

# CO adsorption on HKUST-1 at RT in drifts-28.07.2023

**Date:** 2023-07-28

**Tags:** HKUST-1 DRIFTS

**Created by:** Shuang Chen

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**Date:** 28.07.2023

**Sample:** HKUST-1 (sample Nr. 22 in the Database)

## **General description of the experiment:**

To evaluate the adsorption bands of CO (1 atm) on HKUST-1 at RT (30 °C)

## **Detailed procedure:**

Preparation: Put the water trap and trap containing active carbon into a oven (425 °C) overnight to remove all water and carbonyls.

### **KBr powders,**

Run a background in an Ar (1 atm, 50 ml/min) atmosphere

Background parameter: 256 scans, 2 cm<sup>-1</sup>

heat 100 °C in Ar for 1 hour and cooled down in Ar to 30 °C

Run a background in an Ar atmosphere to compare the water/solvent content.

At rt switch to CO (1 atm, 200 ml/min), measure CO adsorption as a function of time up to 1 h.

parameter: 8 scans, 2cm<sup>-1</sup>

Switch to Ar, flush out CO.

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## Change sample to HKUST-1,

Run a background in an Ar atmosphere (1 atm, 50 ml/min)

parameter: 256 scans, 2cm<sup>-1</sup>

heat 100 °C in Ar for 1 hour and cooled down in Ar to 30 °C

Run a background in an Ar atmosphere to compare cleanliness of the sample

At rt switch to CO (1 atm, 200 ml/min), measure CO adsorption as a function of time up to 1 h.

parameter: 8 scans, 2cm<sup>-1</sup>

Switch to Ar, flush out CO.

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Clean the sample chamber.

## Settings

### File settings:

Computer: for drift experiment

Folder: D:\data\shuangchen\20230728-HKUST-1

Spectra names: SC0001---

### Opus settings:

Resolution	2
Phase resolution	4
Acquisition Mode	Double Sided, Forward-Backward
Aperture	8mm
Mode	Absorbance

Detector	LN MCT Narrow [Internal Pos.2]
Gain	Automatic
ADC-counts	
Polarization	no
Scanner velocity	40

### **Protocol of the experiment:**

Action/Spectrum	Name	Temperature °C	Time	Comments
Action	Take traps out of the oven and cool down to RT	23	08:53	
Action	Load the KBr into the DRIFTS cell	23	09:00	
Action	Check for leaks using Ar (1 atm/ 50 ml/min)	23	10:18	
Action	test an initial background of KBr in Ar	23	10:45	
Action	test the sample in Ar at 100 °C for 1h (to clean sample)	500	11:45	
Action	Cool down the sample in Ar to 23 °C	23	12:19	
Action	test a background of KBr in Ar (after heating to check cleanliness)	23	12:20	
Action	Run the experiment of CO (1 atm/ 200 ml/min) adsorption for 1 hours at 23 °C	23	12:33	
Action	Switch to Ar flush 10min to remove CO	23	12:40	
Action	Change sample to HKUST-1 and put it into the DRIFTS cell	23	14:19	
Action	test a background of HKUST-1 in Ar (same parameter)	23	14:20	
Action	Heat the HKUST-1 in Ar at 100 °C for 1h	100	15:20	
Action				
Action				
Action				
Action				
Action				


## Results :

## Comments:

## Steps

Put traps into the oven / clean at 425°C over night (2023-07-28 08:46:09)

Load the KBr into the DRIFTS cell (2023-07-28 10:17:12)

Check for leaks using Ar (1 atm/ 50 ml/min) (2023-07-28 10:17:14)

test an initial background of KBr in Ar (2023-07-28 10:56:46)

Heat the sample in Ar at 100 °C for 1h (to clean sample) (2023-07-28 15:01:56)

Cool down the sample in Ar to 30 °C (2023-07-28 15:01:57)

test a background of KBr in Ar (after heating to check cleanliness) (2023-07-28 15:01:58)

Run the experiment of CO (1 atm/ 200 ml/min) adsorption for 1 hours at 30 °C (2023-07-28 15:02:00)

Switch to Ar flush 10min to remove CO (2023-07-28 15:02:02)

Change sample to HKUST-1 and put it into the DRIFTS cell (2023-07-28 15:02:03)

test a background of HKUST-1 in Ar (same parameter) (2023-07-28 15:02:04)

Heat the HKUST-1 in Ar at 100 °C for 1h

Cool down the HKUST-1 in Ar to 30 °C

test a background of HKUST-1 in Ar after heating to check cleanliness

Switch to CO and run the experiment of CO adsorption on HKUST-1 for 1 hours at 30 °C

Flow Ar for 10min to remove CO

Remove sample and clean out DRIFTS cell with water

## Comment

On Alexei Nefedov wrote:

Now it looks absolutely acceptable. We with Eric checked the Entry, you have a permission to carry out all activities corresponding to this experiments.

I added in the sample name line the number of this sample in corresponding Database. Please, let provide this information for all experiments in a future.



Unique eLabID: 20230727-c49b380b6d8e3ba7d4b16eea7f647c66afdbb1a1

Link: <https://ifgselabftw.ifg.kit.edu/experiments.php?mode=view&id=2399>