

Practical examples 2

Ex.1) Load “mol1.pdb” as a Molecule (in the Python code). Using the following periodic table, create a function that receives a Molecule as input and outputs each atom’s species number, in a list.

Element Symbol	Species Number
H	1
C	6
N	7
O	8

Ex.2) Create a function that receives a Molecule as input and outputs each atom’s cartesian coordinates, in a list.

Ex.3) Using the previous exercises functions, follow the example described in the TorchANI documentation (https://aiqm.github.io/torchani/examples/energy_force.html) to create and test a new function in order to calculate the energy of a Molecule.