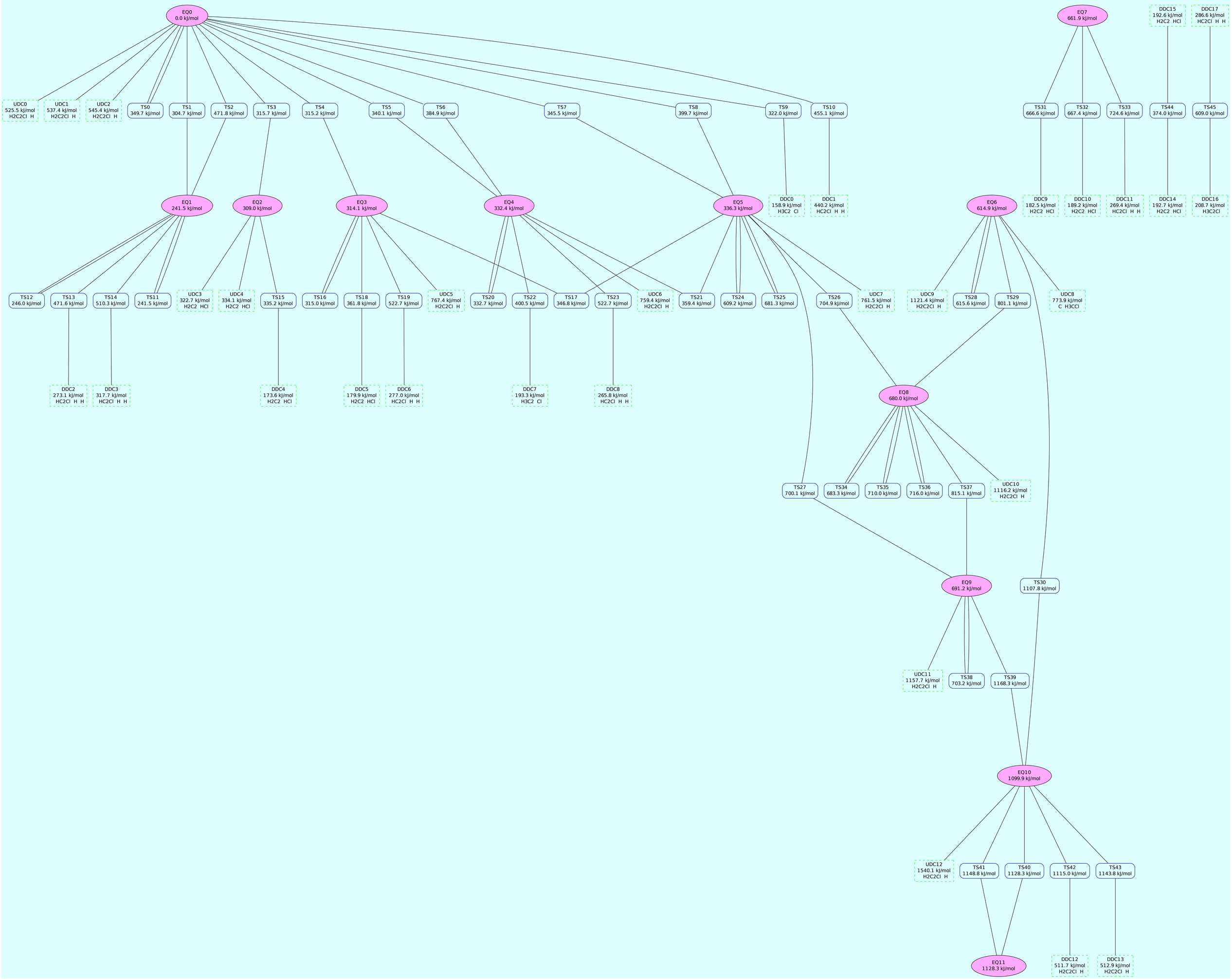H3C2Cl B3LYP/6-31G*