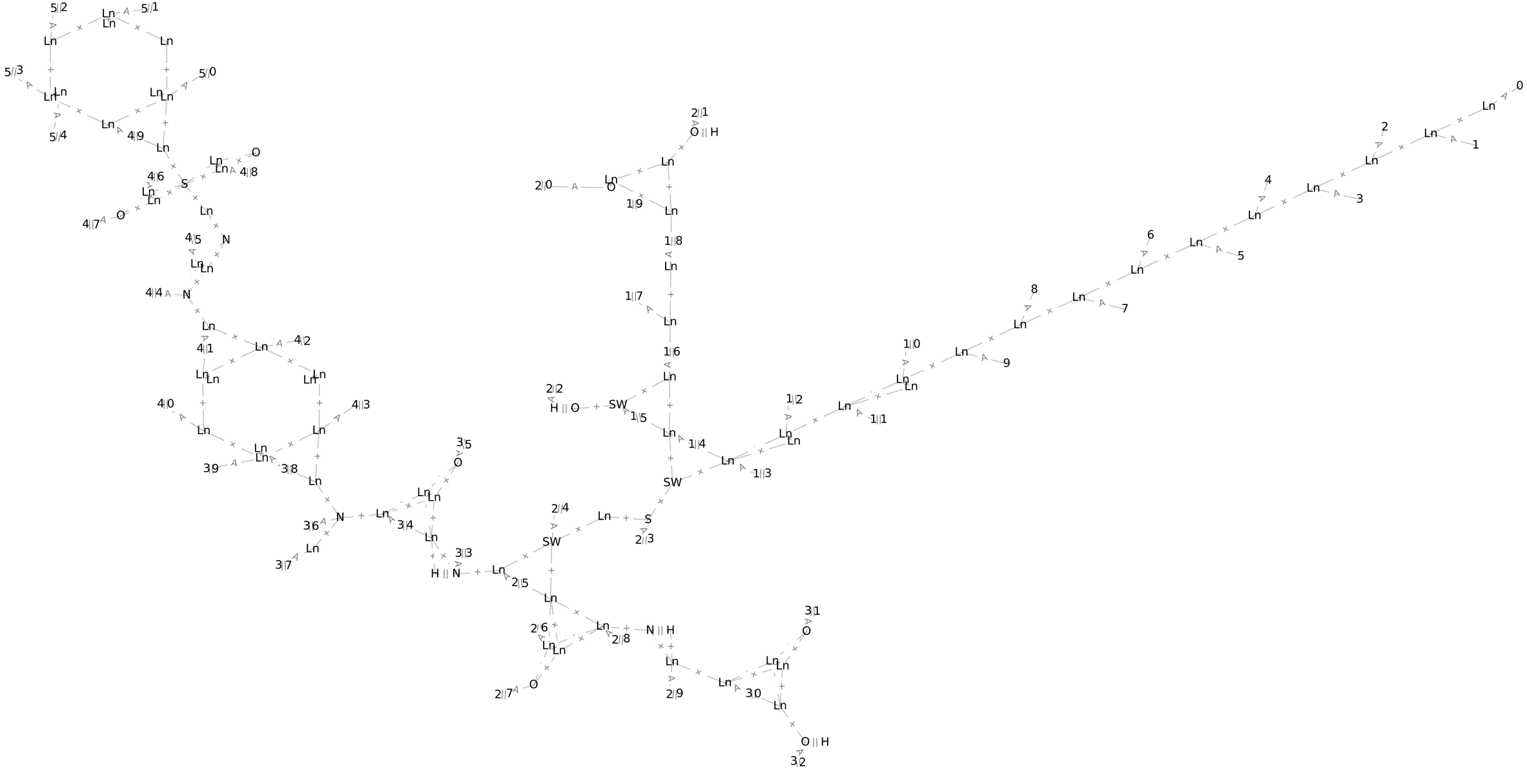10328004_rdkit