

Configuration from
mindlessgen.toml
and CLI

Possible Options:

- Fixed element composition
- Forbidden elements
- Range of occurrences

- Pull atoms towards origin
- Check for clashes with covalent radii

Generator (parallelized instances)

(Random) Atom
List Generation

Random
Coordinate
Generation

Coordinate
Contraction

Restart **Generator**



ORCA Geometry
Optimization



Restart **Generator**



xtb Geometry
Optimization



If DFT check == True

Else

molecules

write successful molecules to
mindless.molecules and export as xyz