# Structural Details of the Activation Process in the Flexible Metal-Organic Framework [Cu(Me-4py-trz-ia)]

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The metal-organic framework [Cu(L1)] (L1 = 3-methyl-5-pyridin-4-yl-1,2,4-triazolyl isophthalate) features outstanding uptake properties for $CO_2$ and $H_2$ at ambient pressure.[1] Activation of this MOF under varying conditions leads to altered X-ray diffraction patterns before reaching the fully desolvated phase. The original diffraction pattern of the as-synthesized phase can be restored by resolvation of the activated material suggesting a flexible structural transformation. These phase transitions and an accompanying colour change between different shades of blue indicate structural changes not only by linker movement but also by a change of the coordination spheres of the $Cu^{2+}$ centres.

Following up these results, we present a detailed structural insight into the behaviour of this flexible MOF during activation by a combination of single crystal structure analyses, Rietveld refinement of high quality powder XRD data and DFT based simulations of the framework structure (Figure 1).

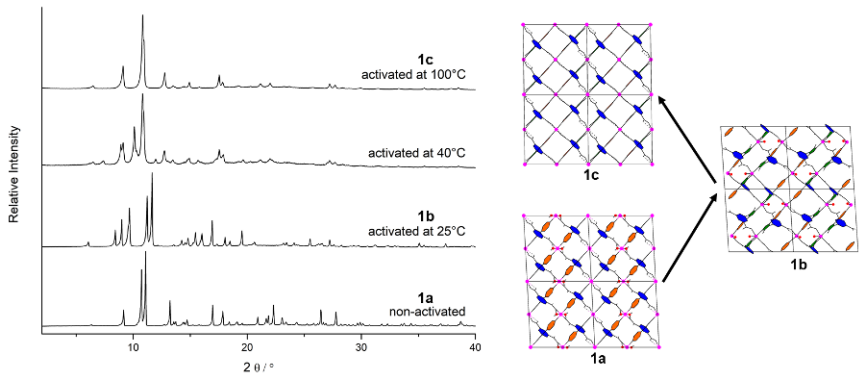


Figure 1, left: X-Ray powder diffraction patterns of the non-activated phase **1a** of [Cu(L1)] and after activation at different temperatures for 24 h in vacuum; right: schematic representation of the frameworks of the phases **1a**, **1b** and **1c** (view along [001]).

[1] D. Lässig, J. Lincke, J. Moellmer, C. Reichenbach, A. Moeller, R. Gläser, G. Kalies, K. A. Cychosz, M. Thommes, R. Staudt, H. Krautscheid, Angew. Chem. 2011, 123, 10528-10532.