in situ ^{13}C CPMAS NMR Study of Porous Coordination Polymer

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Metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) are microporous crystalline materials composed by metal ions acting as nodes (or connectors) and bridging organic ligands acting as linkers. Fig. 1 shows the schematics of such materials. MOFs are able to undergo reversible structural contraction or expansion after adsorption of a guest molecule or if a “gate-opening” pressure is attained, suitable for applications such as adsorption-based separations, molecular storage, catalysis, and *in situ* polymerization

Fig. 2 shows the in situ ^{13}C CPMAS spectra of a CPL-2, i.e. $Cu_2(pzdc)_2(bpy)$, showing the thermally induced structural changes. The appearance of the non-reversible bpy resonances at 423K indicates the collapse of the pores at this degassing temperature, which is way below the decomposition point of the framework, evidencing how sensible this material is to thermal preactivation.

High-resolution solid-state MAS NMR is an invaluable tool capable of probing local coordination environments and physical properties of the MOF/PCP materials. Understanding the relationship between the local structural details and functionalities during the thermal processes is crucial to elucidate the potential of these materials for adsorption and catalysis applications.

Formed by the Cu^{2+} and the anionic pyrazine-2,3-dicarboxylate ($pzdc^{2-}$)

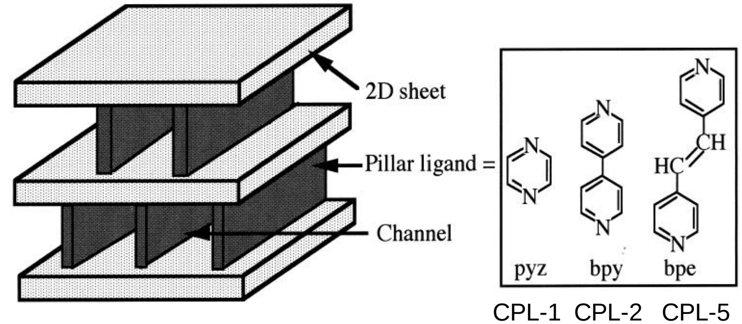

Fig. 1 Schematics of atomic structure of Cu complexes.

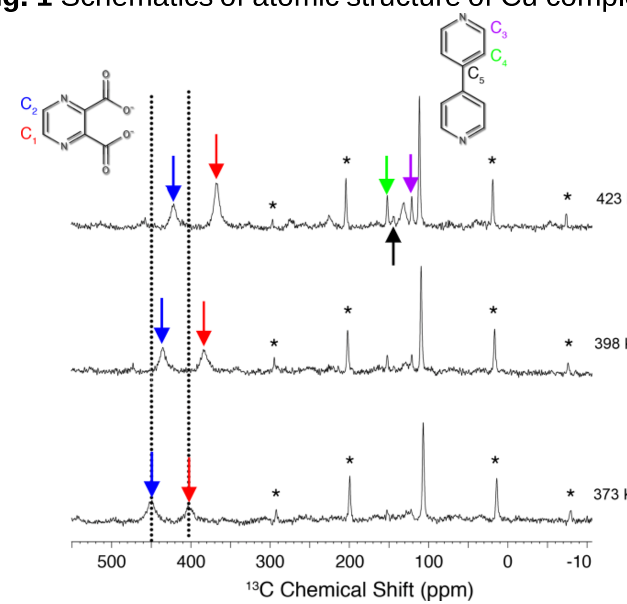

Fig. 2 in situ ^{13}C CPMAS NMR spectra showing the displacement of the pzdc carbons and appearance of the non-reversible bpy pillar ligand resonances at 423K.

Facilities: NMR facility.

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