

COSMObase Installation Guide

Version C2.1 Revision 01.08

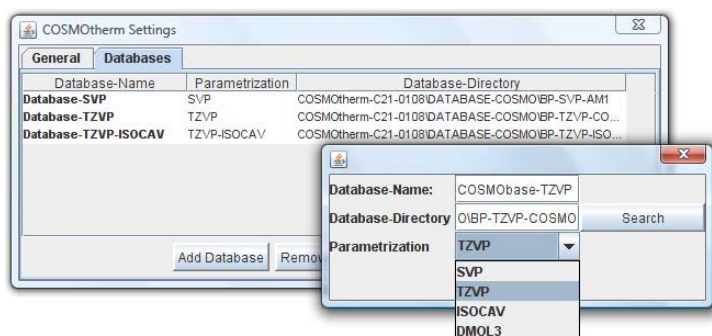
COSMObase (Database of COSMO-files) Installation

To install **COSMObase**, the database of COSMO-files for the usage within the **COSMOtherm** program please unzip the **COSMObase-C21-0108-QMLEVEL.zip** file for the quantum chemistry level that you want to install to a local directory on your computer. Currently four different quantum chemistry level cosmo-files are shipped within **COSMObase**: "QMLEVEL" can be "BP-TZVP-COSMO", "BP-SVP-AM1", "BP-TZVP-ISOCAV", and "DMOL3-PBE" (for details on the quantum chemistry levels, see **COSMOtherm** User's Manual; note that extent of **COSMObase** for the different computational levels may differ). Unzipping the archive file will create the **COSMObase** database index files QMLEVEL.csv, an index Excel-sheet as well as the subdirectory /QMLEVEL/ where the compound cosmo-files name.cosmo, gas phase energy files name.energy, and vapor pressure/property files name.vap of over 10000 molecules/conformers (corresponding to over 4500 compounds) of the given quantum chemistry level are extracted to.

COSMObase Usage in COSMOthermX (Graphical User Interface)

To be able to use **COSMObase** within **COSMOthermX**, the graphical user interface to **COSMOtherm**, you may either directly extract **COSMObase** into the basis directory of your **COSMOthermX** / **COSMOtherm** release installation (~\COSMOthermX-C21-0108\COSMOtherm-C21-0108\) and replace the files that are already given in the **COSMOtherm** release directory /DATABASE-COSMO/.

Alternatively, you may extract the **COSMObase** file archive to a separate directory. In this case you may add the COSMO-file subdirectories /BP-TZVP-COSMO/, /BP-SVP-AM1/, /BP-TZVP-ISOCAV/, or /DMOL3-PBE/ to **COSMOthermX** by choosing the "Add Database" button in the "Databases" card of the "Run"/"Settings" menu of **COSMOthermX** (please note that this process may take a up to few minutes due to the large number of files that have to be processed):



The "Add Database" option allows you to add a COSMO-file directory to the **COSMOthermX** database index. It can be used only locally (with the "Use in this Session" button in the "General" card of the "Run"/"Settings" menu) or added permanently (using the "Save" button in the "General" card of the "Run"/"Settings" menu):

