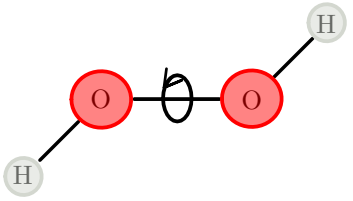
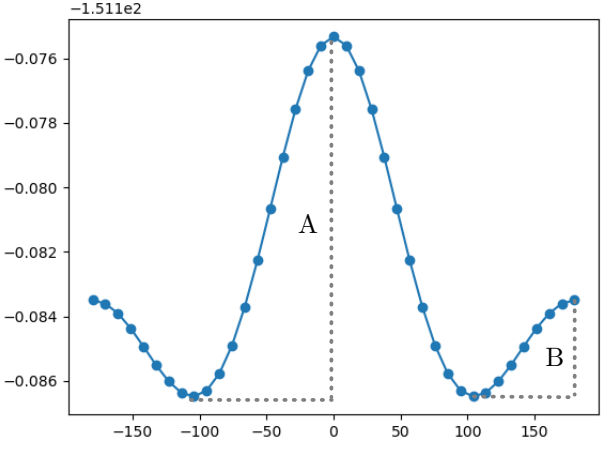
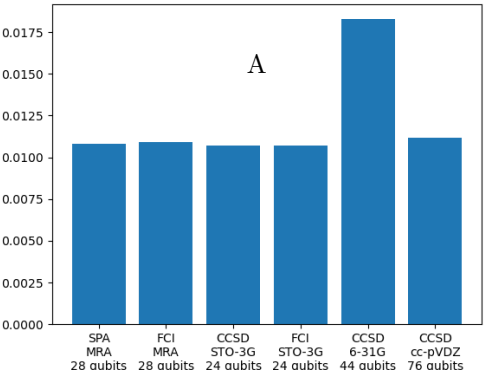
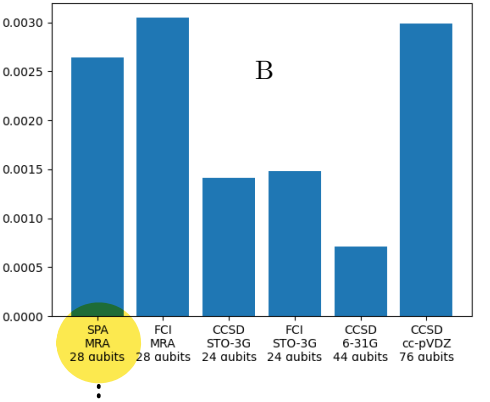




HOOH dihedral angle






```
import tequila as tq

mol = tq.Molecule(geometry="h2o2.xyz", n_pno=7, pno={"maxrank":1})
H = mol.make_hardcore_boson_hamiltonian()
U = mol.make_upccgsd_ansatz(name="HCB-SPA")
E = tq.ExpectationValue(H=H,U=U)

result=tq.minimize(E)
energy=result.energy
```