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

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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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