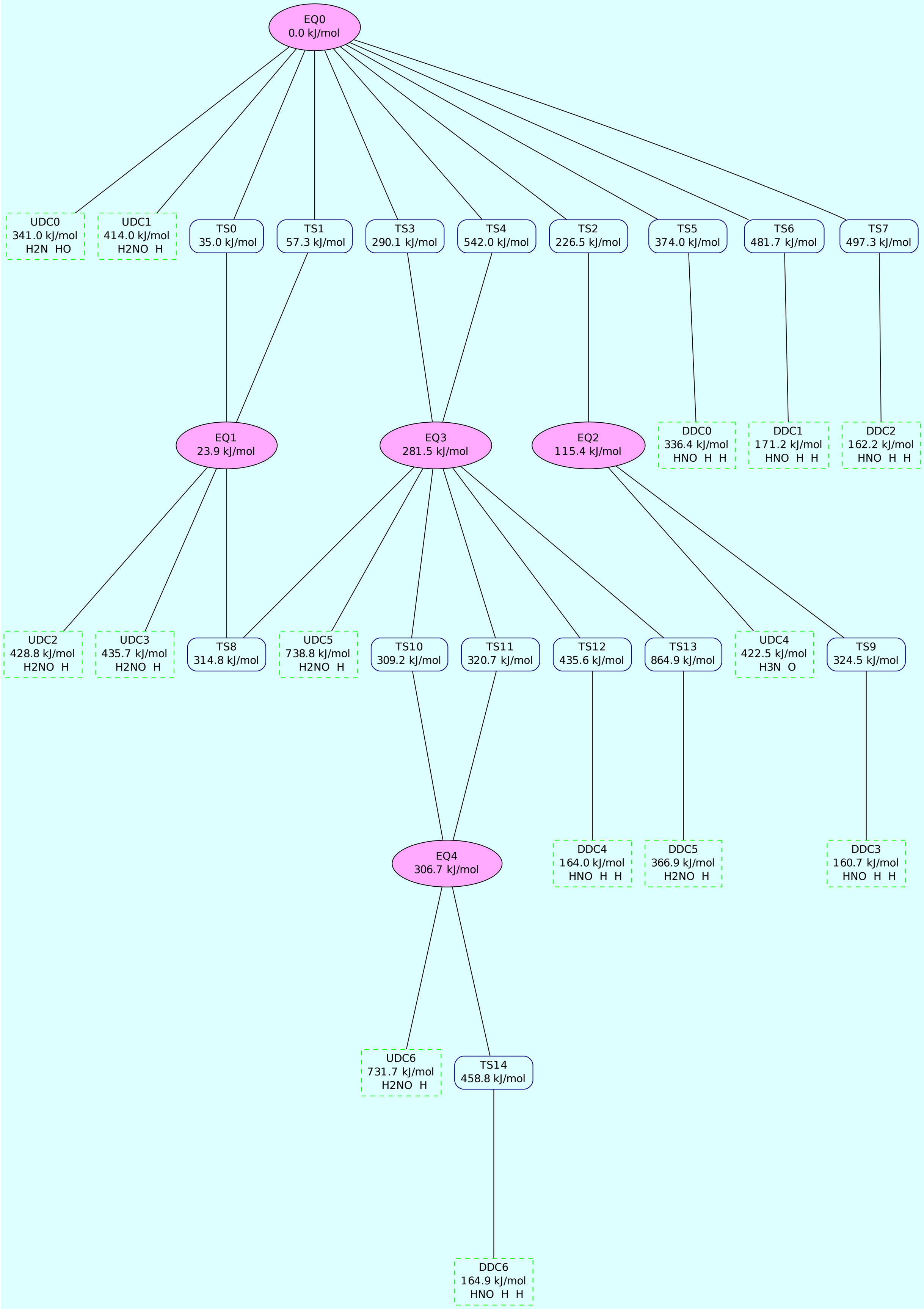H3NO B3LYP/6-31G*