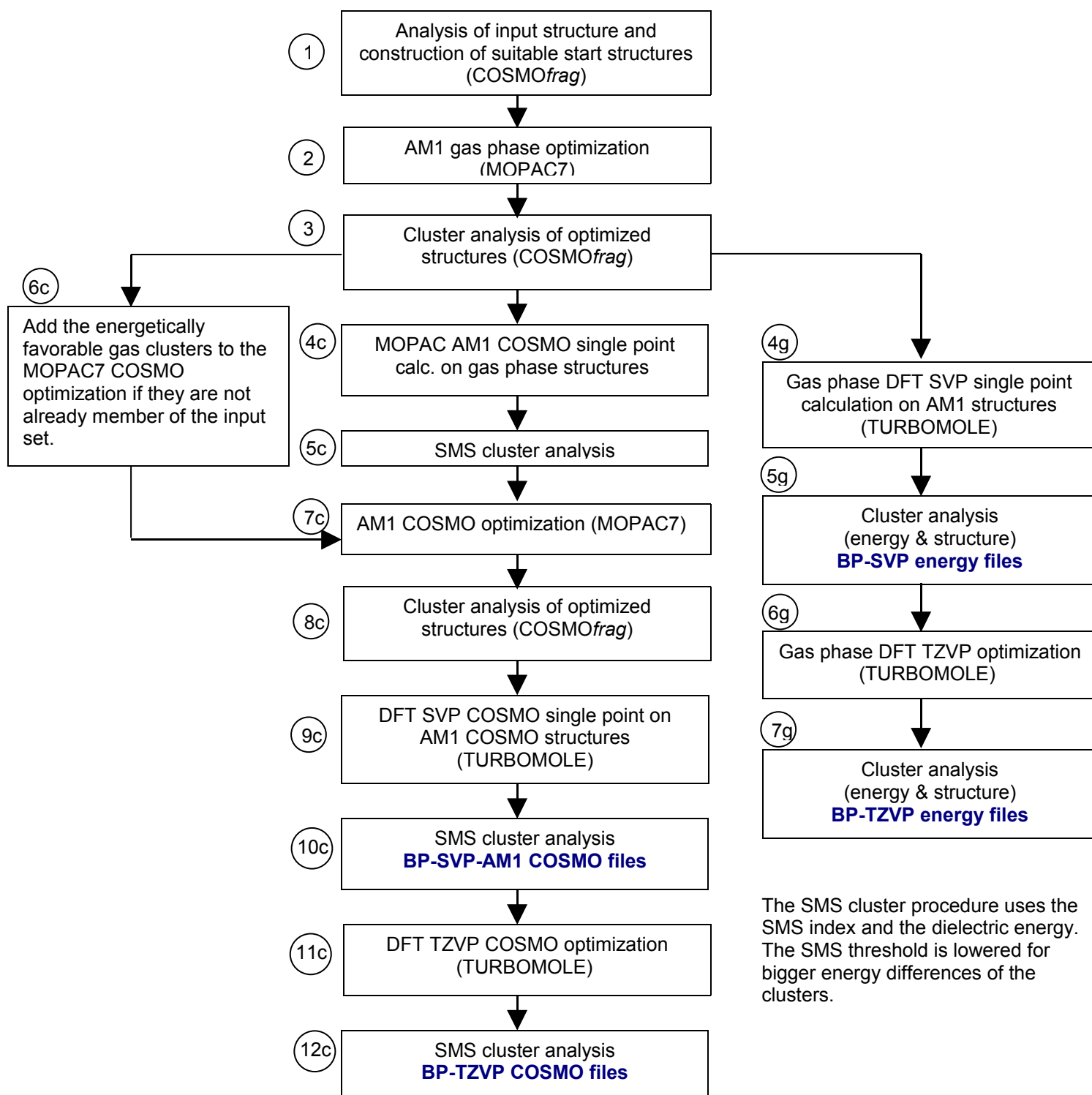


COSMOconf Reference

The *COSMOconf* script automates the creation of COSMO and energy files under consideration of COSMO relevant conformers. The procedure cannot be used for ions or radicals. The current version uses semi empirical AM1 (program: MOPAC [1]) calculations followed by a more accurate Density Functional (DFT) (program: TURBOMOLE [2]) treatment of the most important AM1 conformers.

COSMOconf flowchart:



The SMS cluster procedure uses the SMS index and the dielectric energy. The SMS threshold is lowered for bigger energy differences of the clusters.

1. How to use the script?

In order to do a series of calculations one needs to provide a directory with 3 D input structures. The script needs a list of the structure input files, e.g.:

water.xyz

methanol.xyz

...

The allowed structure file formats are listed in table 1.

The script can be started as follows:

```
COSMOconf -l <input list> -m <method> [-cross -stati -din  
<input file directory> ] > <logfile>
```

Parameters in brackets are optional.

Tab1. List of parameters

Parameter	Description
<method string>	Describes the quantum mechanical level (see table 2)
<list file>	File name of input structure list. The list consists of names of the 3D structure files (inclusive suffix), e.g.: water.xxx methanol.xxx ... The suffix has to be consistent with the file format. Allowed file formats are: sdf : MDL Isis SDF file (3D) car : MSI Biosym/Insight II CAR file xyz : XYZ file ccf : compressed cosmo format ml2: mol2 files cosmo : normal cosmo file
Optional Parameters	
-stati	Statistics run only.
-cross	Crosscheck: the min. of the gas phase calc. will be included in the TZVP cosmo opt. and vice versa (step 11c). Therefore, the cosmo calc. needs a finished gas phase run and the gas calc. needs a finished cosmo run. (BP-TZVP level only)
<input file directory>	Complete path of input file directory

Tab. 2 Methods

Method String	Description
BP-SVP-AM1-GAS	DFT energy calculation with SVP basis and BP functional on a structure that has been optimized on the AM1 level of theory.
BP-SVP-AM1-COSMO	Same strategy as BP-SVP-AM1-GAS. In addition the COSMO model is used in all calculations.
BP-TZVP-GAS	DFT optimization with TZVP basis and BP functional. The optimization starts with the AM1 optimized start structure.
BP-TZVP-COSMO	Similar to BP-TZVP-GAS. In addition the COSMO model is used in all calculations.

Directories and file names

A calculation creates the following directories:

CMcal

This directory holds the subdirectories of the molecules, which contain all MOPAC, COSMO*frag*, and TURBOMOLE calculations.

COSMOconfBP-SVP-SP and COSMOconfBP-TZVP

These directories hold the final *.cosmo and *.energy files, respectively. The different conformers are numbered (0...n) accordingly to the COSMO data base convention. The conformers are ordered with respect to increasing energy. The file glucose0.cosmo, for instance, corresponds to the energetically (DFT energies) favorable conformer. **Please note:** the gas phase energies (*.energy files) are collected in the same directory and have similar names. But the order corresponds to the gas phase energies in this case. Therefore, the gas phase structure of conformer name0.energy does not necessarily correspond to the COSMO conformer structure name0.cosmo.

Restart

The calculations can be restarted by using the same command in the same start directory. COSMO*conf* examines the already existent files and decides what to do. It also allows for a recalculation using a different method on top of a finished run. E.g. a BP-TZVP-GAS run on top of a BP-SVP-AM1-GAS run. In this case the BP-SVP-AM1-GAS results are used as a starting point for the BP-TZVP gas phase optimizations.

Example

The following scheme explains the creation of COSMO files on the BP-TZVP-COSMO level:

- 1) Create 3D input structures, e.g. XYZ files.
- 2) Create a directory and copy the 3D files into this directory e.g.:

```
mkdir new_calc
cd new_calc
copy the files
```

- 3) Create a list of the input file names (the file is called list hereafter).

```
Content of the file list:
ethanol.xyz
methanol.xyz
water.xyz
...
```

- 4) Start the script:

```
COSMOconf -l list -m BP-TZVP-COSMO >list.log
```

The output of the script can be found in the file list.log. The COSMO files are collected in the COSMOconfBP-TZVP directory.

Installation and technical information

Prerequisites:

TURBOMOLE (Version 5.9 or higher) should be installed properly.

Installation:

The installation should be done by a member of the user group (the group that will use the script later on). The installation script tries to copy a file to the TURBOMOLE directory (\$TURBOMOLE). Therefore, the right to write in the TURBOMOLE directory is needed. You TURBOMOLE administrator should have this right.

1)unpack the *COSMOconf* archive into a chosen directory

```
gunzip COSMOconf_....tar.gz  
tar -xvf COSMOconf_....tar
```

2)copy the *COSMOfrag* license to the calculate installation directory. Please ensure read permission for the user group.

3)Start the *COSMOconf* installation script

```
./install
```

The *COSMOconf* directory (the one where you executed install) can be included in the `PATH`. We recommend to define the new `PATH` in the local environment of the user (`.bashrc`, `.cshrc` etc.). For a bash user the entry looks like:

```
export PATH=<path to COSMOconf>:$PATH
```

The calculate script (see `calculate..._manual.pdf`) is part of the distribution and will be installed automatically by `install`. It can be used for a batch generation of COSMO/energy files without conformer treatment. The input structures will be used as starting structures for the optimizations.

Some Technical Details

Some *COSMOconf* settings are defined in the `*.def` files, which can be found in the `DEF_CC` subdirectory. These files contain a description method. The file base names (or method names) and the description section of all `*.def` files of the `DEF_CC` subdirectory are shown in the *COSMOconf* help message. If a new method should be created we recommend to copy an existent method to a new `*.def` file and to change the setting of this new definition file. This should be done by expert users only!

Glossary

DFT	Density Functional Theory
COSMO	Conductor like Screening Model
SMS	Sigma Match Similarity
BP	Gradient corrected function of Becke & Perdew [3]
TZVP	Basis Sets of Triple Zeta Valence Quality [4]
SVP	Basis Sets of Double Zeta Valence Quality [5]
AM1	Austin Model 1 [6]

References

[1] . MOPAC7

MOPAC7 is the public domain version of:

MOPAC - A GENERAL MOLECULAR ORBITAL PACKAGE
ORIGINAL VERSION WRITTEN IN 1983
BY JAMES J. P. STEWART AT THE
UNIVERSITY OF TEXAS AT AUSTIN
AUSTIN, TEXAS
MODIFIED TO DO ESP CALCULATIONS BY
BRENT H. BESLER AND K. M. MERZ JR. 1989

locally modified by Andreas Klamt, COSMOlogic.

For more details about MOPAC7, please visit <http://sourceforge.net/projects/mopac7/>

- [2]. TURBOMOLE, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; <http://www.turbomole.com/>
- [3] Dirac, P.A.M., *Proc. Royal Soc. (London)* **A 123** (1929), 714. Slater, J.C., *Phys. Rev.* **81** (1951), 385. Vosko, S.H., Wilk, L., Nusair, M., *Can. J. Phys.* **58** (1980), 1200. Becke, A.D., *Phys. Rev. A* **38** (1988), 3098. Perdew, J.P., *Phys. Rev. B* **33** (1986), 8822.
- [4] Fully Optimized Contracted Gaussian Basis Sets of Triple Zeta Valence Quality for Atoms Li to Kr. A. Schäfer, C. Huber and R. Ahlrichs; *J. Chem. Phys.* **100**, 5829 (1994).
- [5] Fully Optimized Contracted Gaussian Basis Sets for Atoms Li to Kr. A. Schäfer, H. Horn and R. Ahlrichs; *J. Chem. Phys.* **97**, 2571 (1992).
- [6] Dewar, M. J. S., Zoebisch, E. G., Healy, E. F. and Stewart, J. J. P., *Journal of the American Chemical Society*, **107**, 3902, (1985).