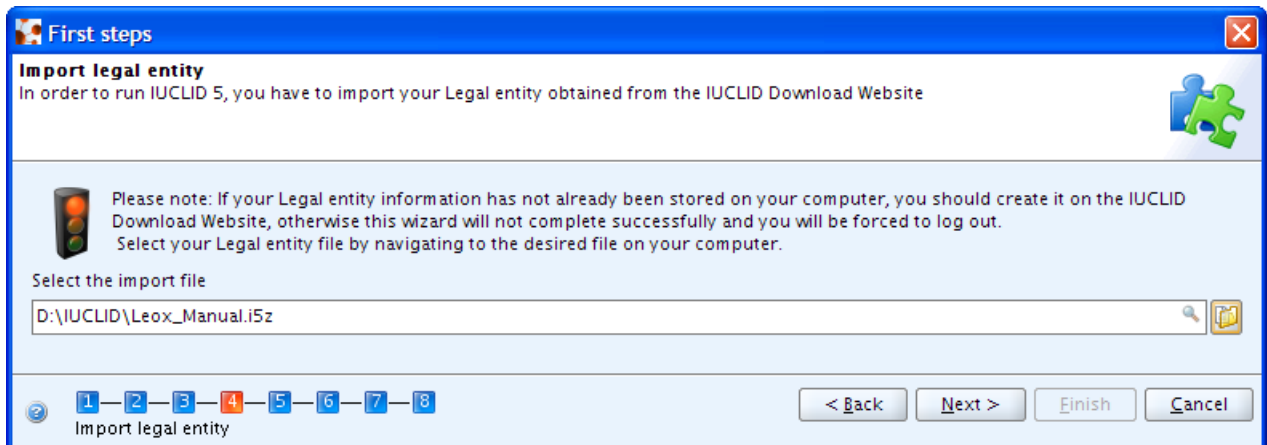


Tip

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

At least one Legal entity must be imported successfully before this wizard can be completed. If there is 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.

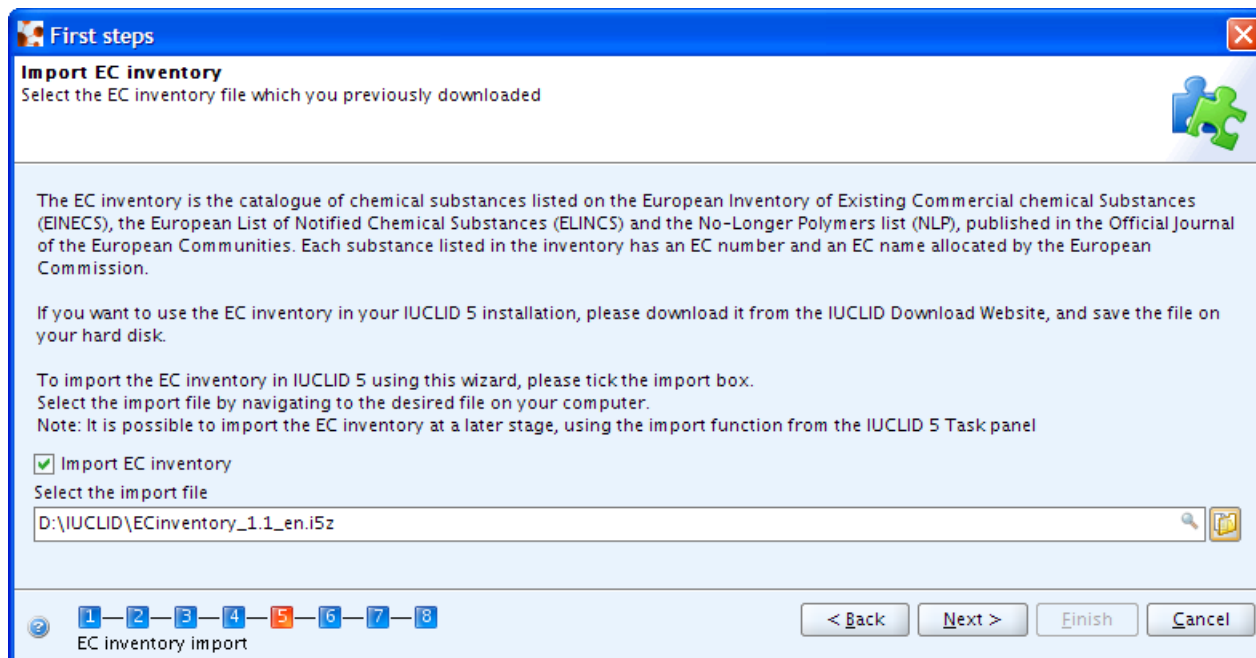
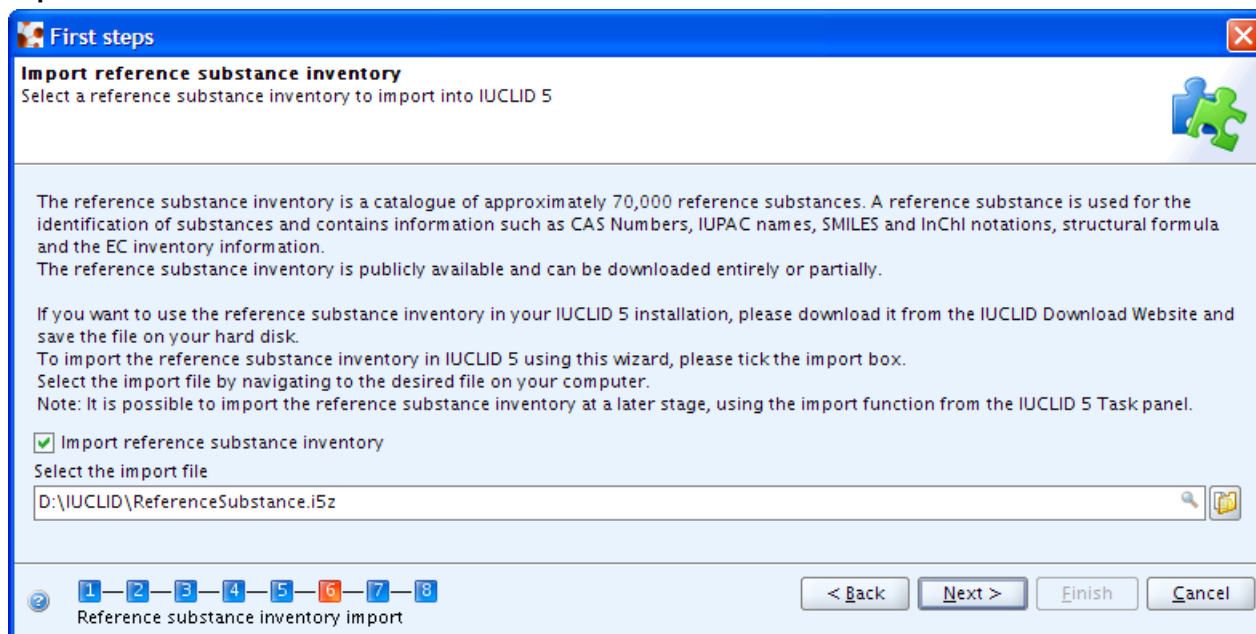


Figure 4.9. Step 6 of the First steps wizard - Import reference substance inventory

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.



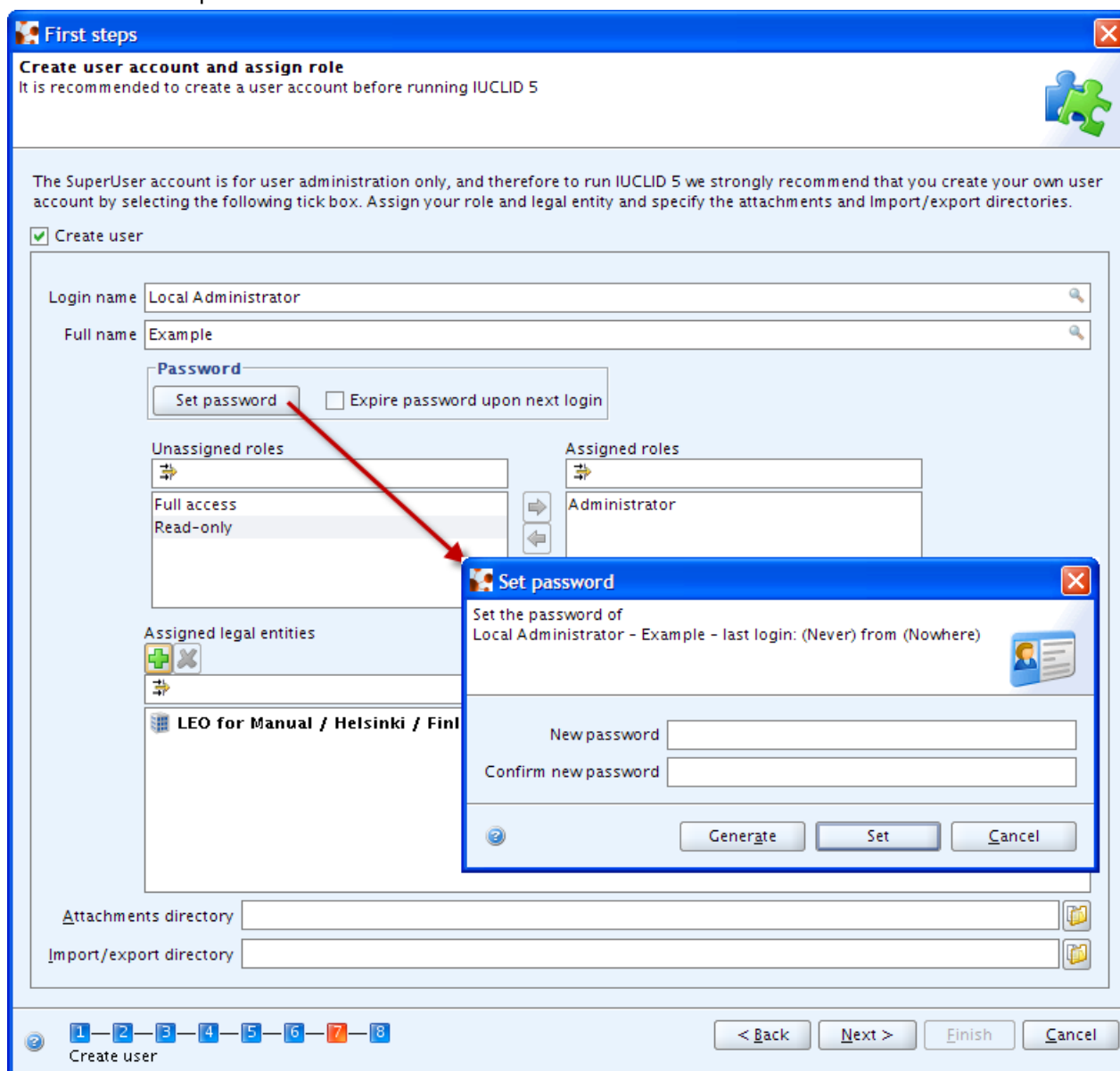


Tip

Time and IT resources can be saved by importing into IUCLID 5 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

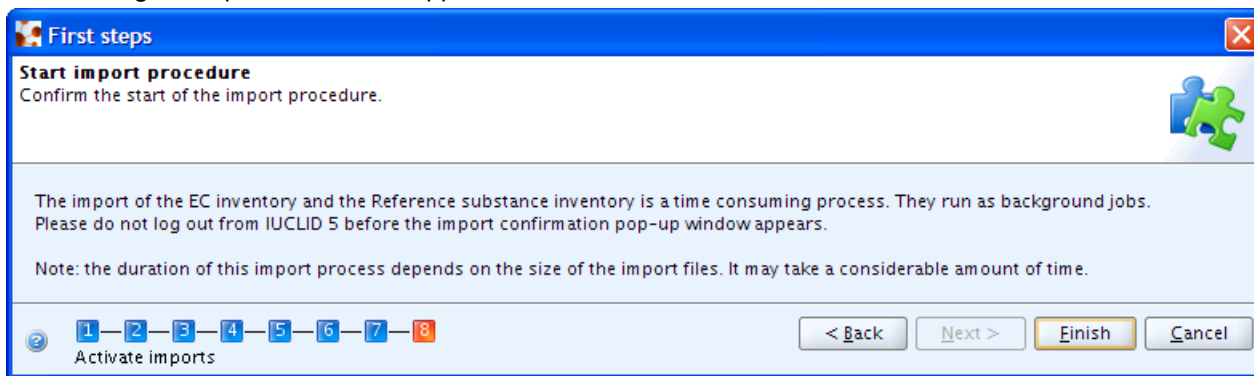
It is recommended to create a user with the *Administrator* Role regardless of whether a stand alone or a distributed version of IUCLID 5 is set up. Once a user has been created, the IUCLID 5 administrator (in case of a distributed version) can define different other user(s) and assign different role(s) 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 document **IUCLID 5 End-user Manual**. Individual users can connect to the IUCLID 5 server using Java Web Start technology, as described in section 3.1 of this document. A convenient way to achieve that is for users to save onto their desktop, one of the files downloaded from the default Java Web Start page. The user would launch IUCLID 5 by simply double-clicking on the icon on his or her desktop. Alternatively, the users could be supplied with the URL *http://<address of your server>:8080/i5server*, and instructions on which link to use.

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>.