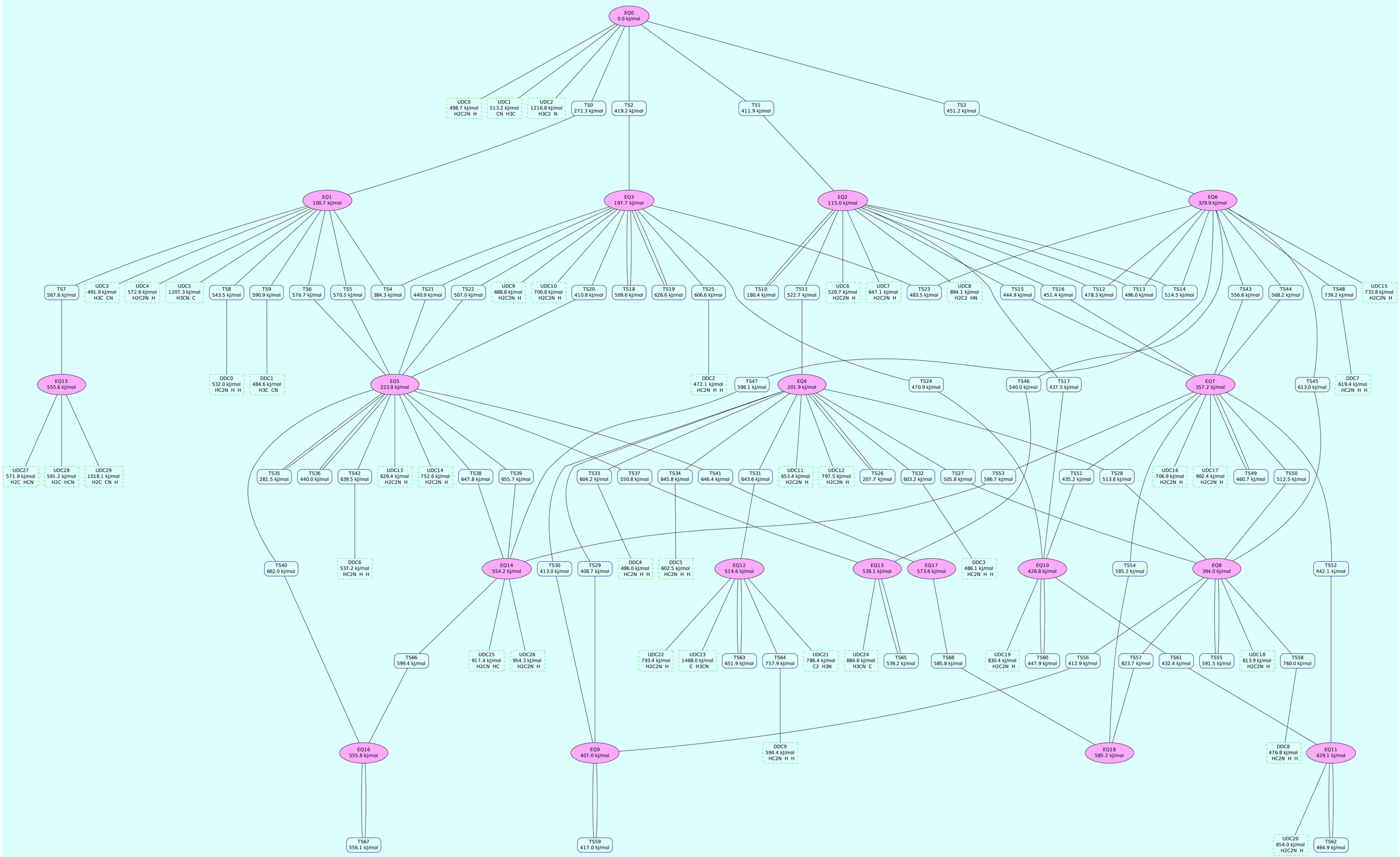H3C2N B3LYP/6-31G*