

GQCP::Molecule

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