Example dataset

If you only want to download or inspect a **single representative case** before using the full repository, a good minimal example is the hydrated dysprosium(III)

System: \[Dy(H2O)9\]^{3+}

Where to look

- **Optimized geometry (single-frame XYZ):**
  `opt-xyz/Ln-xyz/Ln-H2O_x/Dy3_9H2O.xyz`
- **NWChem optimization input:**
  `nwchem-inputs/Ln-9H2O/opt-Dy3+.nw`
- **NWChem AIMD input (qmd):**
  `nwchem-inputs/Ln-9H2O/MD-Dy3+.nw`
- **Representative AIMD trajectory (multi-frame XYZ):**
  `MD-traj/9H2O-Dy3+.xyz`

What this example demonstrates

- A complete “opt → AIMD” workflow for a hydrated Ln(III) complex using consistent settings.
- How optimized motifs (from `opt-xyz/`) relate to the short AIMD stability checks (in `MD-traj/`).

Typical checks users run on this example

- Dy–O distance distributions and their short-time stability
- Coordination number classification (8 vs 9) and transient exchange events (if any)
- Comparison of optimized geometry vs trajectory-averaged structure

Sample of the AIMD trajectory file format (`MD-traj/9H2O-Dy3+.xyz`)

Trajectories are stored as **multi-frame XYZ** files (frames concatenated).

Each frame begins with:

1. The number of atoms (here `28` = 1 Dy + 9 O + 18 H)

2. A comment line that starts with the frame index and may include additional **NWChem `qmd` diagnostics** (e.g., total electronic energy and thermostat/integration-related fields as printed by NWChem)

3. The atomic coordinates in Å

Below is a short excerpt showing the first few frames. See **`README.md`** for the full description of directory layout, naming conventions, and how this file connects to the matching `opt-*.nw` / `MD-*.nw` inputs and the optimized geometry.

```text
28
0 -1572.4479926813 1.938974E-01 7.354739E-02
Dy -0.01243265 -0.03441430 0.34372318
O 0.84109235 1.38291364 2.12233230
O 0.81382756 -1.47589527 2.10062677
O -1.68834432 0.06124921 -1.42546616
O -1.24314185 2.09533379 0.27057318
O -1.59533144 0.03929822 2.20111067
O -1.42875407 -2.03389966 0.26660593
O 2.44381912 -0.06760761 0.21136394
O 0.80183262 -1.66051994 -1.24175085
O 0.90021928 1.51752964 -1.28628342
H 1.85669248 1.40271789 -1.39638300
H 0.53192840 1.60058407 -2.17833957
H -2.26320443 -1.87881758 -0.20282614
H -1.66809716 -2.48771961 1.08861842
H -1.44307156 0.75087000 2.84097727
```

H -2.55649948 -0.02465348 2.09645640

H 1.20014407 2.25881358 1.91603463

H 1.44643990 0.98770143 2.76850625

H 0.16934376 -1.89515072 2.69111129

H 1.43965974 -2.17476116 1.85669290

H -1.52048943 -0.32982631 -2.29578705

H -2.03791960 0.95062999 -1.58550767

H -1.75755550 2.36208955 1.04664522

H -0.74360245 2.87872289 -0.00267883

H 2.98893727 0.30536633 0.91903744

H 2.89018835 -0.88174551 -0.06493481

H 0.19647519 -2.38458487 -1.46197991

H 1.23252644 -1.40411715 -2.07136152

28

1 -1572.4480634496 1.782585E-01 3.286302E-02

Dy -0.01230385 -0.03477194 0.34370832

O 0.83708736 1.38176939 2.12116229

O 0.81632324 -1.47399277 2.10197747

O -1.69059708 0.06210942 -1.42608686

O -1.24156102 2.09541870 0.26972813

O -1.59392389 0.03944874 2.20007142

O -1.43142988 -2.03554766 0.26595559

O 2.44516986 -0.06778995 0.21338372

O 0.80159059 -1.65870243 -1.23926910

O 0.90272118 1.52204102 -1.28673585

H 1.84069751 1.39751440 -1.39230336

H 0.52876669 1.59996166 -2.18333726

H -2.27734753 -1.88549872 -0.20773946

H -1.66665721 -2.48327865 1.09532797

H -1.44067338 0.75454541 2.84454629

H -2.55100815 -0.02894939 2.11598363

H 1.19447807 2.26293441 1.91098634

H 1.45479609 0.98132971 2.75563865

H 0.17571055 -1.89183005 2.68434111

H 1.43810335 -2.17858263 1.83898470

H -1.50542488 -0.32219512 -2.29701914

H -2.03020362 0.94892358 -1.57453900

H -1.75925022 2.35605713 1.05075046

H -0.75010142 2.88218895 -0.00925854

H 2.97584171 0.29648654 0.91544855

H 2.89121690 -0.88615986 -0.06585357

H 0.19395143 -2.38669510 -1.46414062

H 1.22549304 -1.42327892 -2.06817163