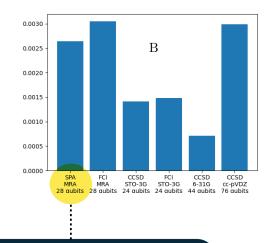


0.0175 Α 0.0150 0.0125 0.0100 0.0075 0.0050 0.0025 0.0000 CCSD CCSD MRA MRA STO-3G STO-3G 6-31G cc-pVDZ 28 aubits 28 aubits 24 aubits 24 aubits 44 aubits 76 aubits



```
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
```