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Adsorption of gases in Cu-BTC

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Introduction

New family of microporous adsorbents: Metal Organic Framework (MOF)

- Highly crystalline with 3D structure
- High surface area and pore volume → good for gas adsorption and storage

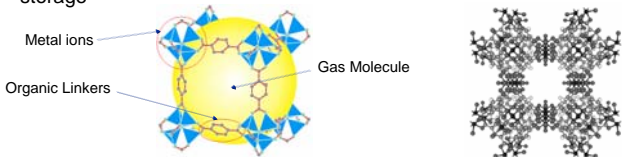


Figure 1. Metal Organic Framework (MOF-5)

Figure 2. Crystal structure of Cu-BTC

- Copper (II) benzene-1,3,5-tricarboxylate (Cu-BTC) has been synthesized
- Some of the Natural Gas components have been selected to conduct adsorption and kinetic measurements: CH₄, CO₂, N₂

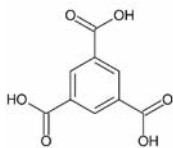


Figure 3. Trimesic acid is an organic linker in Cu-BTC structure

Materials and methods

- **Synthesis:** Cu-BTC synthesized in our laboratory

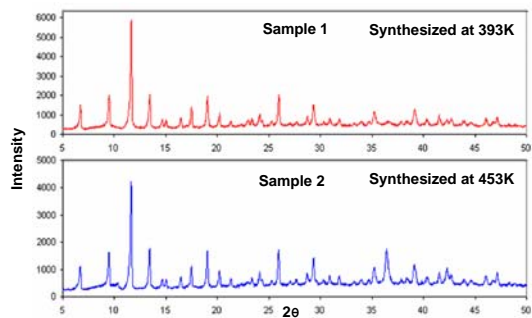
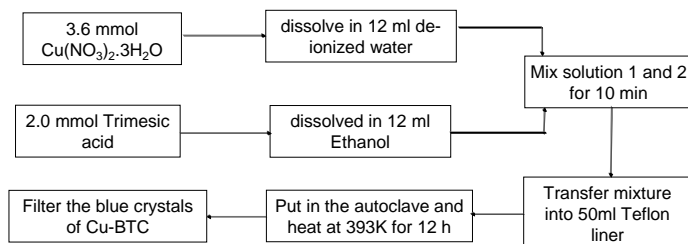


Figure 3. X-ray diffraction (XRD) of Cu-BTC synthesized at two different temperatures

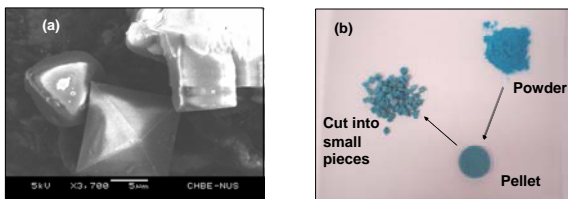


Figure 5. (a) Scanning Electron Microscopy (SEM) of synthesized Cu-BTC and (b) Preparing synthesized powder for adsorption experiments



Figure 6. Experimental Setup (Constant Volume)

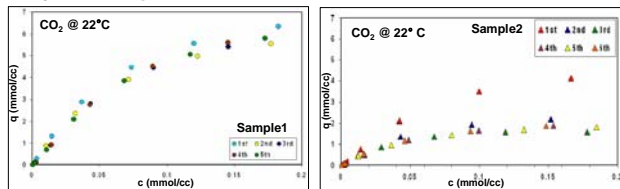
• **Langmuir isotherm:**

$$\frac{q}{q_s} = \frac{bC}{1+bC} \Rightarrow q = \frac{q_s b C}{1+bC} = \frac{Kc}{1+bC}$$

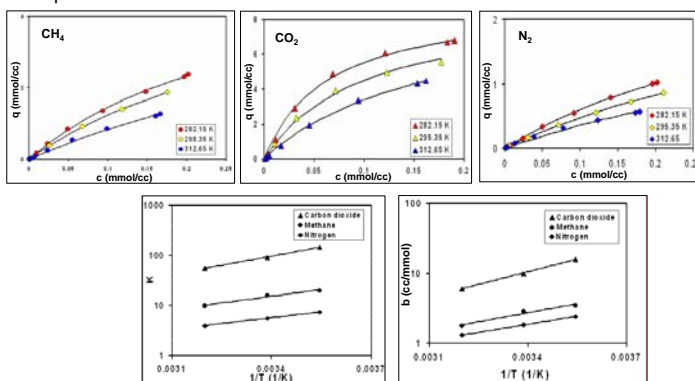
$$b = b_0 e^{-\Delta H_i / R_i T}$$

Results

Stability and sample selection :



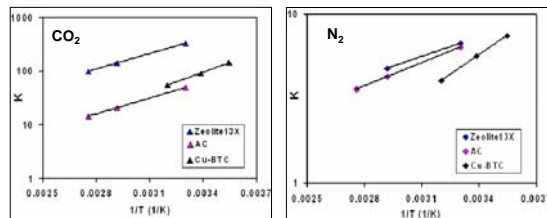
- **Equilibrium measurements:** The Langmuir model fits well to all equilibrium data



• **Comparison of Cu-BTC with AC & Zeolite13X:**

Adsorbent	Adsorbate	q _s	b ₀ (cm ³ /mmol)	-ΔH _i (kJ/mol)	Residual
Activated carbon	Nitrogen	3.17	0.0626	2.09	0.07318
	carbon dioxide	6.17	0.00451	4.51	0.41876
Zeolite 13X	Nitrogen	6.15	0.0574	1.78	0.02935
	carbon dioxide	6.81	0.0333	4.39	3.27684
Cu-BTC	Nitrogen	3.09	4.30E-03	3.66	4.38E-03
	carbon dioxide	9.05	8.00E-04	4.52	3.37E-01
	Methane	5.61	3.20E-03	3.94	9.11E-03

Adsorbent	Temperature	η _{CO₂/N₂}	η _{CO₂/CH₄}
Activated carbon	303	7.77	
	343	4.86	
	363	4.02	
Zeolite 13X	303	49.3	
	343	20.8	
Cu-BTC	282.15	19.25	7.31
	295.35	15.99	5.66
	312.65	13.66	5.52



Conclusions and Future Works:

- ✓ MOFs are promising materials for gas separation and storage
- ✓ Lower temperature synthesis favors better crystallinity
- ✓ Langmuir model fits well to N₂, CH₄ and CO₂ equilibrium data
- ✓ Cu-BTC is good for CO₂/N₂ and CO₂/CH₄ separation

- ➔ Kinetic measurements of mentioned gases on Cu-BTC are in progress
- ➔ H₂S and SO₂ will come to the picture as Natural Gas components in future measurements

References:

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3. H. Dathe, A. Jentsy and J. A. Lercher, "Sulfate formation on SOx trapping materials studied by Cu and S K-edge XAFS", 2005
4. Wong Ian Rhee, "Development of an adsorption based process for CO₂ capture from flue gas", FYP Thesis, 2007