Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Liquid self-diffusion of H_2O and DMF molecules in Co-MOF-74: molecular dynamics simulations and dielectric spectroscopy studies

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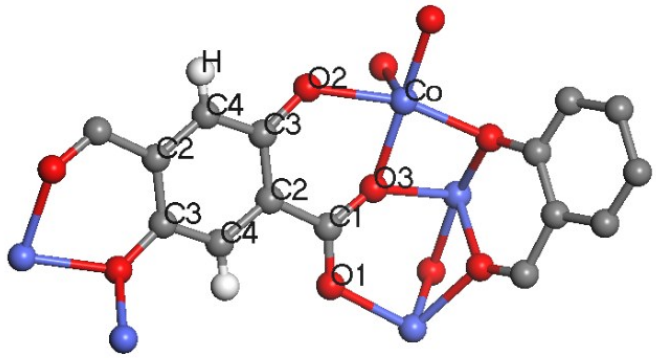

Atom Type	Partial Charge [e-]
Co	1.101
C1	0.817
C2	-0.302
C3	0.376
C4	-0.163
O1	-0.716
O2	-0.643
O3	-0.645
H	0.175

Figure S1. Partial charges of the Co-MOF-74 metal-organic framework used in this work.

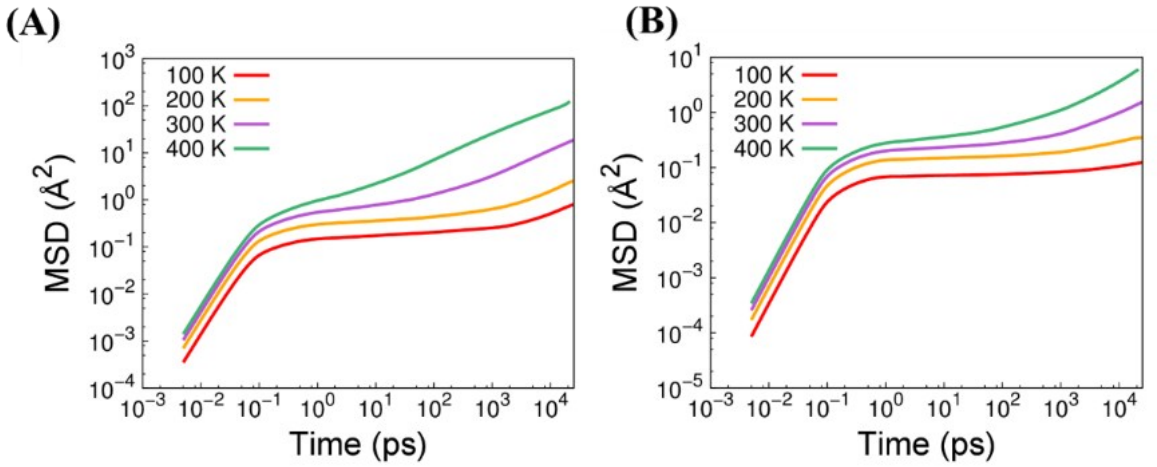

Figure S2. Mean squared displacement versus time of (A) H_2O and (B) DMF for different temperatures as obtained from MD simulations.

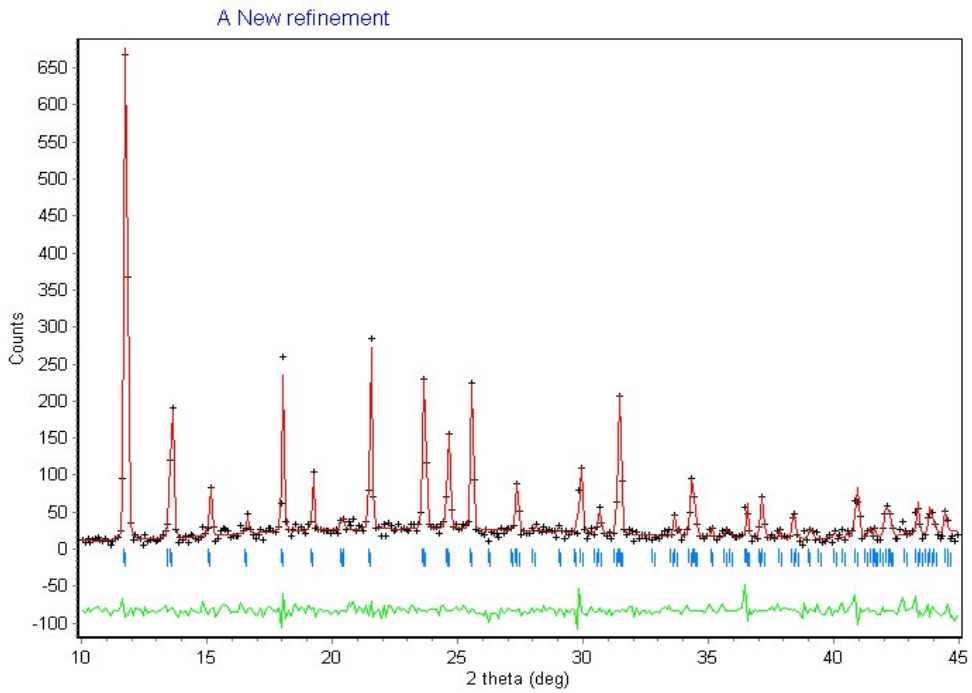

Figure S3. Le Bail refinement of the Co-MOF-74 sample. Key: Observed (black dots), calculated (solid red line) and difference (bottom green line) profiles. The blue tick marks indicate the positions of the allowed Bragg reflections.

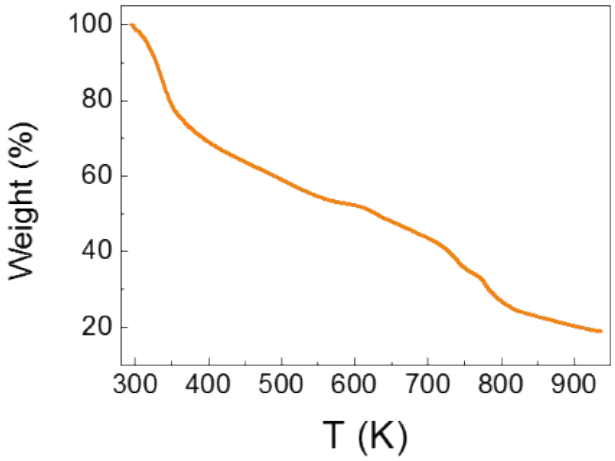

Figure S4. TGA curve of Co-MOF74 (Co_2(dobdc)·[2DMF.1H_2O]).

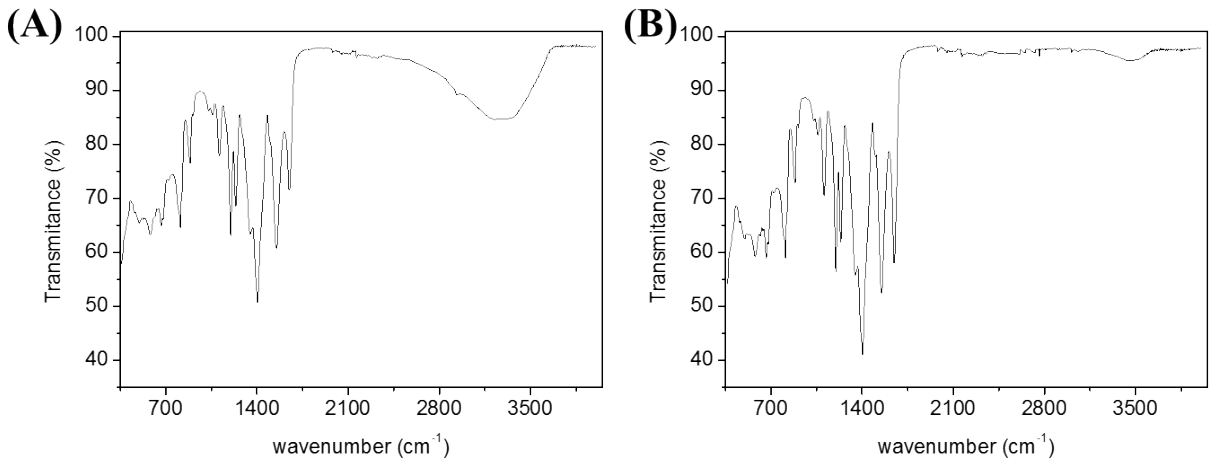

Figure S5. Infrared spectra of (A) Co-MOF-74, (Co_2(dobdc)·[2DMF.1H_2O]), and (B) Co-MOF-74(ev), (Co_2(dobdc)·[0.5DMF]). Band around 3500 cm^{-1} correspond to the presence of water, which is almost negligible for Co-MOF-74(ev).

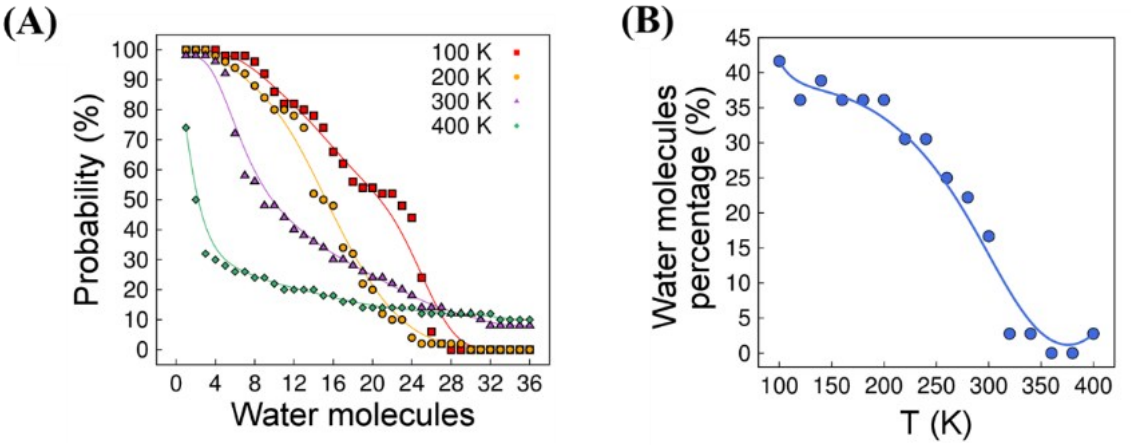

Figure S6. (A) Probability of finding water molecules at CoMOF-O_{H2O} distances less than 4 Å, for several temperatures. (B) Percentage of water molecules with probability P > 70 % of being located at CoMOF-O_{H2O} distance less than 4Å, as obtained from MD simulations. Solid lines are shown as guide for the eyes.

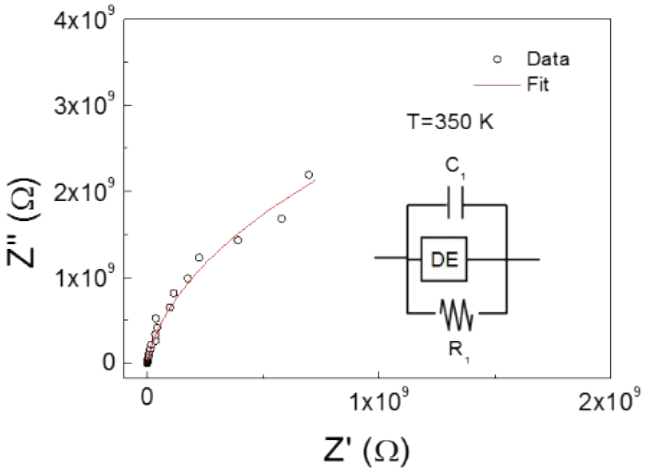

Figure S7. Typical impedance complex plane plot for Co-MOF-74(ev) at 350 K.