

CENSO 3.0.5

Webpage

<https://github.com/grimme-lab/CENSO>

https://xtb-docs.readthedocs.io/en/latest/CENSO_docs/censo.html

Version

3.0.5

Installation Environment

- Python 3.14.2 (pyenv 2.6.17)
- anmr (enso 2.0.2)
- other dependent packages

Brief Installation Procedure

```
$ module purge
$ module load pyenv/2.6.17
$ export PYENV_ROOT=/apl/pyenv/repos/2.6.17
$ pyenv virtualenv 3.14.2 3.14.2-censo-3.0.5
$ pyenv activate 3.14.2-censo-3.0.5
(3.14.2-censo-3.0.5) $ eval "$(pyenv init -)"
(3.14.2-censo-3.0.5) $ pip install censo pytest matplotlib pandas
```

Notes

- This is installed in the pyenv environment prepared on the shared area.
- Settings like PATH are described in "censo/3.0.5" module. Please check samples in /apl/censo/3.0.5/samples.
- Executable of anmr (from ENSO 2.0.2) is available in /apl/censo/3.0.5/bin.
- ORCA 6.1.1 and Turbomole 8.0 work fine with CENSO 3.0.5.
 - xTB 6.7.x may not work with this version.