

Supporting Information

Cyclic gas-phase heterogeneous process in a metal-organic framework involving a nickel nitrosyl complex

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FT-IR spectra

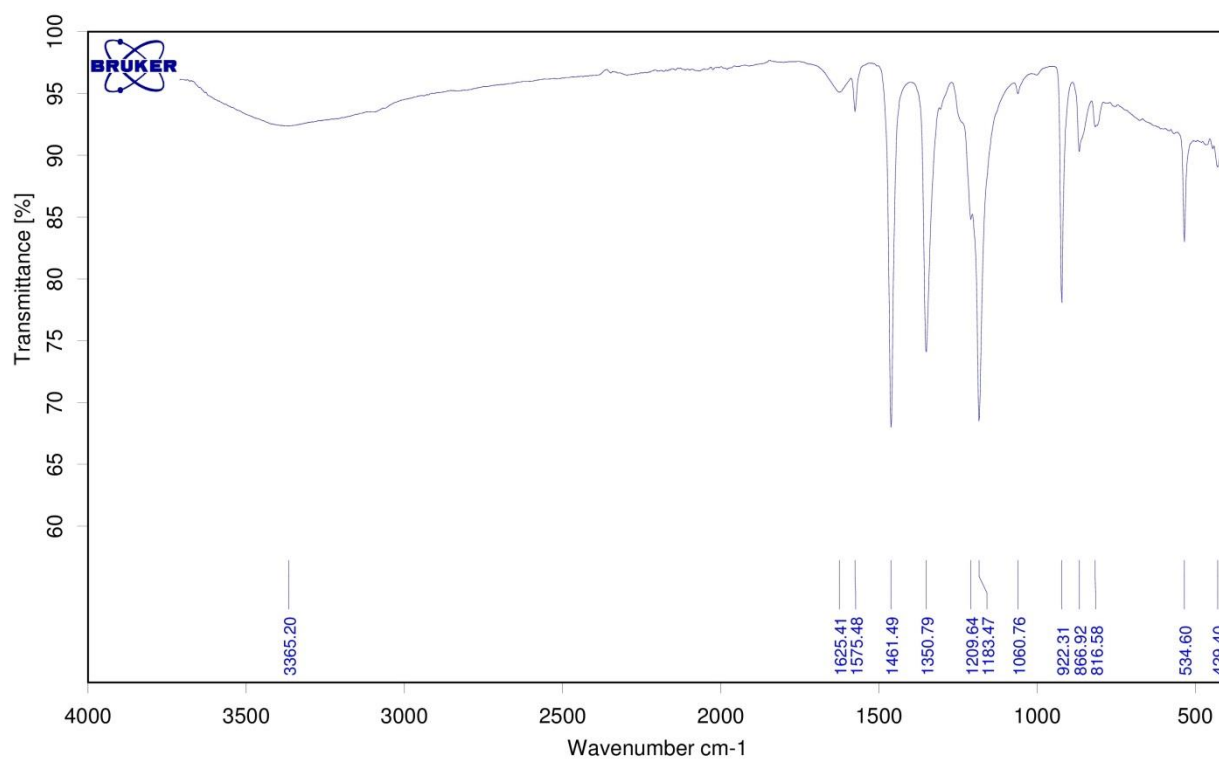


Fig. S1 FT-IR spectrum of Ni-MFU-4/-NO₂.

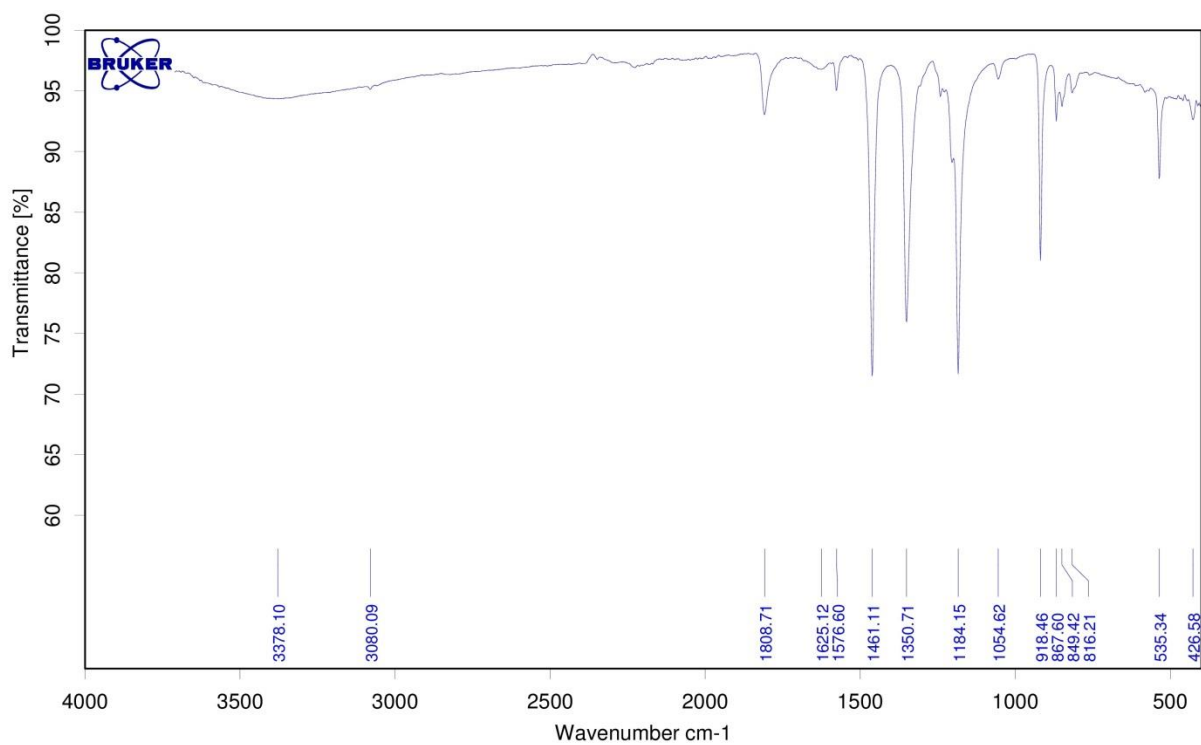


Fig. S2 FT-IR spectrum of Ni-MFU-4/-NO.

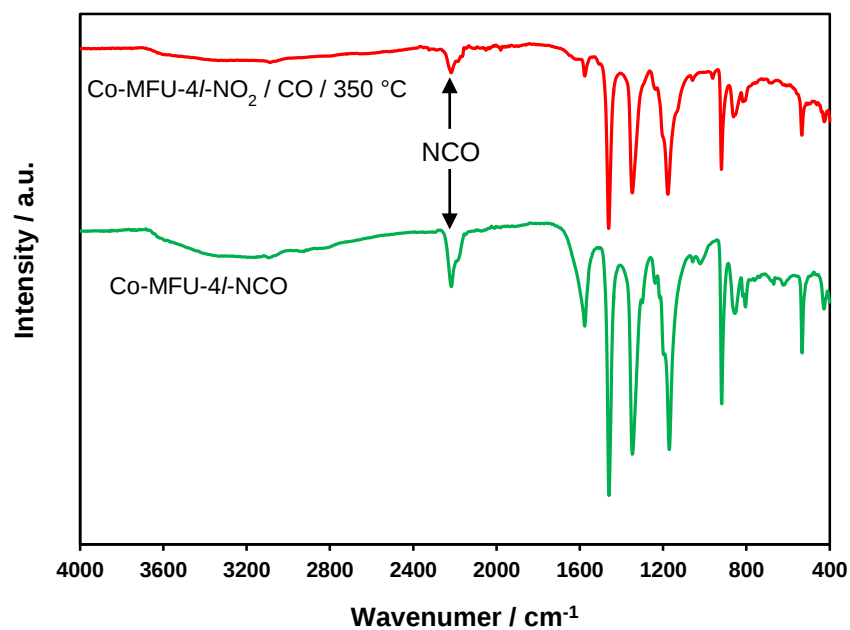


Fig. S3 FT-IR spectra of Co-MFU-4l-NCO (green) and Co-MFU-4l-NO₂ after treatment with CO at 350 °C (red).

DRIFT spectra

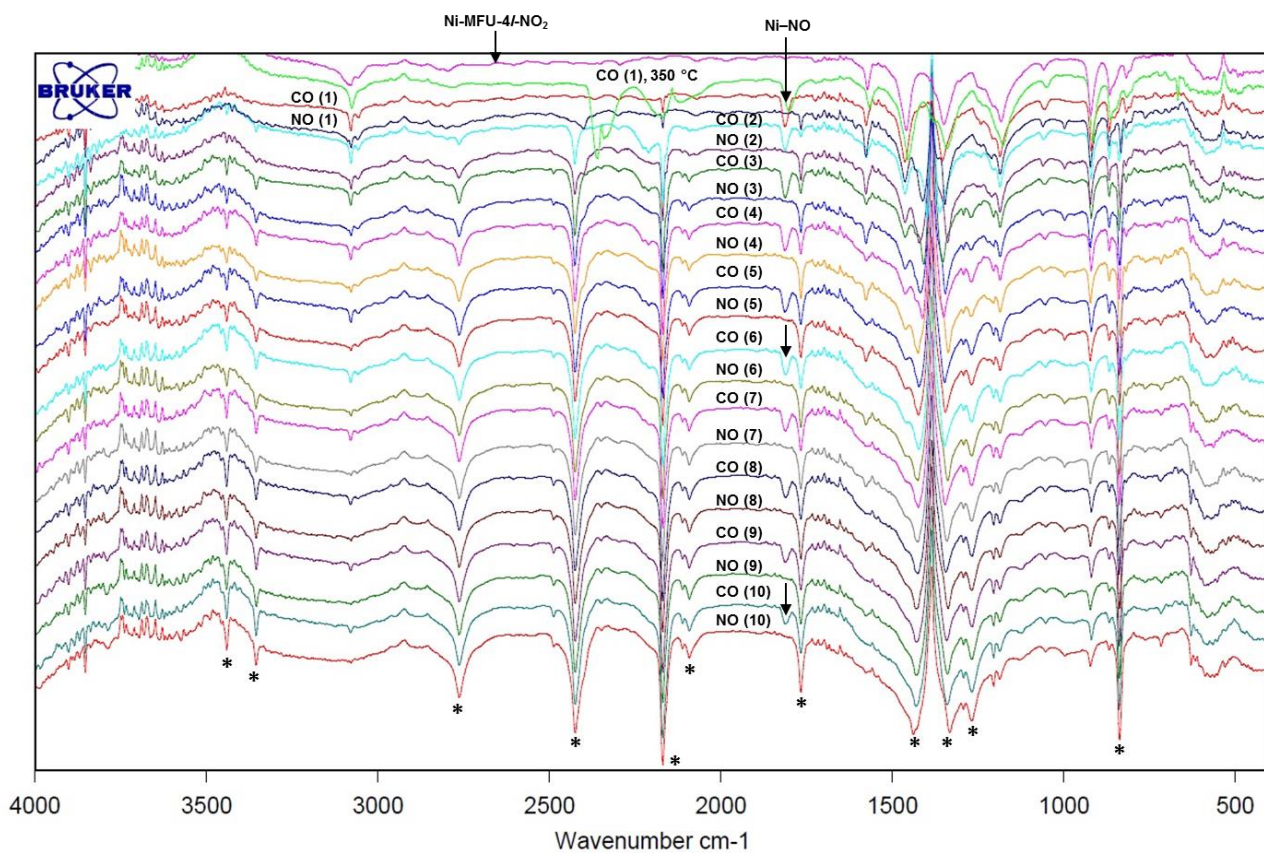


Fig. S4 DRIFT spectra of Ni-MFU-4l-NO₂ after treatment with CO at 350 °C and subsequent treatment with NO at 40 °C (marks over the spectrum indicate a gas and cycle number); * - bands, accumulating due to NO₂ / N₂O₄ impurities.

UV-vis-NIR spectra

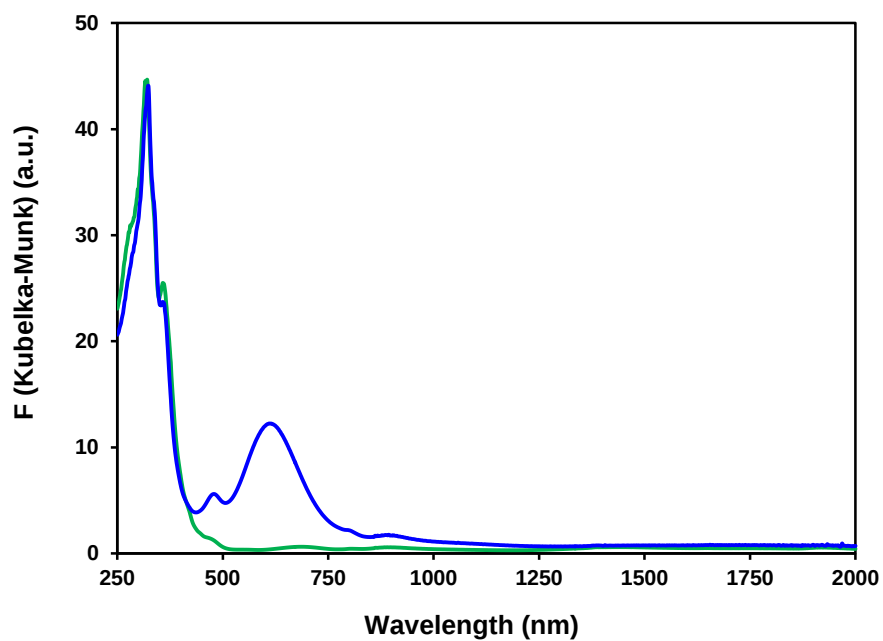


Fig. S5 UV-vis-NIR spectra of Ni-MFU-4l-NO₂ (green) and Ni-MFU-4l-NO (blue).

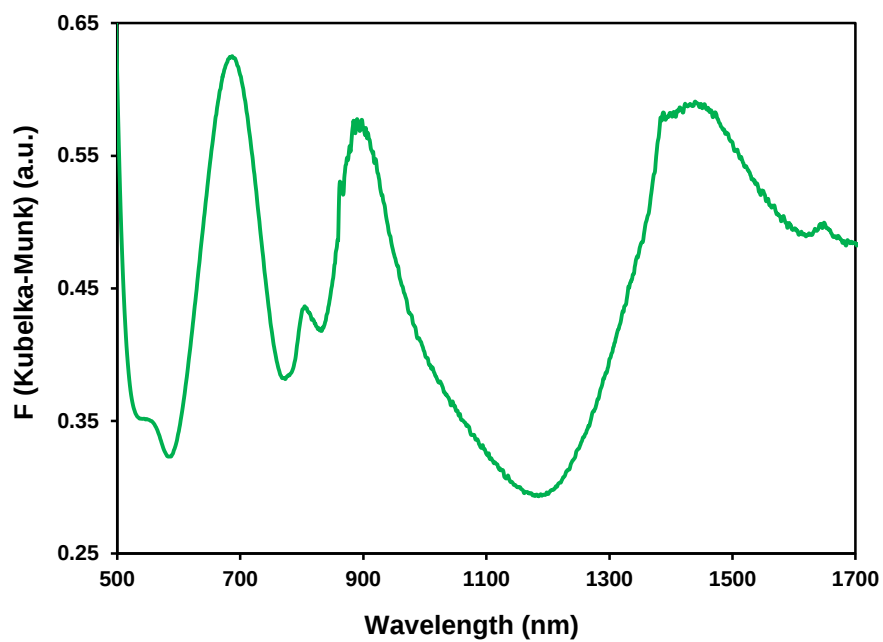


Fig. S6 UV-vis-NIR spectrum of Ni-MFU-4l-NO₂.

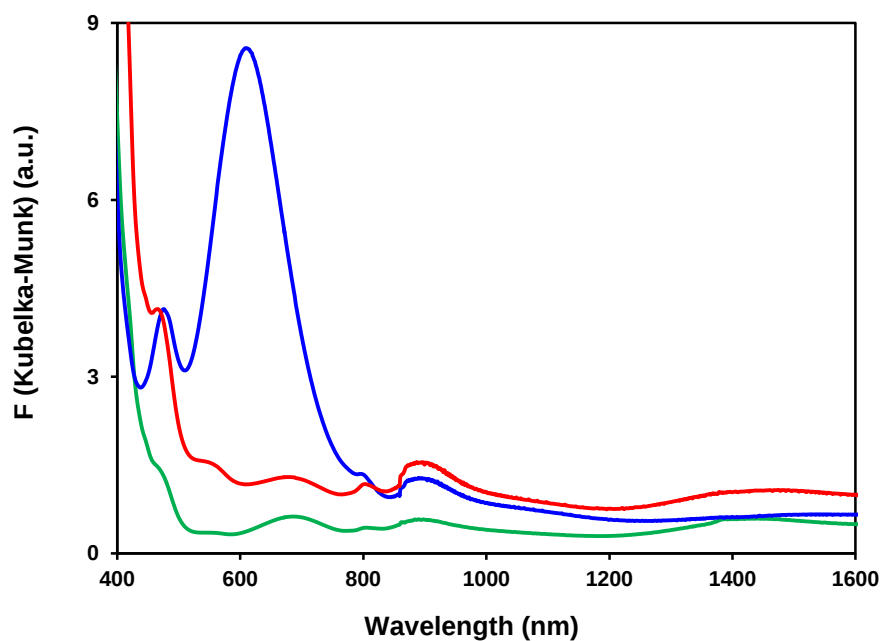


Fig. S7 In situ UV-vis-NIR spectra of Ni-MFU-4l-NO before (blue) and after (red) reaction with 5% NO in Ar; green curve shows a reference spectrum of Ni-MFU-4l-NO₂.

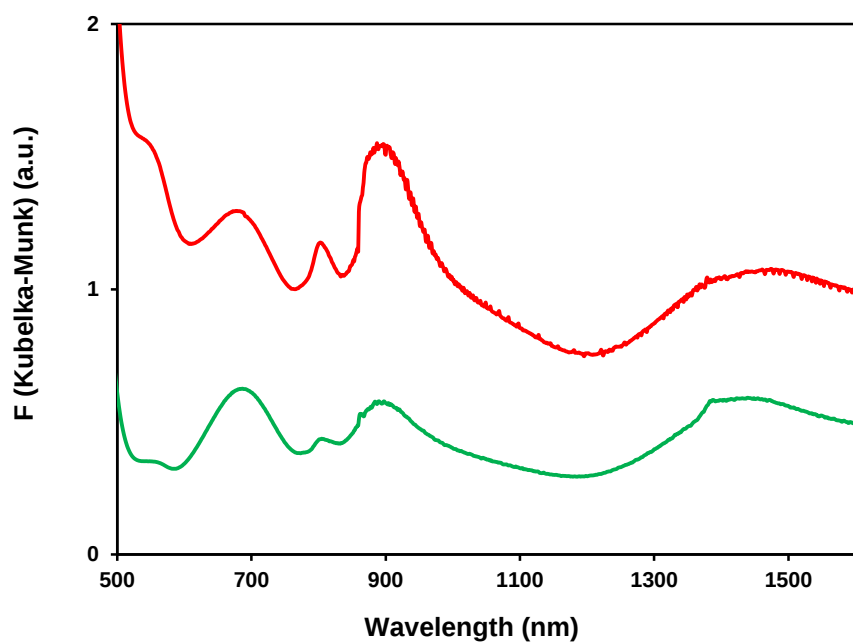


Fig. S8 Zoom of the in situ UV-vis-NIR spectra shown in Fig. S7 (the spectrum of Ni-MFU-4l-NO is not shown).

Powder X-ray diffraction measurements

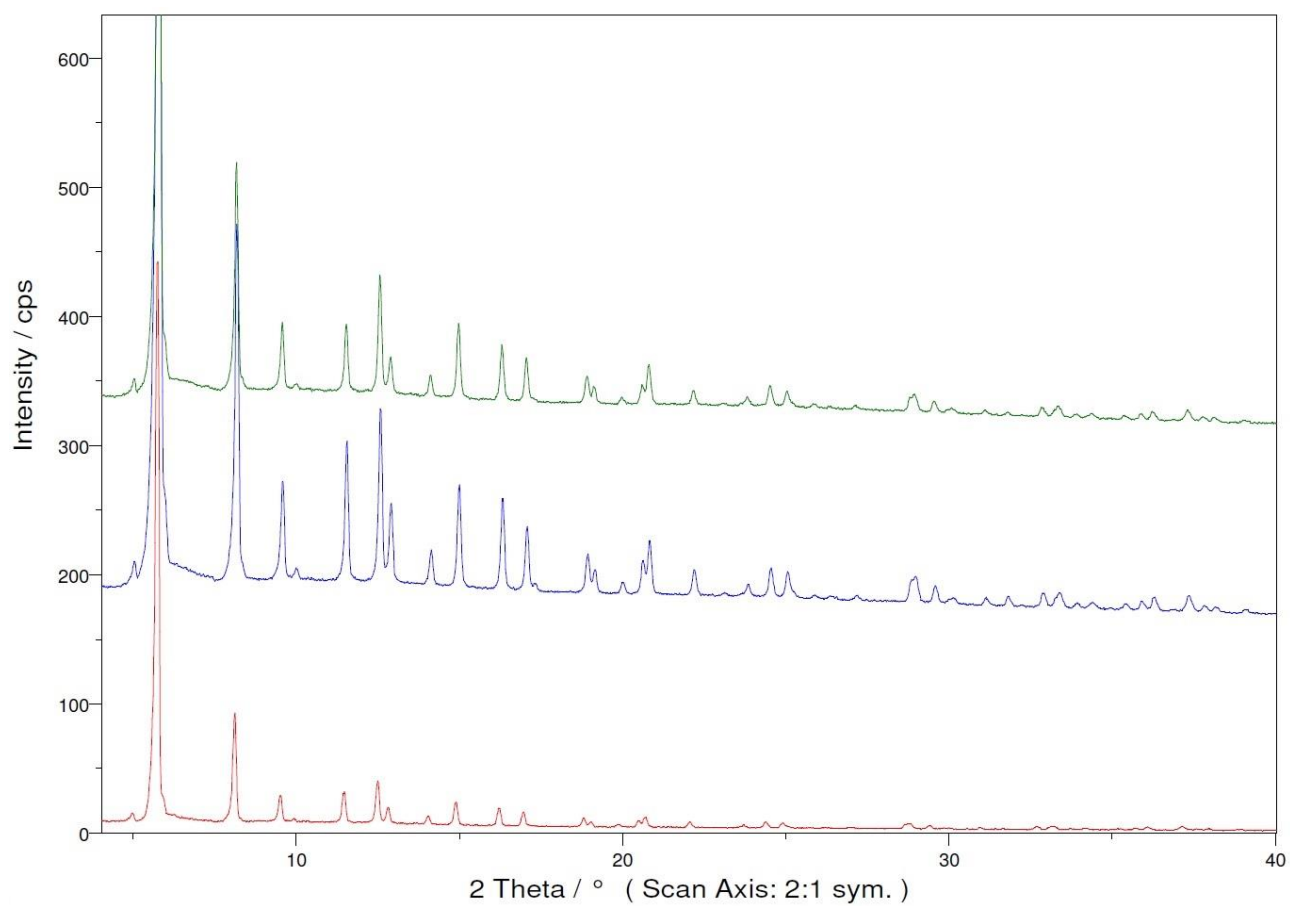


Fig. S9 XRPD patterns of MFU-4l (red), Ni-MFU-4l-NO₂ (green) and Ni-MFU-4l-NO (blue).

Gas sorption measurements

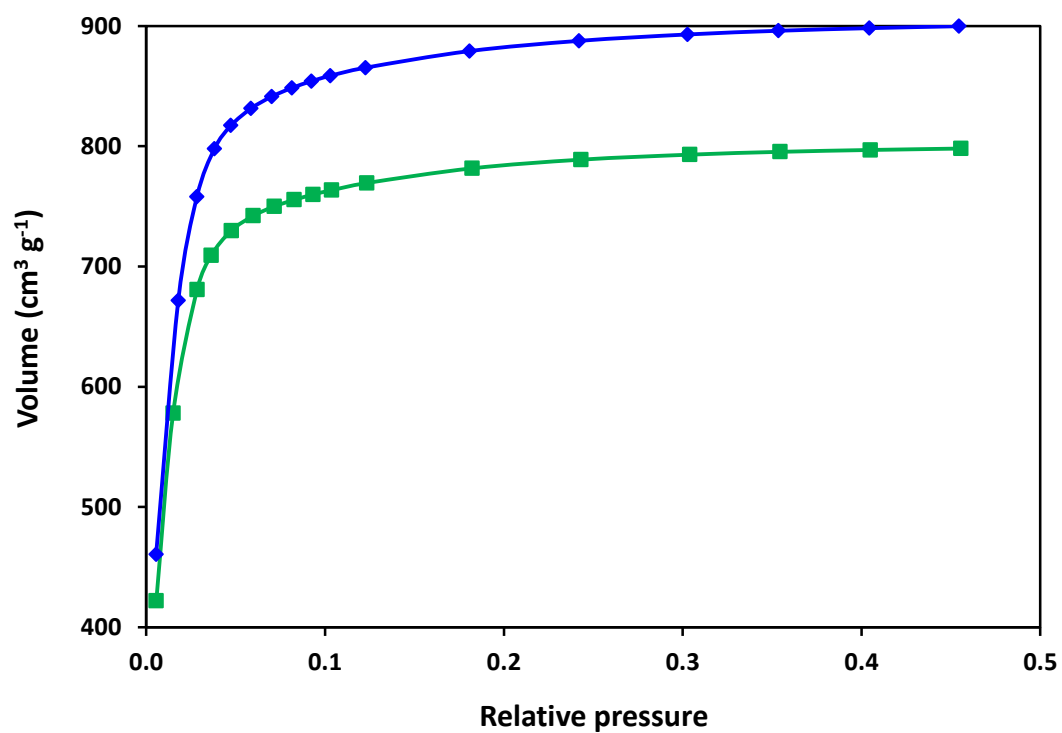


Fig. S10 Nitrogen adsorption isotherms at 77.3 K for Ni-MFU-4l-NO₂ (green) and Ni-MFU-4l-NO (blue).