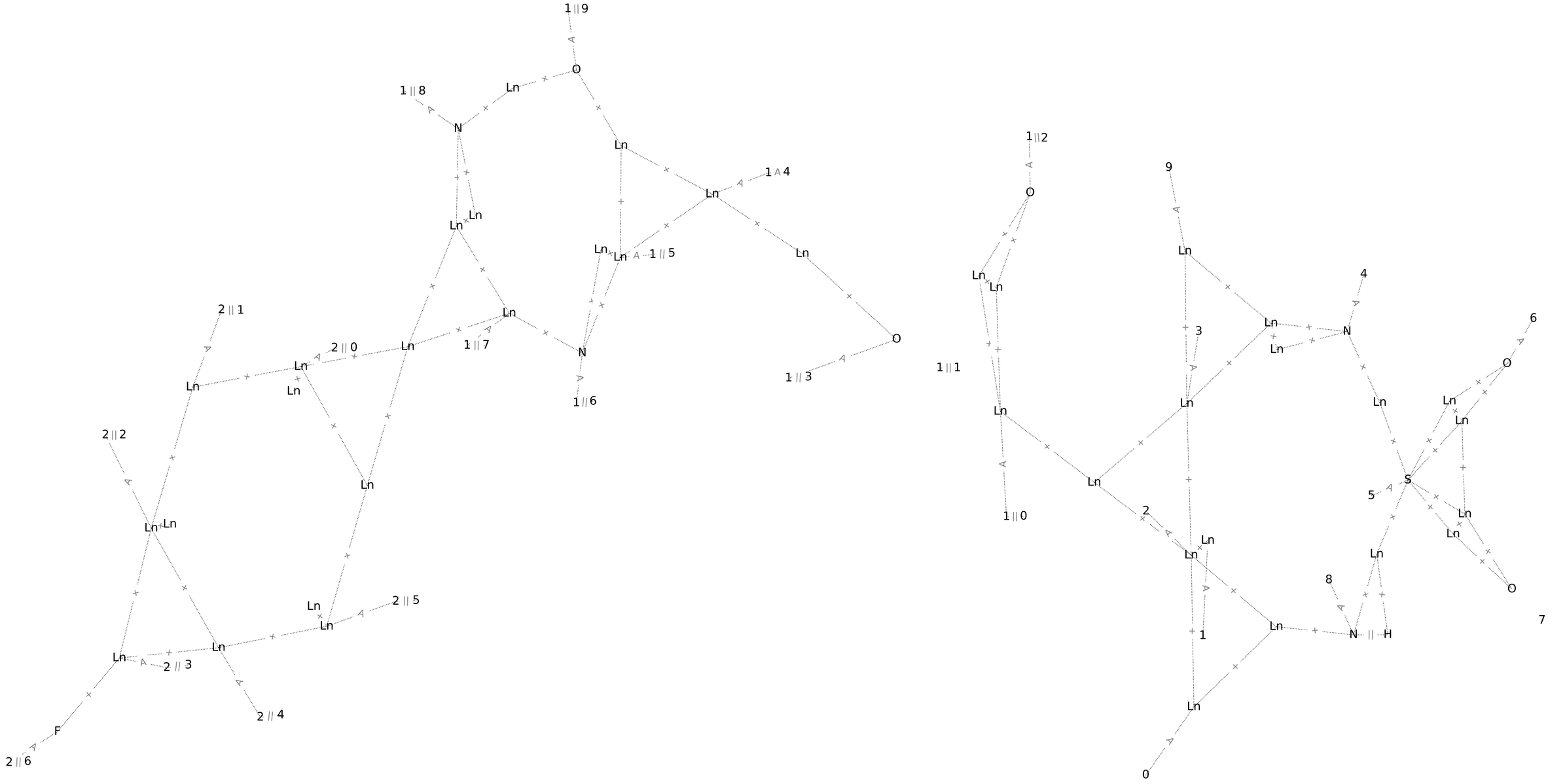9474047_rdkit