GQCP::Molecule

+ Molecule()
+ Molecule()
+ calculateInternuclearDistance
Between()
+ charge()
+ description()
+ nuclearFramework()
+ numberOfAtoms()
+ numberOfElectronPairs()
+ numberOfElectrons()
+ totalNucleicCharge()
+ HChain()
+ H2Chain()
+ HRingFromDistance()
+ HRingFromRadius()
+ ReadXYZ()