Chemselect Manual for administrators

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1. Installation

The Debian package `chemselect_<version>-1_amd64.deb` is provided by the Federal Environment Agency (UBA) at the address https://repo.chemselect.uba.de.

The software package requires a computer based on AMD64 or EM64T architecture with the Ubuntu Server 22.04. All software packages required by CHEMSELECT are automatically loaded and installed during the installation of CHEMSELECT, if this has not already been done.

The initial installation requires 3 steps

Step 1: Load the UBA signature

```
wget-O-https://repo.chemselect.uba.de/UBA-Repo-Chemselect.gpg    |
gpg --dearmor | sudo tee /etc/apt/keyrings/UBA-RepoChemselect.gpg
> /dev/null
```

The public key of the UBA is retrieved, translated into a binary format and stored appropriately.

Step 2: Extend the list of data sources

```
echo     "deb     [signed-by=/etc/apt/keyrings/UBA-Repo-Chemselect.gpg]
http://repo.chemselect.uba.de/ubuntu jammy contrib" |   sudo tee
/etc/ apt/sources.list.d/chemselect.list
```

Step 3: Update the list of available packages and install CHEMSELECT

```
sudo apt update && apt install chemselect
```

Future updates of CHEMSELECT will be loaded and installed automatically by repeating step 3.

The CHEMSELECT package requires some other services and ensures their automatic installation if necessary. These are:

- apache2 (web server)
- mariadb-server (database)
- postfix (mail server)

The configuration of these services is not carried out completely automatically, but is the responsibility of the server administrator.

2. Configuration

Two parameters are requested during the initial installation:

- The privileged user.

  CHEMSELECT recognizes a privileged user who is identified by his e-mail address.

- The host name.

  CHEMSELECT attempts to determine its own host name automatically. If this is not possible, e.g. for virtual hosts, the hostname must be entered in the format `hostname:port` hostname and - if the default is not used - the port must be specified.

You can change these parameters with the command

```
sudo dpkg-reconfigure chemselect
```

Web server certificate

After successful installation, the application can be accessed with a web browser at the address `https://example.intern`. The configuration for this can be found in the file:

`/etc/apache2/sites-available/011-chemselect.conf`

```
 1 ###
 2 # a2enmod proxy, proxy_http, headers, ssl
 3 ### drop this in /etc/apache2/sites-available
 4 # enable with a2ensite
 5
...
 9
10 VirtualHost *:443>
11     ServerAdmin ${webmaster}
12     ServerName ${servername}
13     SSLEngine on
14     SSLProxyEngine On
15     SSLProxyCheckPeerName off
16     SSLCertificateFile      /etc/ssl/certs/ssl-cert-snakeoil.pem
17     SSLCertificateKeyFile /etc/ssl/private/ssl-cert-snakeoil.key
18     ProxyPass / https://127.0.0.1:${serverport}/
19     ProxyPassReverse / https://127.0.0.1:${serverport}/
...
24 </VirtualHost>
```

Lines 16 and 17 point to a self-issued certificate that is either not accepted by the web or is classified as insecure. This certificate must be replaced by your own certificate.

You must activate all changes with the command

```
sudo systemctl restart apache2
```

Data protection and imprint

You can create your own privacy policy and legal notice instead of the pre-installed declarations.

To do this, create a file in the /etc/chemselect/local directory with the name Privacy.html or Imprint.html. You can find samples of these files in the file /usr/share/chemselect.

Database

CHEMSELECT assumes that the *Mariadb* database is operated in its standard mode, i.e. that the database can be accessed by the root user without a password.

If this is not the case, the file `/etc/chemselect/config.json` must be changed:

```
{
  "Database": {
    "Server": "localhost",
    "Name": "chemselect",
    "User": "chemselect",
    "Password": "*******"
  },
  "AdminEmail": "*****",
  "Realhost": "*****"
}
```

You must activate all changes with the command

```
sudo systemctl restart chemselect
```

Mailserver

CHEMSELECT would also like to send emails and therefore assumes a local *Postfix* installation that allows an SMTP connection from *localhost*. The Postfix configuration must ensure that emails are sent to CHEMSELECT users via the Internet and that local emails are distributed to postmaster appropriately. You can make changes with the command

```
sudo dpkg-reconfigure postfix
```

Troubleshooting

You can recognize a successful installation by calling `https://<ihr-server>` in your web browser. The image displayed should look like that of the reference server https://

At the end of the installation, an e-mail is sent to the e-mail address of the privileged user and to the postmaster of the server with the subject "chemselect has been successfully installed". Check whether this mail is delivered.

Relevant configuration files are:
- `/etc/chemselect/config.json`
- `/etc/apache2/sites-enabled/011-chemselect.conf`

Relevant log files are:

- `/var/log/kestrel/*`
- `/var/log/apache2/*`
- `/var/log/syslog*`