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Water cluster structure in the MOF CAU-10-H: a powder diffraction perspective

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Several metal-organic frameworks (MOF) excel in harvesting water from the air or as heat pumps as they show a steep step in the water isotherm at 10-30 RH% [1]. Yet, a precise understanding of the water structure within the confined space of such MOF is still lacking. Here, we unravel the structural properties of CAU-10-H under various water content. We show that the water content can be tuned using the relative humidity, temperature and history of the sample. Previous studies have shown a structural phase transition from hydrated (non-centrosymmetric structure) to dry (centrosymmetric structure) [2]. Here in this contribution, we show that high resolution powder diffraction can allow to locate water molecules and the existence of various states of hydrated phases including centrosymmetric one.

This study besides bringing further insight into the water clusters present in this MOF enlightens also the powerfulness of powder diffraction in the study of MOF materials.

[1] Wentao Xu, Omar M. Yaghi, ACS Cent. Sci. 2020, 6, 8, 1348–1354

[2] Dominik Fröhlich et al. J. Mater. Chem. A, 2016,4, 11859-11869

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