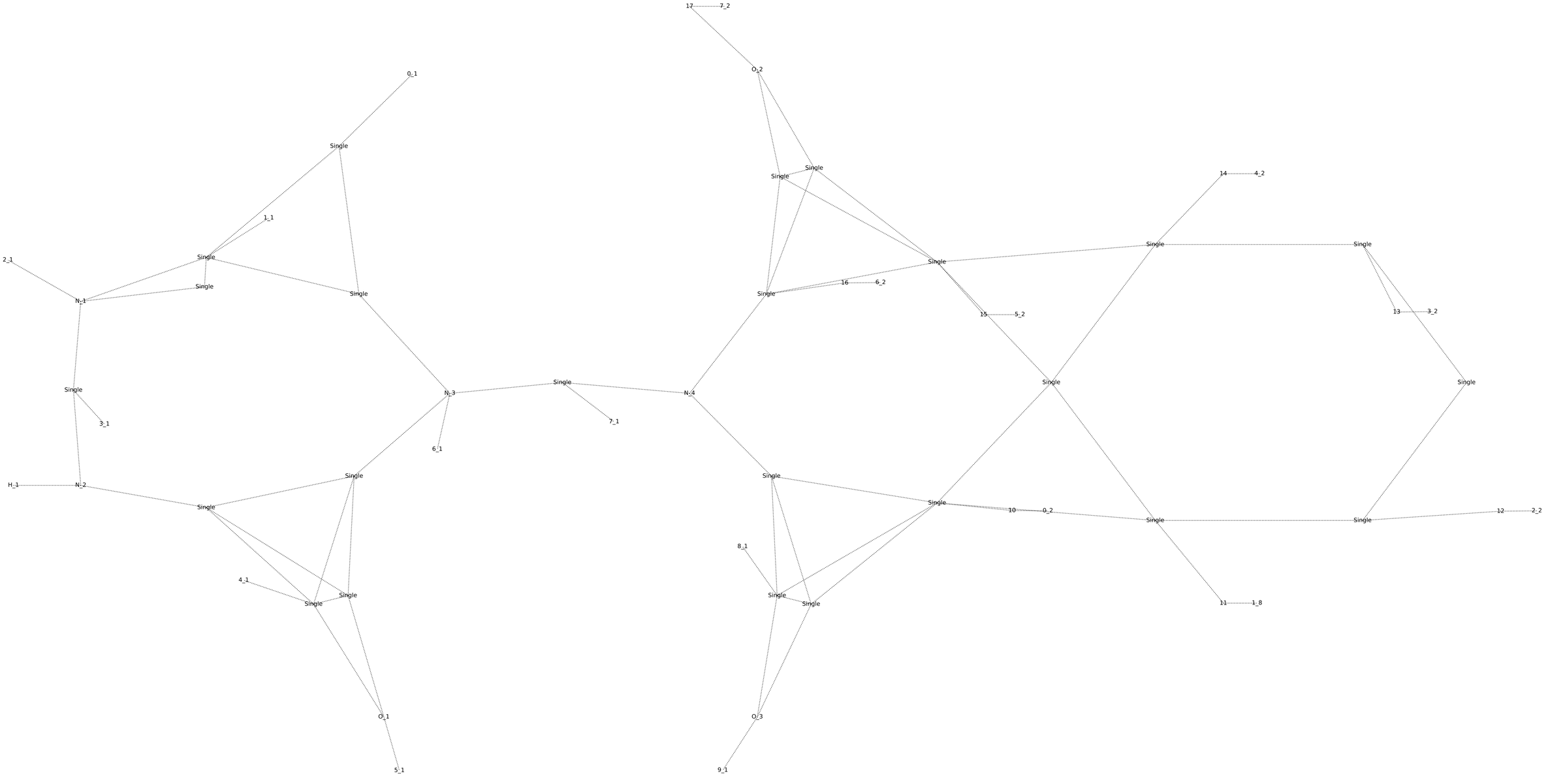10705789_rdkit