

# Data Statement

All the datasets mentioned in the paper are shipped with this package.

## QM7

The raw [extxyz](#) file of the QM7 dataset, the [input](#) and the training script are all included.

## SNAP

The converted ASE Sqlite3 databases (Ni, Mo, Mo-Ni) are included in directory [datasets](#). The corresponding trained models can be found in directory [models](#).