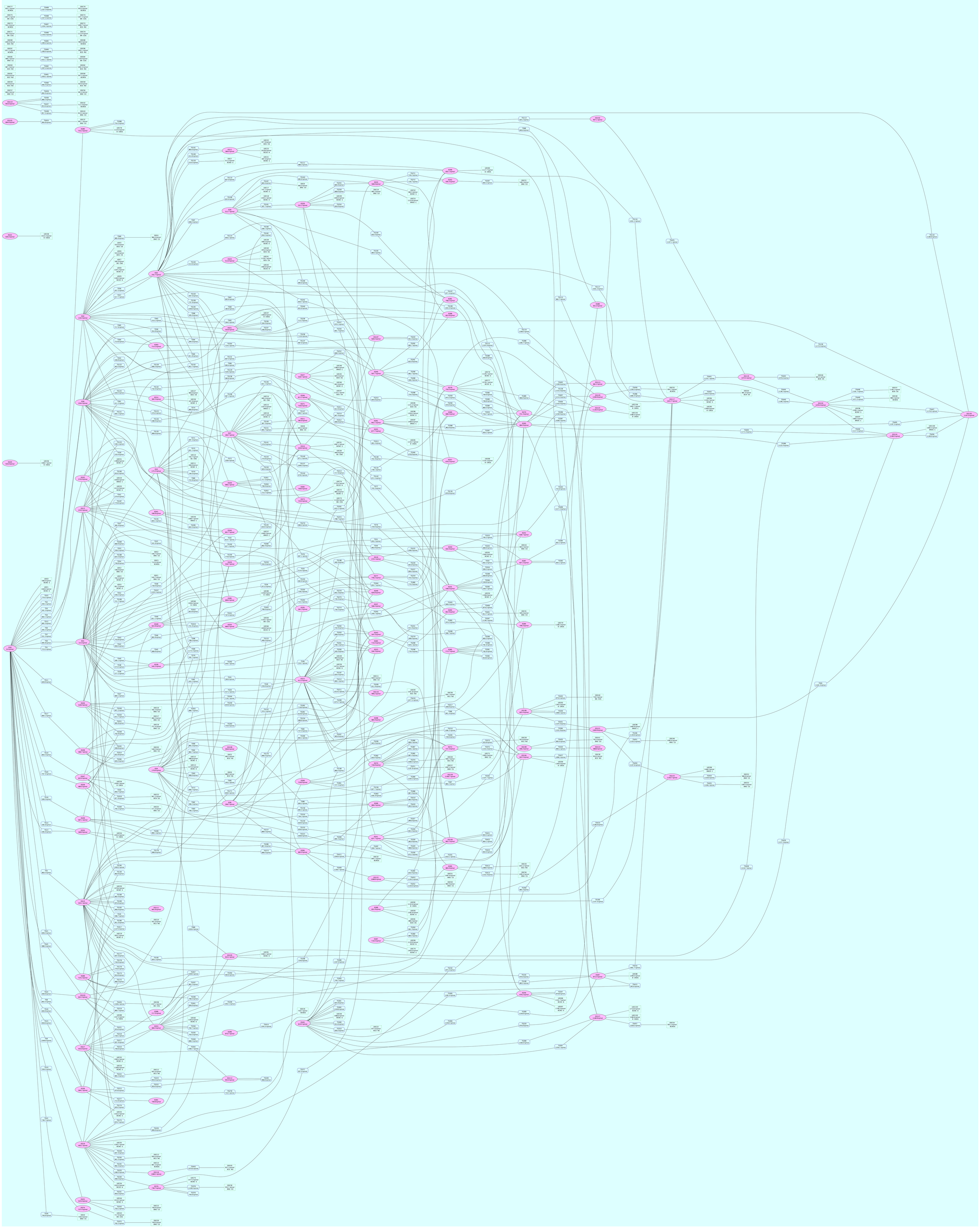BCNOS B3LYP/6-31G*