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In situ High Pressure Powder Diffraction study of proton conductors based on metal phosphonates

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Soft Porous Metal Organic frameworks (MOFs) are referred to as a class of coordination polymers that exhibit structural flexibility in response to guest interactions or physical stimuli [1]. By combining softness and regularity, the responsive crystalline frameworks show, for instance, unique mechanisms of separation and storage of gases.

Here we report the effects of high pressures of CO₂ on the frameworks of two types of coordination polymers based on multifunctional metal phosphonates, which exhibit proton conductivity at high relative humidity in addition to porous properties. The first one, Ni₂(H₂O)₂(O₃PCH₂N(C₄H₈)NCH₂PO₃)·8H₂O (Ni-STA-12) is a well-known MOF material structural featured by 1D channels build from MO₅N octahedra linked by the piperazinyl moieties [2]. The second solid, Mg[(HO₃PCH₂)₂NHCH₂C₆H₄CH₂NH-(CH₂PO₃H)₂]·2H₂O, (MgHDTMP·2H₂O), is a pillared layer metal phosphonate containing flexible alkyldiaminetetraphosphonate as linker of the inorganic layers. For both solids, *in situ* synchrotron powder diffraction data were collected on BL04-MSPD under different pressures of CO₂ (up to ~10 bar) and temperatures at ALBA (Barcelona, Spain). The resulting structural changes observed on their frameworks as well as their proton conductivities will be discussed.

References

- [1] S. Horike, S. Shimomura, S. Kitagawa, *Nature Chemistry* **2009**, 1, 695-704.
- [2] S.R. Miller, G.M. Pearce, P.A. Wright, F. Bonino, S. Chavan, S. Bordiga, I. Margiolaki, N. Guillou, G. Férey, S. Bourrelly and P.L. Llewellyn, *J. Am. Chem. Soc.* **2008**, 130, 15967–15981.

Caption (s) - Add figures as attached files (2 fig. max)

Figure 1. X-ray diffraction patterns of MgHDTMP at different CO₂ pressures. The inset shows the evolution of the peaks upon CO₂ adsorption/desorption. (*desorption).

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