

# Isorecticular Isomerism in 4,4-connected Paddlewheel Metal-Organic Frameworks: Structural Prediction by the Reverse Topological Approach

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## PXRD Data

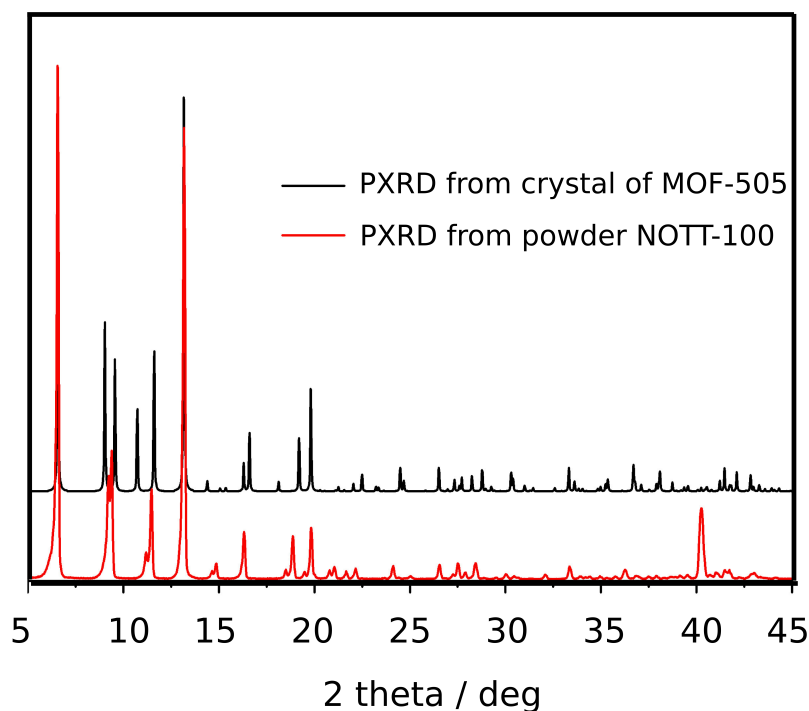


Figure 1: XRPD patterns obtained from the powder sample NOTT-101<sup>1</sup> (red) and the single crystal MOF-505<sup>2</sup> (black).

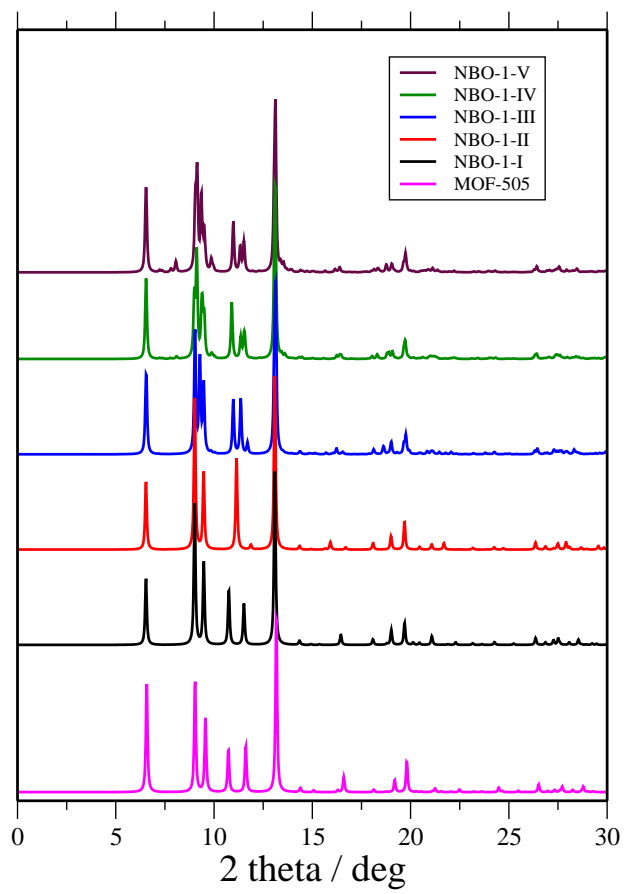


Figure 2: XRPD patterns of the five most stable structures of NBO-1 obtained from the calculation compared with that of MOF-505<sup>2</sup>.

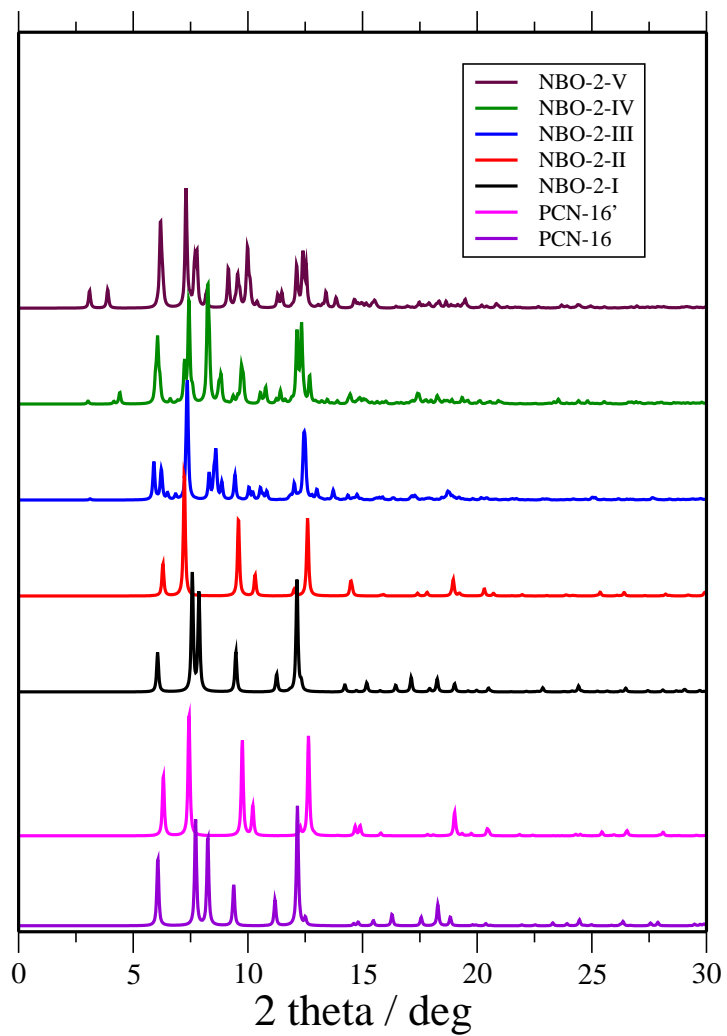


Figure 3: XRPD patterns of the five most stable structures of NBO-2 obtained from the calculation. The patterns of two phases (PCN-16 and PCN-16')<sup>3</sup> from the experiment are shown for comparison.

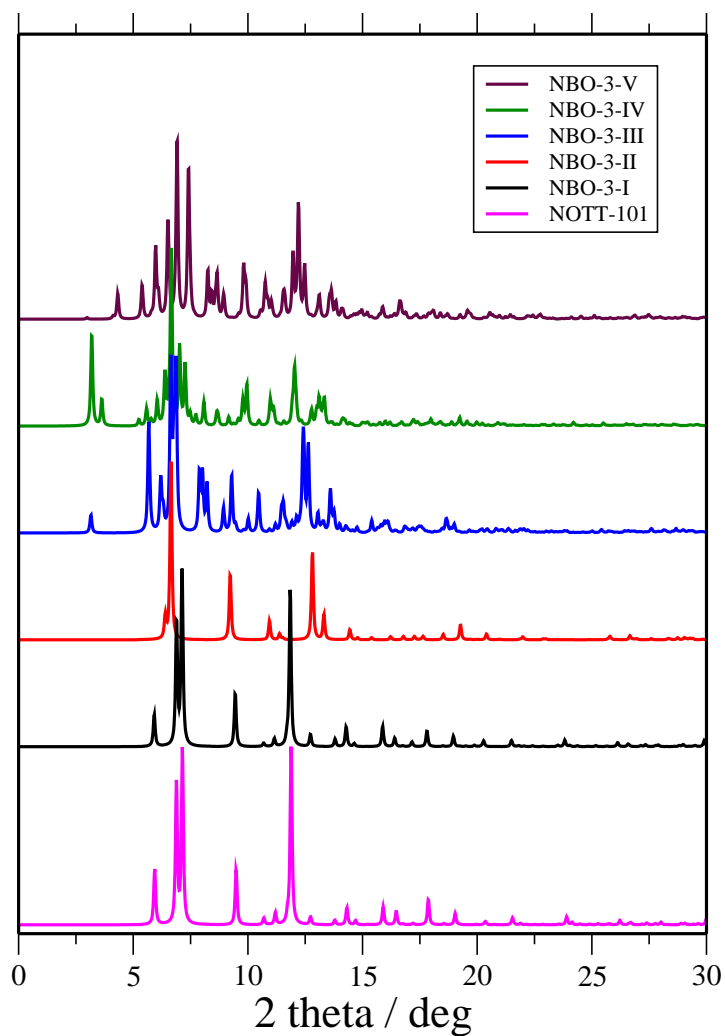


Figure 4: XRPD patterns of the five most stable structures of NBO-3 obtained from the calculation compared with that of NOTT-101<sup>1</sup>.

## References

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