Align two molecules

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Aim and References

- Overlap two rigid bodies by translation followed by rotation (Kabsch algorithm).
- Supporting information of Construction of Two-Dimensional Potential Energy Surfaces of Reactions with Post-Transition-State Bifurcations.
- Appendix A of author's dissertation.
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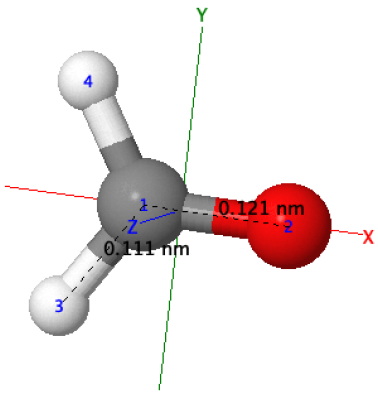
Usage

- In /src, both `overlap.f90` and `overlap.py` do the same things; overlap two ridge bodies.
- Use `makefile` to compile Fortran code.
- Input:
  1. Structure to be varied: $1, extension: .xyz
  2. Reference structure; $2, extension: .xyz

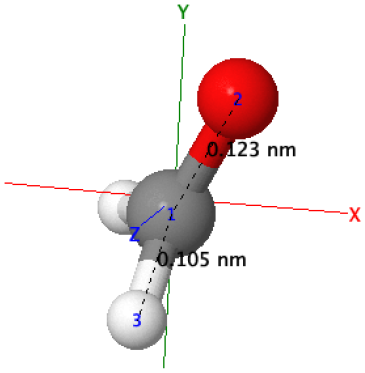
Examples with Screenshots

Prepare two input files for program `overlap.py` or `overlap.f90`, and above input files follow the standard file format which can also be executed by general visualizer, like `jmol`.

The first input file is `coord_from_output_S0.xyz` in folder `./run`, which has C-O bond length as 0.121 nm. This is the structure to be varied.



The second input file is `coord_from_input_S0.xyz` in the same folder as above file, which has C-O bond length as 0.123 nm. This is the reference structure.



Execute the program and change the coordinate of `coords_from_output_S0.xyz` into `shifted.coords_from_output_S0.xyz`. The screenshots of python and Fortran are shown as followed.

Execute the python code `overlap.py`, and it prints out the initial/final RMSD and also produces shifted structure as followed.

```
(base) GracedeMacBook-Pro-2:run Grace$ ../src/overlap.py coords_from_output_S0.xyz coords_from_input_S0.xyz
 1.1677  0.0482
(base) GracedeMacBook-Pro-2:run Grace$ cat shifted.coords_from_output_S0.xyz
4
shifted.coords_from_output_S0.xyz
C -0.002550887498442524 -0.003874579064632166 -0.0009796060938770121
O 0.5961592376433993 1.010971826147303 0.2582916304090838
H -0.05245610801037635 -0.8611467830178539 0.7029848888914599
H -0.5431522421345802 -0.14695046406481668 -0.9602969132066667
```

And then, Fortran code is executed to compare with python result, which is the same for both initial/final RMSD and shifted structure.

```
(base) GracedeMacBook-Pro-2:run Grace$ ../src/overlap coords_from_output_S0.xyz coords_from_input_S0.xyz
 1.1677 0.0482
(base) GracedeMacBook-Pro-2:run Grace$ cat shifted.coords_from_output_S0.xyz
           4
shifted.coords_from_output_S0.xyz
 C -2.707762329462154E-003 -3.801813303707957E-003 -9.020802505374016E-004
 O  0.596209775357381       1.010948384431145       0.258266655217898
 H -5.240113679783330E-002 -0.861172281194226       0.702957722713277
 H -0.543100876230085      -0.146974289933516      -0.960322297680638
```

After translation and rotation, RMSD changes from 1.1677 to 0.0482, and the characteristic bond length of C-O is still reserved.