GQCP::Molecule

+ Molecule() + Molecule() + calculateInternuclearDistance

Between() + charge() + description()

+ nuclearFramework() + numberOfAtoms()

+ numberOfElectronPairs() + numberOfElectrons() + totalNucleicCharge()

+ HChain() + H2Chain() + HRingFromDistance()

+ HRingFromRadius()

+ ReadXYZ()