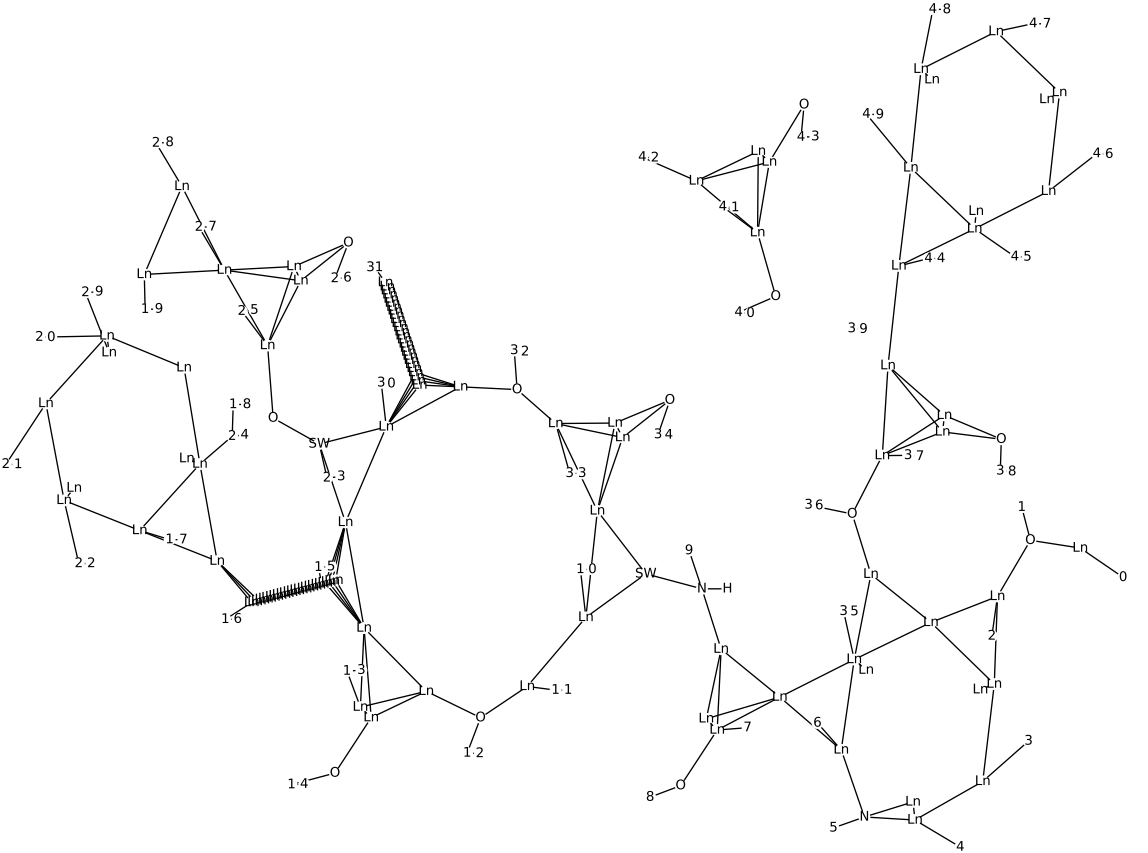USRE039991-20080101-C00553_rdkit