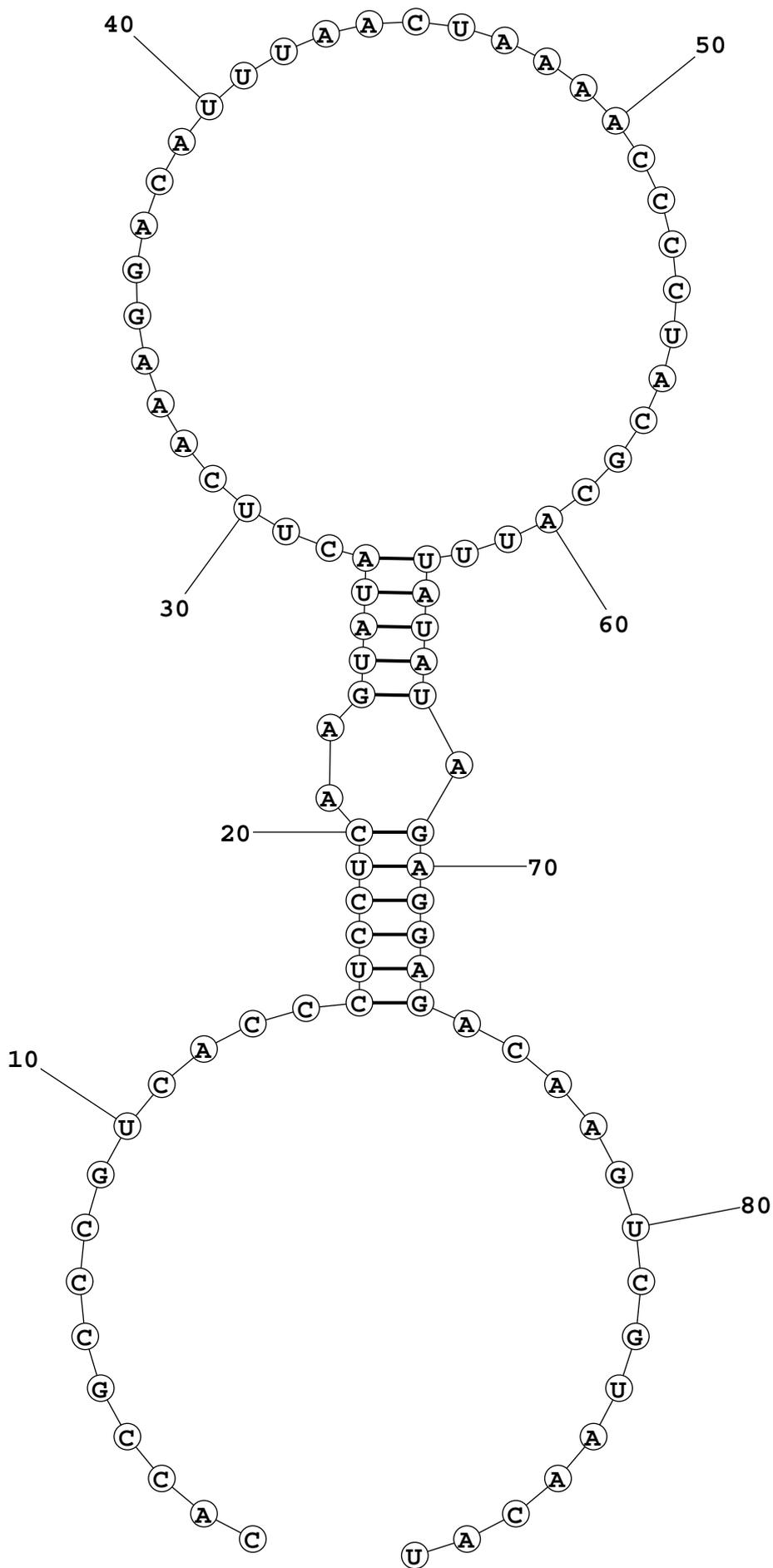ENERGY = -14.0   12S

ENERGY = -13.5 12S