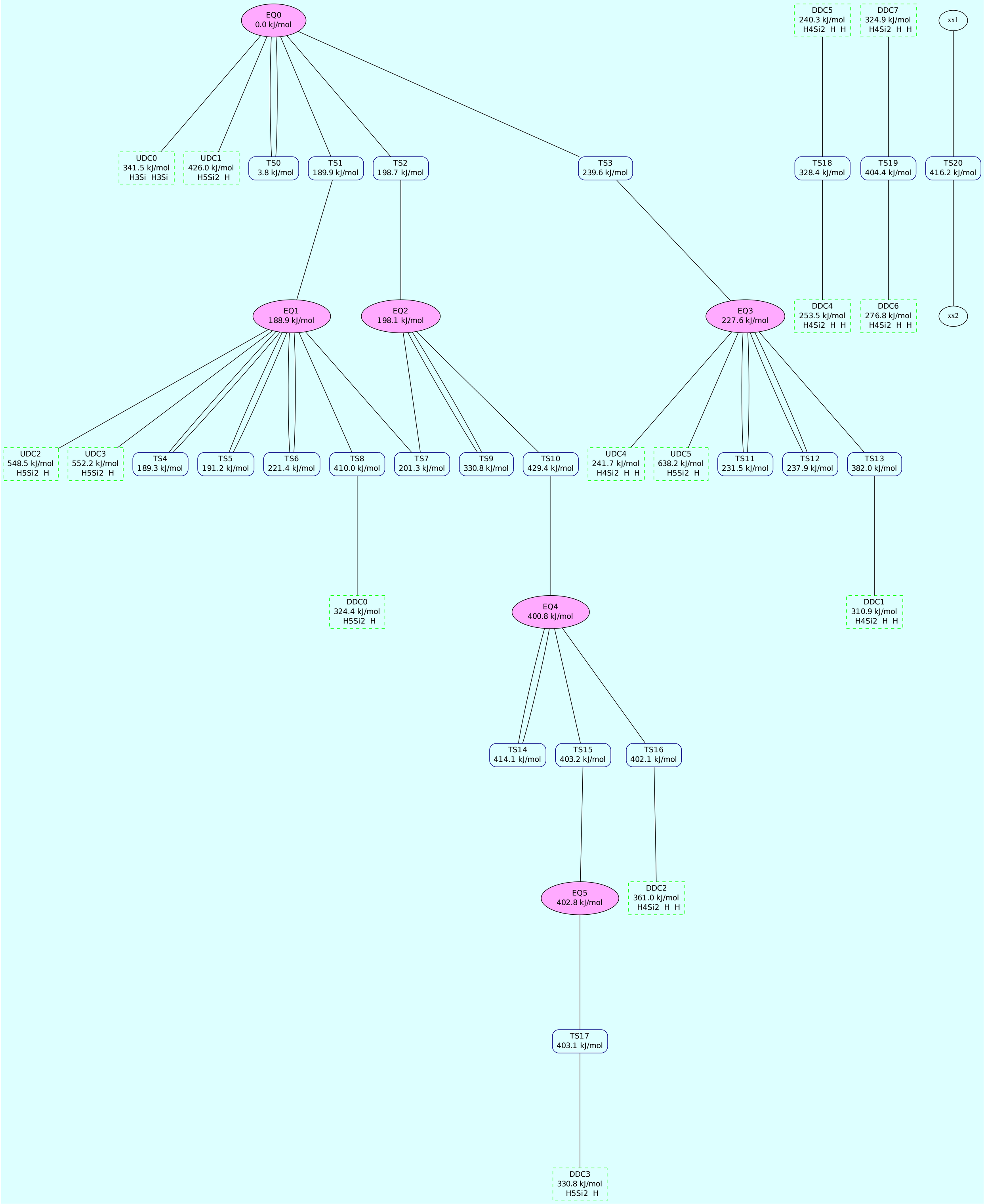H6Si2 B3LYP/6-31G*