Low-wavenumber vibrational spectroscopy study of the metal-organic frameworks DUT-8

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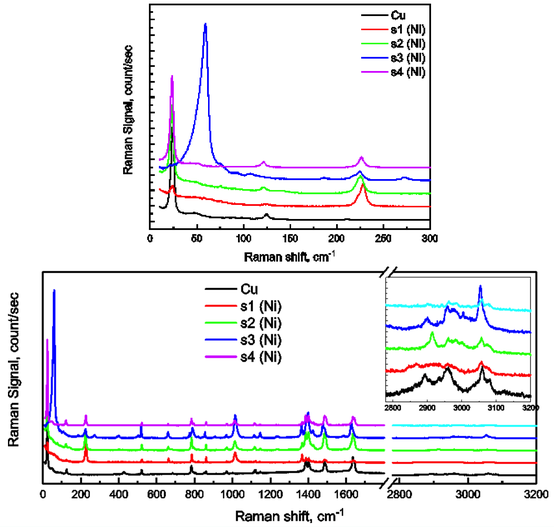
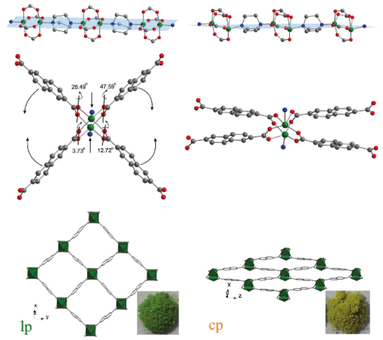
INTRODUCTION

Soft porous crystals are defined as porous solids that possess both a highly ordered network and structural transformability. They are bistable or multistable crystalline materials with long range structural ordering, a reversible transformability between states, and permanent porosity. The term porosity means that at least one crystal phase possesses space that can be occupied by guest molecules. The aim of our investigation is studying possible transitions between open and closed phases in DUT-8 (Ni) with DCM and DMF. The low-frequency Ramanis used as a tool since it has been established recently that in this region of the spectra, the lines characterize the open and closed forms.

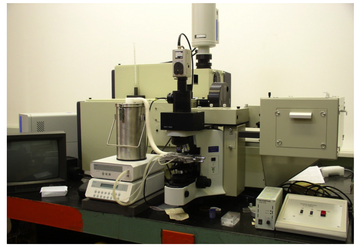
DUT-8(Ni)_flex and DUT-8(Ni)_rigid were synthesized and activated according to a previously published procedure.[1] X-ray powder diffraction patterns were measured to prove the sample's phase purity. The samples are denoted as follows: S1 – as made DUT-8(Ni)_flex; S2 – as made DUT-8(Ni)_rigid; S3 – desolvated DUT-8(Ni)_flex; S4 – desolvated DUT-8(Ni)_rigid.The strongest line around 23 cm^{-1} characteristic for the open structure disappears and a new band at 59.8 cm^{-1} is observed in the spectrum of desolvated DUT-8(Ni). Thus, this characteristic band can unambiguously characterize the state of the system (open/closed). The open system shows the typical line at *ca.* 23 cm^{-1}, the closed system – at *ca.* 60 cm^{-1}.



STRUCTURE



EQUIPMENT

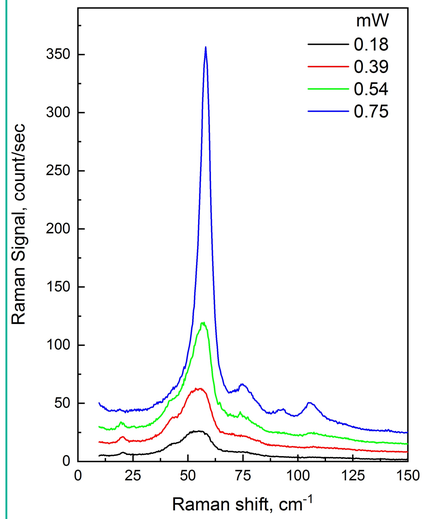


HORIBA Jobin Yvon T64000

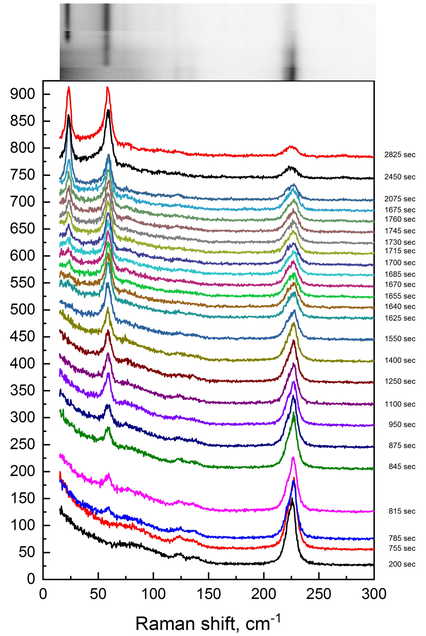
Exitation: Ar+ 514.5 nm
Power: 10 mW on sample
Spectral resolution: 0.3 $см^{-1}$
Scan time: 40 sec
Accumulations: 2 scan
Geometry: Backscattering

DYNAMICAL PROCESSES

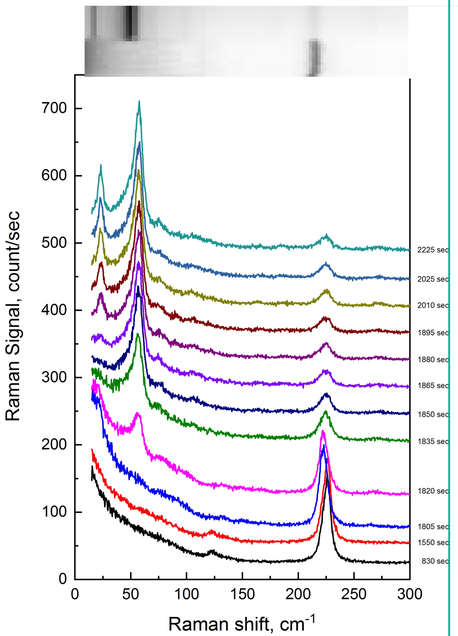
Heating by laser



Evaporation of dichloromethane (DCM)



Evaporation dimethyl formamide (DMF)



The low-wavenumber region is important for the vibrational spectra study and should not be ignored at the planning and carrying out of spectral experiments. The present Raman scattering study on the DUT-8 (Ni) metal– organic framework system shows a significant difference in the low-frequency region for open (23 cm^{-1}) and closed (60 cm^{-1}) pore forms of DUT-8(Ni). The applied technique can be further established for monitoring the phase transitions in flexible MOF materials.