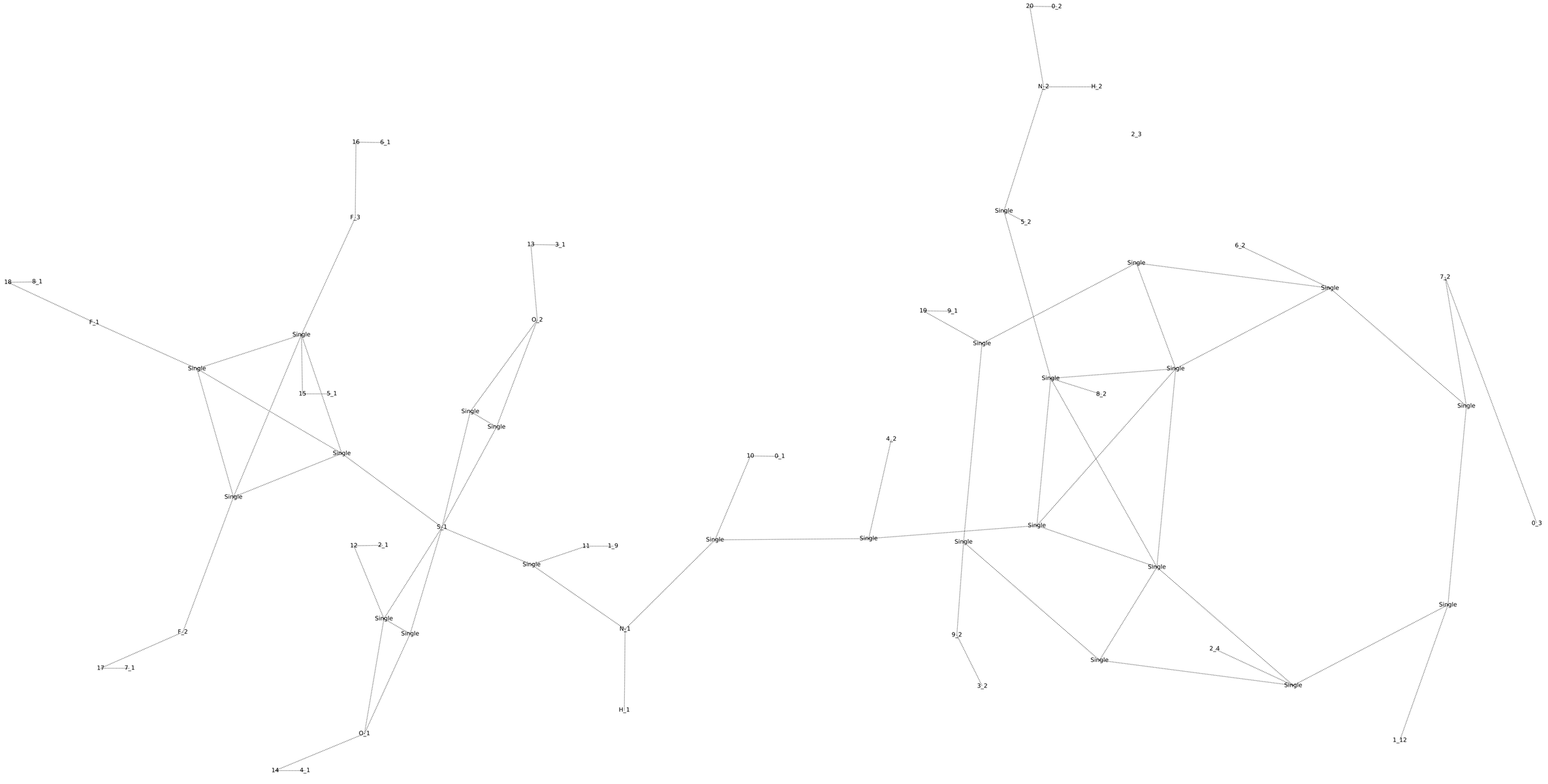9880495_rdkit