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...:| CAST :: CHARMm ATOM ASSIGNMENT |:|:..
      version 0.1 -- Fabian Dey
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CAST is a small and simple tool, which takes a molecule in Sybyl-MOL2 format with TAFF atom types and assigns CHARMm atom types according to rules defined in the folder "castdata/atomtyp.txt". The lines containing CHARMm atom assignment rules start with the tag "EXTTYP". CAST was written using the OpenBabel C++ source kit (version 2.2.3) and uses its SMILES definition for the assignment rules. Assignment rules are applied in order of appearance, thus successive rules might overwrite previously defined atoms (thus default atom types appear first in the respective atom element section).

In order to run cast you first have to export the castdata folder:

```
export CAST_DATADIR=[LOCATION_OF_CAST]/castdata/      (bash,ksh)
setenv CAST_DATADIR [LOCATION_OF_CAST]/castdata/      (tcsh,csh)
```

and then run (in a shell):

```
cast [FILELIST] [OUTPUTFOLDER]
```

```
where: - FILELIST      is a list of mol2 files
       - OUTPUTFOLDER  the folder cast should write the files to
       -> CAST will overwrite any files without warning!
```

see also :

OpenBabel  
<http://openbabel.org>

SMILES tutorial by Daylight:  
[http://www.daylight.com/dayhtml\\_tutorials/languages/smiles/index.html](http://www.daylight.com/dayhtml_tutorials/languages/smiles/index.html)

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General remarks:

- CAST is under development, assignment rules are probably neither complete nor perfect and might change in the future!

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