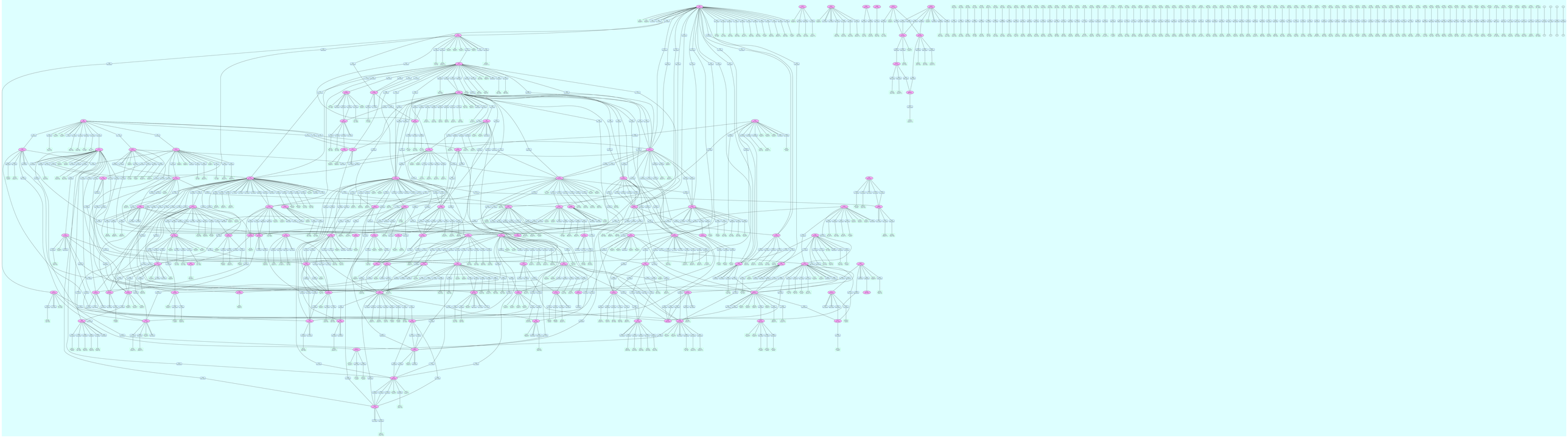HCN32 B3LYP/6-31G*