

# IUCLID 5

## Guidance and support

### Installation Guide

### Distributed Version

Linux - Apache Tomcat - PostgreSQL



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It can be accessed at the addresses:

<http://iuclid.echa.europa.eu>.

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# Introduction

IUCLID 5 has two different installation architectures:

- Standalone installation

The IUCLID 5 application connects directly to the database which usually resides on the same computer. Using this installation not more than one user can work simultaneously on the same database.

- Distributed installation

In this architecture the database and the application server resides on a server computer and the user works with another computer called client. It is similar to a web based application with the only difference that the user interface of the application (buttons, text boxes etc.) is not a series of web pages but a specific Java application called "IUCLID 5 client" downloaded automatically from the server.

This document describes how to download, install and configure the necessary open source software products and the IUCLID 5 application itself on a Linux server. Only the distributed installation is described.

The aim of this document is that a user with basic computer skills would be able to install and run IUCLID 5. The following is a list of items NOT covered in this document:

- Complete and detailed installation and configuration procedure of the operating system (GNU/Linux).
- A detailed configuration of the Database Management System (PostgreSQL) and the Application Server (Tomcat)

## 1. Conventions of this document

All the commands required to install IUCLID 5 have to be entered into the shell console which is a text mode screen. The graphical user interface is not required. In this mode the system writes on the screen a short text called prompt when the previous command is finished and the system is ready to execute another command. The prompt is different on each computer. It might provide information about the computer's name, the currently logged in user, the current directory etc. This document uses the current directory name followed by the "#" sign to represent the prompt. The "~" sign means the home directory (/root).

```
~#
```

The commands you have to enter is printed with bold characters. You must copy the commands *exactly* as written, upper and lowercase does matter. At the end press the enter key.

```
~#command
output
~#
```

In many cases the commands do not have any output but some commands write also the output on the screen, for example the **ls** command lists the content of a directory.

If an error message appears, read it carefully and try to correct the problem. For example if the **cp** (copy) command cannot find the required file, it reports the error.

```
~#cp iuclid5 root
cp: cannot stat 'iuclid5': No such file or directory
~#
```

## 2. Prerequisites

### 2.1. Hardware requirements

The server hosting IUCLID 5 must have at least:

- RAM: 1 GB (recommended 2 GB)
- Hard disk space: 200 GB
- CPU: 2 GHz, 32 or 64 bit architecture
- Network adapter 100 Mbps (recommended 1Gbps)

### 2.2. Software requirements

- Java Runtime Environment (JRE) or Java Software Development Kit (SDK) 6
- PostgreSQL 8.2 or 8.3
- Tomcat 5.5 or 6.0

# Chapter 1. Installation



## Note

If you have already installed a previous version of IUCLID you have to follow the upgrade procedure described in the chapter Upgrade.

## 1.1. Operating system

IUCLID 5 has been tested thoroughly using the CentOS Linux distribution. CentOS is an Enterprise-class Linux Distribution derived from sources freely provided to the public by a Linux vendor. You can download it from <http://www.centos.org>. It is sufficient to download the `server-cd` because IUCLID 5 server requires only the minimal operating system installation without any optional software.

Other distributions may be used as well. In that case the file locations might be different from the ones used in this document.

It is recommended to select the minimum configuration when the installation program asks to select the software components to be installed. You may want to install the applications you need, but keep in mind that it is not a good practice to install not necessary software on the server.

### 1.1.1. Opening the network port for IUCLID 5 server

In order to establish the connection from the workstation computer to the server, the server's firewall must be configured to allow the IUCLID 5 server to accept connections on port 8080.

It is not recommended to completely disable the firewall. In CentOS for example the `system-config-securitylevel-tui` tool allows you to easily modify the firewall settings. On other Linux distributions please refer to the documentation of the operating system.

```
~#system-config-securitylevel-tui
```

Be cautious! You should not trust any network interface. In the "Allow incoming" section set SSH (secure shell) and 8080 port. For security reasons do not allow any other traffic like telnet, http or ftp.

Before you start the installation procedure you have to download the required components for IUCLID 5. In order to select the correct files, you should know the architecture (platform) of your server computer. Please consult the user manual of your computer. If the Linux operating system is already installed, write the following command. The command will write the platform's name on the screen, for example `i386`.

```
~#uname -i
i386
~#
```

## 1.2. JAVA Development Kit

The simplest way to install Java is using the package manager of your operating system. In this way you do not need to download Java manually.

In case no appropriate Java runtime environment is available in the package manager, download the JAVA Development Kit (JDK) 6 or JAVA Runtime Environment (JRE) 6 according to the operating system distribution and architecture of your computer from <http://java.sun.com/javase/downloads/index.jsp>. Select the latest available update.

For example for a 32 bit computer download the i586 version.

```
jdk-6u11-linux-i586.bin
```

If you have a computer with 64 bit processor(s) and the 64 bit version of Linux installed on it then download the 64 bit Java SDK or JRE.

```
jre-6u11-linux-x64.bin
```

If you selected Java in the package manager, it should be installed already. Otherwise run the installer.

Make the JDK file executable and start it.

```
iuclid5#chmod +x jdk-6u11-linux-i586.bin  
iuclid5#./jdk-6u11-linux-i586.bin
```

The Sun binary code License Agreement prompt is displayed. Press the enter button to scroll down to the end. You are asked to accept the license. Answer "yes".

```
Do you agree to the above license terms? [yes or no]  
yes
```

Status messages are displayed as the installation proceeds. Warning messages can be ignored. After the installation check the Java environment by displaying the version.

```
iuclid5#java -version  
java version "1.6.0"  
Java(TM) SE Runtime Environment (build 1.6.0-b105)  
Java HotSpot(TM) Server VM (build 1.6.0-b105, mixed mode)
```

For more information please consult the Java SE 6 Platform installation instructions at <http://java.sun.com/javase/6/webnotes/install/index.html>.

## 1.3. PostgreSQL

PostgreSQL is the database management system (DBMS) used by IUCLID 5 to store all data.

Most likely PostgreSQL 8.2 or 8.3 is included in your distribution. It is recommended to install the distribution specific packages.

You can find the installation packages on <http://www.postgresql.org>. The required version is 8.2.x or 8.3.x where x is the highest available number.

You do not need to download all the installation packages. Only the files with the name starting with `postgresql-libs`, `postgresql-server` and `postgresql` are required.

### 1.3.1. Creating the iuclid5 database user

A new Linux user "postgres" has been created during installation process. "postgres" user has no password so you can not log in using this user name. Its purpose is performing database administrative tasks. To act as postgres user you have to use the "su" command.

Change the current directory and current user.

```
$cd /  
$su postgres  
$
```



## Note

By changing the user, the prompt is also changed to the \$ sign (and usually "bash-3.00\$" is displayed).

Now each command you type is executed as postgres user. The first thing to do is to create a database user that allows IUCLID 5 application to connect to the database. Type a password, confirm the password and answer "n" to all subsequent questions. (Press enter after each answer).



## Note

Remember the password you give to iuclid5 user, it will be needed later.

```
$createuser -EP iuclid5  
Enter password for new role:  
Enter it again:  
Shall the new role be a superuser? (y/n) n  
Shall the new role be allowed to create databases? (y/n) n  
Shall the new role be allowed to create more new roles? (y/n) n  
CREATE ROLE  
$
```

## 1.3.2. Creating the iuclid5 database

Create a new database specifying the owner, encoding and the name of the database.

```
$createdb --owner=iuclid5 --encoding=UTF-8 iuclid5  
CREATE DATABASE  
$
```

Once the database preparation tasks are, change back to the root user.

```
$exit  
/#
```

For security reasons by default database users are not enabled to connect to the database even if they provide the correct password. It is necessary to configure PostgreSQL in order to enable IUCLID 5 to connect.

Open the configuration file using a text editor for example **nano**.

```
iuclid5#nano /var/lib/pgsql/data/pg_hba.conf  
# PostgreSQL Client Authentication Configuration File  
# =====  
#
```

Move the cursor to the end of the file using the down arrow button until the line "# IPv4 local connections:".

```
# IPv4 local connections:
host      all             all             127.0.0.1/32      ident sameuser
```

Insert a new line just after the "IPv4 local connections" and type "host iuclid5 iuclid5 127.0.0.1/32 md5". This line tells PostgreSQL that iuclid5 user is allowed to connect to iuclid5 database from the local computer using the encrypted password authentication.

```
# IPv4 local connections:
host      iuclid5      iuclid5      127.0.0.1/32      md5
host      all             all             127.0.0.1/32      ident sameuser
```

Press CONTROL-X to exit from the editor, type "y" to save the file and confirm the file name by pressing the enter key.

```
Save modified buffer (ANSWERING "No" WILL DESTROY CHANGES) ? y
Y Yes
N No          ^C Cancel
```

```
File Name to Write: /var/lib/pgsql/data/pg_hba.conf
^G Get Help          M-D DOS Format      M-A Append          M-B Backup File
^T To Files          M-O Mac Format      M-P Prepend         ^C Cancel
```

Restart PostgreSQL to load the new configuration.

Your iuclid5 database is now ready to serve the IUCLID 5 application.

For more information about installing PostgreSQL and administer the server look for the <http://www.postgresql.org/docs/documentation> page.

## 1.3.3. Set up daily backup of the database

The data you store into IUCLID 5 might be very important for your organisation. A user may accidentally delete valuable data or a system failure could cause loss of data. To prevent this situation and prepare a smooth recovery, it is vital to schedule a daily backup.

## 1.4. Tomcat

The preferred way to install Tomcat is by using the package manager of your operating system. The required version is 5.5.x or 6.0.x where x is the highest available number.

### 1.4.1. Manual installation

Distribution independent packages can be downloaded from the Tomcat website [<http://tomcat.apache.org/>].

The file to download is for example:

```
apache-tomcat-5.5.26.tar.gz
```

The installation of Tomcat is extracting a set of files and setting up the starting parameters. Extract the downloaded archive into the directory /opt (use the version number of your downloaded Tomcat).

```
iuclid5#tar -xzf apache-tomcat-5.5.26.tar.gz -C /opt
iuclid5#
```

It is convenient to create a version independent symbolic link pointing to the actual tomcat directory. It will be used to find the location of Tomcat, whichever version is installed.

```
iuclid5#ln -s apache-tomcat-5.5.26 /opt/apache-tomcat"
iuclid5#
```



## Tip

Tomcat contains some example applications which are not needed. You can delete them in order to save resources. Do not delete the ROOT directory!

For more information visit the Tomcat website [<http://tomcat.apache.org/>].

## 1.4.2. Memory settings



## Important

IUCLID 5 requires at least 512 MB RAM to be allocated to Tomcat.

Check the amount of memory allocated on the server status page of the Tomcat manager application. The "Max Memory" parameter under JVM should show a value of at least 512 MB.

## 1.5. Deploying IUCLID 5

Before downloading IUCLID 5 you need to register as a IUCLID user on the IUCLID website [<http://iuclid.eu/>]. The application itself is packaged into the `iuclid5_server_yyyy-mm-dd.zip` file.

### 1.5.1. Deployment in Tomcat

Deployment is the term used for the process of installing a web application into the Tomcat server.

Web application deployment may be accomplished in two ways.

- Statically - the web application is set up before Tomcat is started
- Dynamically - in conjunction with the Tomcat Manager web application or manipulating already deployed web applications

You can find more information on how to deploy in tomcat a web application on the Tomcat deployment [<http://tomcat.apache.org/tomcat-5.5-doc/deployer-howto.html>] web page.

In this document only the Static deployment is described. However the dynamic deployment may be used as well.

Tomcat has to be stopped using the command specific to your distribution.

```
~#service tomcat stop
```

The deployment of IUCLID 5 actually consists of extracting the `i5server.war` archive into the `webapps` directory of Tomcat.

```
iuclid5#unzip i5server.war -d /opt/apache-tomcat/webapps/i5server
Archive:  i5server.war
...
  inflating: /opt/apache-tomcat/webapps/i5server/WEB-INF/web.xml
iuclid5#
```

Open the `server.properties` file in the `webapps/i5server/WEB-INF/classes` directory.

The `server.properties` file is the configuration of IUCLID 5 server. In order to connect to the database correctly it is necessary to modify the `server.properties` configuration file. The default configuration file contains settings for connect to a PostgreSQL database on the same computer. Usually it is sufficient to specify the database password.

```
#
# 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
```

If your database server is running on another computer or database name, user name are different, modify the settings accordingly. For example your database server's name is `dbserver`, PostgreSQL is accepting connections on port `12345`, the database name is `chemdb` and the user is `joe` with password `xyz`, then your configuration is:

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

The IUCLID 5 server registers activities into a log file which helps the system administrator. The configuration file setting the logging is `i5server.logging.properties` in the `WEB-INF/classes` directory.

Start the Tomcat service using the command specific to your distribution.



## Note

When IUCLID 5 is started the first time it creates new tables in the database which might take up to 30 seconds.

```
iuclid5#service tomcat start
Starting Tomcat - IUCLID5 server [ OK ]
iuclid5#
```

The installation is completed. You can connect to the application with your browser by typing the address `http://your_server:8080/i5server []`.

## Chapter 2. Upgrade

Upgrading IUCLID 5 to version 5.1.1 from a previous version consists of replacing the application's program files while keeping the current configuration and database.

1. Close all IUCLID 5 client applications.

2. Shut down Tomcat

3. Copy the following configuration files to a backup directory

```
<Tomcat>/webapps/i5server/WEB-INF/classes/server.properties
```

```
<Tomcat>/webapps/i5server/WEB-INF/classes/i5server.logging.properties (if exists)
```

4. Delete `i5server` from `<Tomcat>/webapps`. (or undeploy the application using the manager)

5. Deploy the new version of IUCLID 5 (as described in the section "Deployment in Tomcat")

6. Replace the previously saved configuration files into the `<Tomcat>/webapps/i5server/WEB-INF/classes` directory.

7. Start Tomcat

