

Quantachrome TouchWin™

version 1.22

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Report date: Tue Mar 17 2020 **Operator:** pwoodell
Filename: MOF - St2_20200316_143047.qcuPhysIso

Analysis Data

Sample

ID hexane Ioaded edot **Weight** 0.1000g
Description 16MAR20

Analysis

Data ID {4bdf261d-d9a0-496d-a122-0fa11f835f60}
Operator pwoodell **Date** 2020.03.16 **Duration** 299.2min
Instrument St 2 on NOVA touch 2LX [s/n:1050005564] **Firmware** 1.05
Comments
Ambient Temp. 24.32 °C **Void Volume Mode** He Measure **Cold Zone** 2.90922 mL
Warm Zone 3.68063 mL **Cell Type** 9mm with rod **Thermal Delay** 120 sec
Po Mode Continuous

Adsorbate

Name Nitrogen **Molecular Weight** 28.013 g/mol **Cross Section Area** 16.2 Å²/mol
Non-ideality 6.580000e-05 1/torr **Bath Temperature** 77.35 K

Degas information

Type Vacuum Degassing
Operator pw
Description
Heating Heat to 120.0 °C at 10.0 °C/min then hold for 180 min

Data Reduction Parameters

Data Reduction Parameters

Thermal Transpiration no

DFT Method

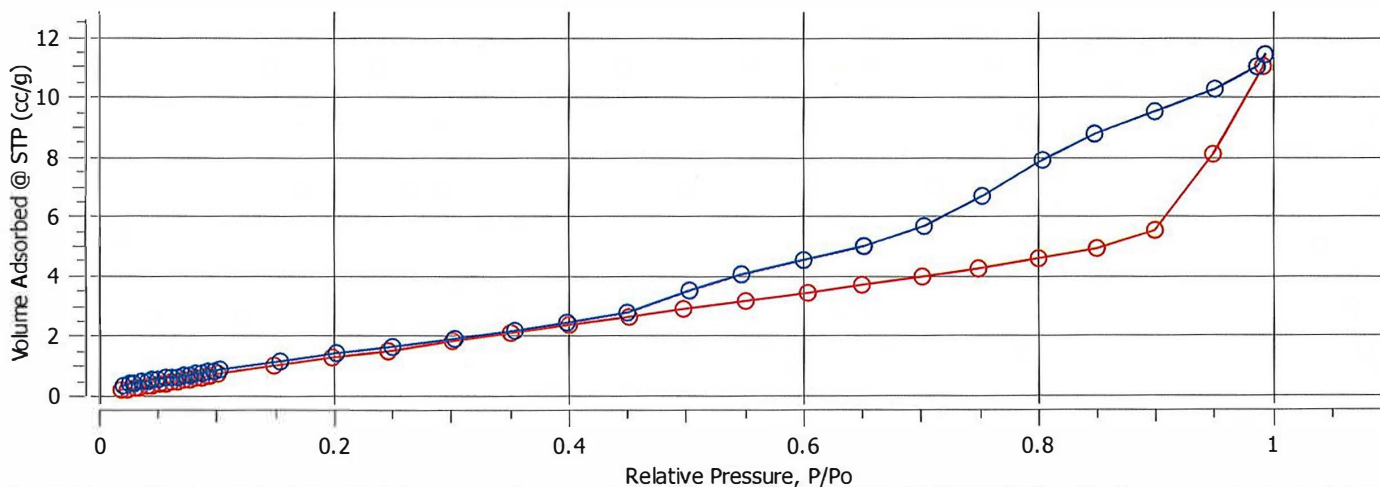
Model N2 @ 77K on silica (cyl./spher. pore)(NLDFT Ads. model)
Min P/Po 0.02 **Max P/Po** 0.99 **Moving pt. avg.** off

Adsorbate Model

Name Nitrogen **Molecular Weight** 28.0134 g **Cross Section Area** 16.2 Å²/molec
Bath Temperature 77.35 K

Isotherm-Isotherm

○ Ads ○ Des



Isotherm Branch Adsorption
Correlation coeff., r 0.990647

Multipoint BET Summary/Results

Slope 471.708
C constant 6.85749

Intercept 80.5308
Surface area 6.306 m²/g

Pore Volume Mode (Pore Width) 0.0098 cc/g
4.7280 nm

DFT method Summary/Results

Surface Area 5.1648 m²/g
Fitting Error 8.1801 %

Lower Confidence Limit 1.7800 nm
Notes Adsorption data

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Report date: Mon Mar 16 2020 **Operator:** pwoodell
Filename: MOF - St2_20200316_073537.qcuPhysIso

Analysis Data

Sample

ID hexane loaded meo **Weight** 0.0510g
Description 16MAR20

Analysis

Data ID {f4df2dac-0488-4d2b-89f6-a641fc8167b7}
Operator pwoodell **Date** 2020.03.16 **Duration** 367.7 min
Instrument St 2 on NOVA touch 2LX [s/n:1050005564] **Firmware** 1.05
Comments
Ambient Temp. 25.83 °C **Void Volume Mode** He Measure **Cold Zone** 3.01097 mL
Warm Zone 3.76154 mL **Cell Type** 9mm with rod **Thermal Delay** 120 sec
Po Mode Continuous

Adsorbate

Name Nitrogen **Molecular Weight** 28.013g/mol **Cross Section Area** 16.2 Å²/mol
Non-ideality 6.580000e-05 1/torr **Bath Temperature** 77.35 K

Degas information

Type Vacuum Degassing
Operator pw
Description
Heating Heat to 120.0 °C at 10.0 °C/min then hold for 180 min

Data Reduction Parameters

Data Reduction Parameters

Thermal Transpiration no

DFT Method

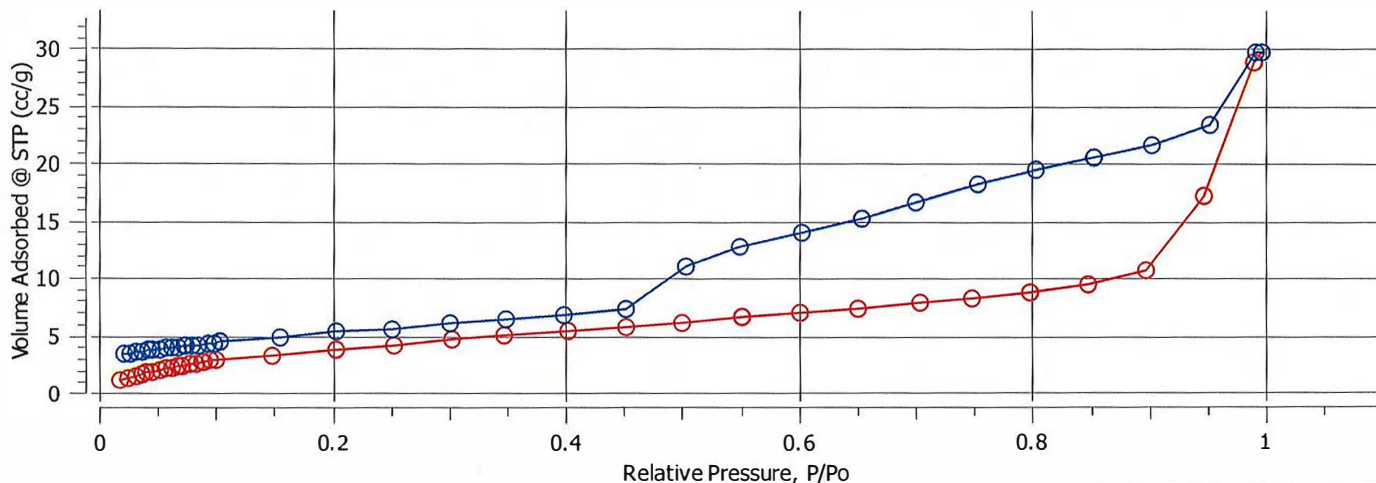
Model N2 @ 77K on silica (cyl./spher. pore)(NLDFT Ads. model)
Min P/Po 0.02 **Max P/Po** 0.99 **Moving pt. avg.** off

Adsorbate Model

Name Nitrogen **Molecular Weight** 28.0134g **Cross Section Area** 16.2 Å²/molec
Bath Temperature 77.35 K

Isotherm-Isotherm

○ Ads ○ Des



Multipoint BET Summary/Results

Isotherm Branch Adsorption
Correlation coeff., r 0.99765

Slope 205.954
C constant 22.6179

Intercept 9.52697
Surface area 16.162 m²/g

DFT method Summary/Results

Pore Volume Mode (Pore Width) 0.0207 cc/g
 3.7750 nm

Surface Area 11.5001 m²/g
Fitting Error 2.9843%

Lower Confidence Limit 1.7800 nm
Notes Adsorption data

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Report date: Mon Mar 16 2020 **Operator:** pwoodell
Filename: MOF - St1_20200316_073537.qcuPhysIso

Analysis Data

Sample

ID hexane loaded hexo **Weight** 0.0490g
Description 16MAR20

Analysis

Data ID	{6e0c98e9-48d0-4dfd-b25c-acc029747f19}			Duration	376.2min
Operator	pwoodell	Date	2020.03.16	Firmware	1.05
Instrument	St 1 on NOVA touch 2LX [s/n:1050005564]			Cold Zone	2.97974mL
Comments		Void Volume Mode	He Measure	Thermal Delay	120sec
Ambient Temp.	25.80°C	Cell Type	9mm with rod		
Warm Zone	3.63928mL				
Po Mode	Continuous				

Adsorbate

Name Nitrogen **Molecular Weight** 28.013g/mol **Cross Section Area** 16.2Å²/mol
Non-ideality 6.580000e-05 1/torr **Bath Temperature** 77.35K

Degas information

Type Vacuum Degassing
Operator pw
Description
Heating Heat to 120.0 °C at 10.0 °C/min then hold for 180 min

Data Reduction Parameters

Data Reduction Parameters

Thermal Transpiration no

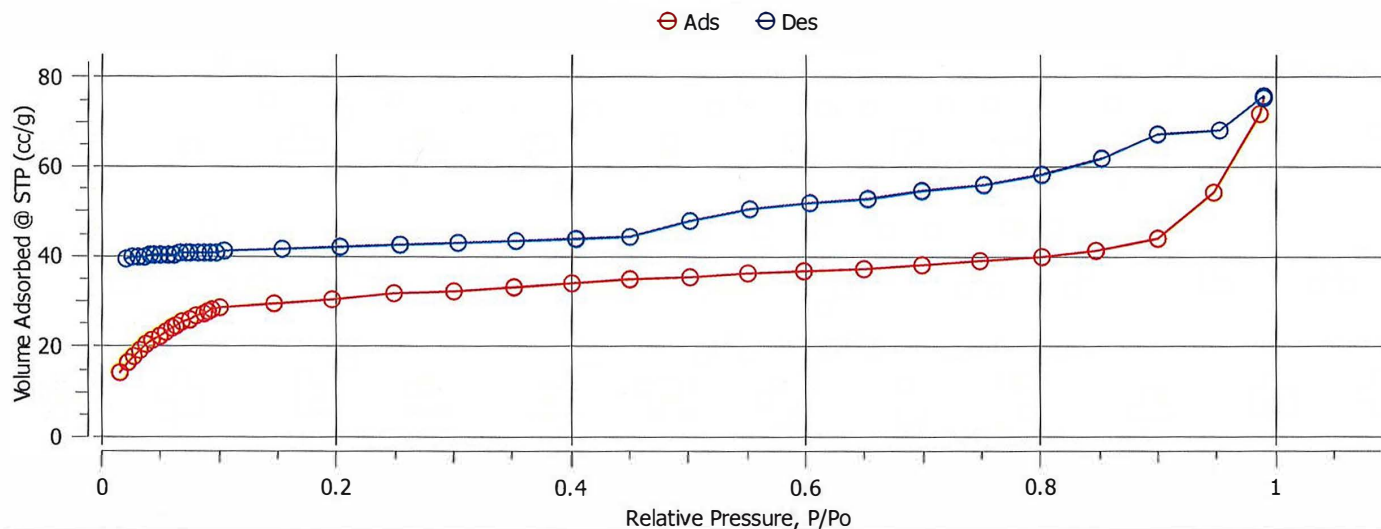
DFT Method

Model N2 @ 77K on silica (cyl. pore)(NLDFT Ads. model)
Min P/Po 0.02 **Max P/Po** 0.99 **Moving pt. avg.** off

Adsorbate Model

Name Nitrogen **Molecular Weight** 28.0134g **Cross Section Area** 16.2Å²/molec
Bath Temperature 77.35K

Isotherm-Isotherm



Multipoint BET Summary/Results

Isotherm Branch	Adsorption	Slope	25.788	Intercept	0.539313
Correlation coeff, r	0.999326	C constant	48.8164	Surface area	132.278 m ² /g

DFT method Summary/Results

Pore Volume Mode (Pore Width)	0.1051 cc/g 2.1860 nm	Surface Area	87.4229 m ² /g	Lower Confidence Limit	1.6310 nm
		Fitting Error	0.4540%	Notes	Adsorption data

1st Run

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Report date: Tue Mar 24 2020 **Operator:** pwoodell
Filename: Neat MEO.qcuPhysIso

Analysis Data

Sample
ID neat meo **Weight** 0.0390g
Description

Analysis
Data ID {94318505-bc7d-42f6-8c7a-d0edabcfb2b9}
Operator pwoodell **Date** 2020.03.23
Instrument St 2 on NOVA touch 2LX [s/n:1050005564] **Duration** 312.5min
Comments **Firmware** 1.05
Ambient Temp. 24.53°C **Void Volume Mode** He Measure **Cold Zone** 2.86585mL
Warm Zone 3.73686mL **Cell Type** 9mm with rod **Thermal Delay** 120sec
Po Mode Continuous

Adsorbate
Name Nitrogen **Molecular Weight** 28.013g/mol **Cross Section Area** 16.2Å²/mol
Non-ideality 6.580000e-05_{1/torr} **Bath Temperature** 77.35K

Degas information
Type Vacuum Degassing
Operator pw
Description
Heating Heat to 120.0 °C at 10.0 °C/min then hold for 180 min
Heat to 200.0 °C at 10.0 °C/min then hold for 1440 min

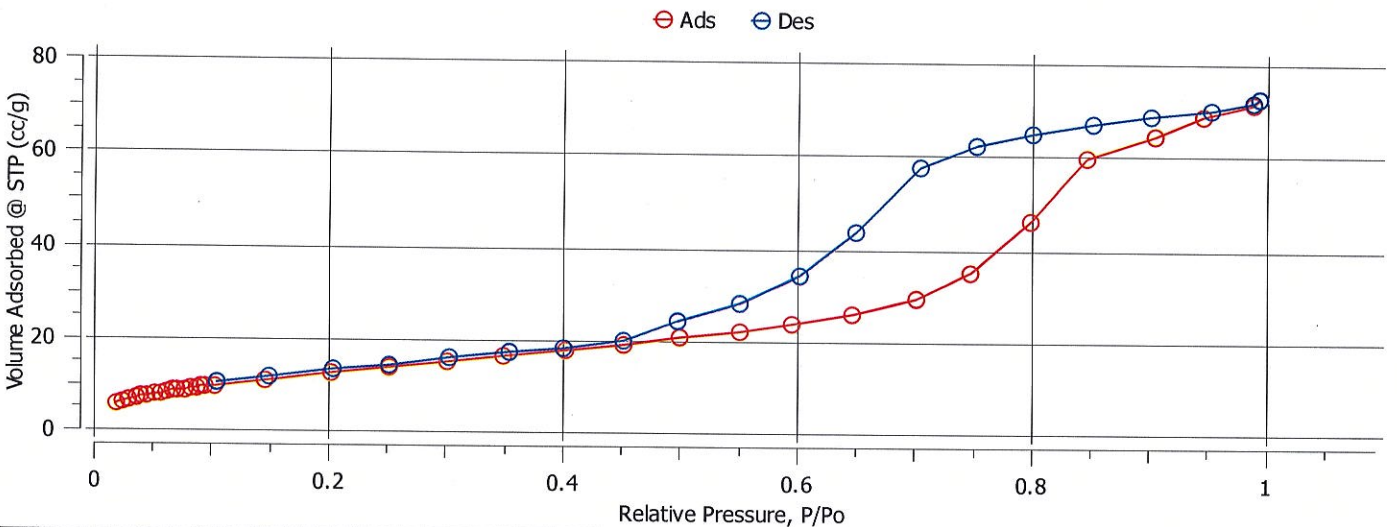
Data Reduction Parameters

Data Reduction Parameters
Thermal Transpiration no

DFT Method
Model N2 @ 77K on silica (cyl./spher. pore)(NLDFT Ads. model)
Min P/Po 0.02 **Max P/Po** 0.99 **Moving pt. avg.** off

Adsorbate Model
Name Nitrogen **Molecular Weight** 28.0134g **Cross Section Area** 16.2Å²/molec
Bath Temperature 77.35K

Isotherm-Isotherm



Multipoint BET Summary/Results

Isotherm Branch Adsorption
Correlation coeff., r 0.99917

Slope 79.0974
C constant 56.9659

Intercept 1.41331
Surface area 43.255 m²/g

DFT method Summary/Results

Pore Volume 0.0992 cc/g
Mode (Pore Width) 12.9910 nm

Surface Area 45.6429 m²/g
Fitting Error 2.6771%

Lower Confidence Limit 1.7800 nm
Notes Adsorption data

1st Run

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Report date: Tue Mar 24 2020 **Operator:** pwoodell
Filename: Neat HEXO.qcuPhysIso

Sample Analysis Data

Sample ID: neat hexo **Weight:** 0.0380g

Analysis Data ID: {451720cf-ee93-43f1-aa07-95b747dc6697}
Operator: pwoodell **Date:** 2020.03.23
Instrument Comments: St 1 on NOVA touch 2LX [s/n:1050005564] **Duration:** 325.3min
Firmware: 1.05

Ambient Temp.: 24.08°C **Void Volume Mode:** He Measure **Cold Zone:** 2.95379mL
Warm Zone: 3.67985mL **Cell Type:** 9mm with rod **Thermal Delay:** 120sec
Po Mode: Continuous

Adsorbate Name: Nitrogen **Molecular Weight:** 28.013g/mol **Cross Section Area:** 16.2Å²/mol
Non-ideality: 6.580000e-05 1/torr **Bath Temperature:** 77.35K

Degas information Type: Vacuum Degassing
Operator: pw
Description: Heat to 120.0 °C at 10.0 °C/min then hold for 180 min
Heat to 200.0 °C at 10.0 °C/min then hold for 1440 min

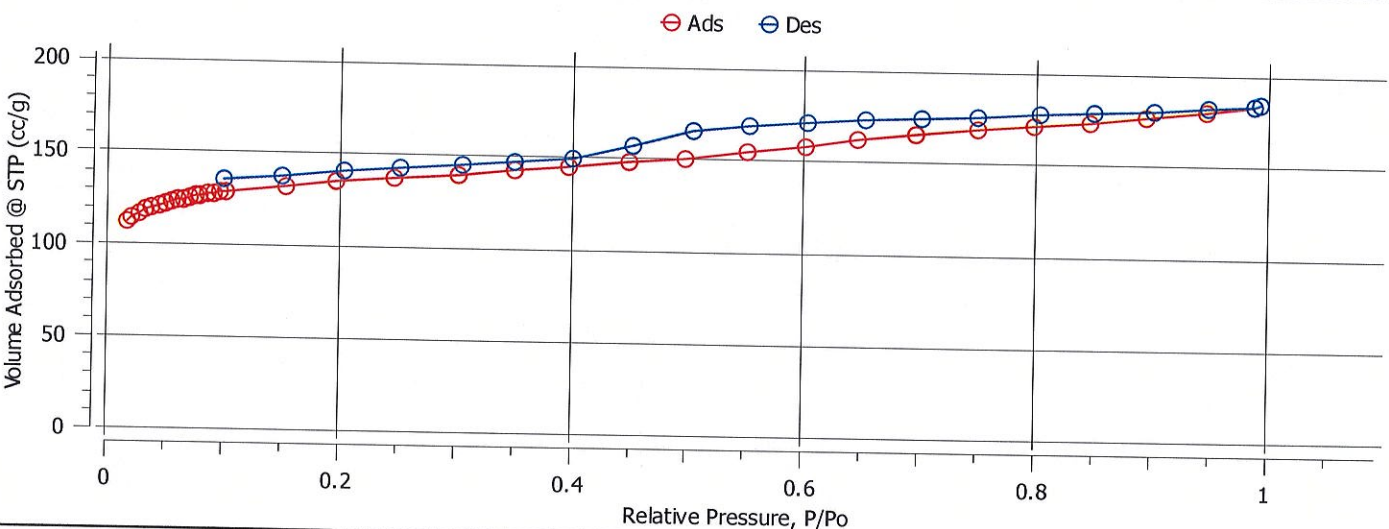
Data Reduction Parameters

Thermal Transpiration: no

DFT Method Model: N2 @ 77K on silica (cyl. pore)(NLDFT Ads. model)
Min P/Po: 0.02 **Max P/Po:** 0.99 **Moving pt. avg.:** off

Adsorbate Model Name: Nitrogen **Molecular Weight:** 28.0134g **Cross Section Area:** 16.2Å²/molec
Bath Temperature: 77.35K

Isotherm-Isotherm



Isotherm Branch: Adsorption
Correlation coeff., r: 0.999956

Multipoint BET Summary/Results
Slope: 6.8271 **Intercept:** 0.00454176
C constant: 1504.18 **Surface area:** 509.763 m²/g

DFT method Summary/Results
Pore Volume Mode (Pore Width): 0.2730cc/g 1.6310nm
Surface Area: 684.4108m²/g **Lower Confidence Limit:** 1.6310nm
Fitting Error: 0.0861% **Notes:** Adsorption data



GAS PHYSISORPTION ISOTHERM DEGASSING CONDITIONS

SAMPLE ID	EXTERNAL DEGASSING CONDITIONS			IN-SITU VACUUM DEGASSING CONDITIONS	
	DURATION	TEMPERATURE	TECHNIQUE	DURATION	TEMPERATURE
HKUST-1 MOF					
HK	2 Hours	150°C	Vacuum	60 Minutes	150°C

GAS PHYSISORPTION ISOTHERM DATA SUMMARY

SAMPLE ID	BET SPECIFIC SURFACE AREA (m ² /g)	BJH PORE VOLUME 1.7 – 300 nm (cm ³ /g)	BJH AVG PORE DIAMETER 1.7 – 300 nm (nm)	ADSORBATE GAS
HKUST-1 MOF				
HK	1993.08	0.13	3.62	Nitrogen

GAS PHYSISORPTION ISOTHERM DATA SUMMARY (continued)

SAMPLE ID	DFT PORE VOLUME		DFT PORE AREA	
	TOTAL VOLUME (cm ³ /g)	PORE SIZE RANGE (nm)	TOTAL AREA (m ² /g)	PORE SIZE RANGE (nm)
HKUST-1 MOF				
HK	0.70	≤ 172.079	2135.53	≥ 0.393

*JF 2010.06.09
CL 2011.06.09*



Particle Technology Labs

UNIVERSITY OF SOUTH CAROLINA AIKEN

3Flex 5.02

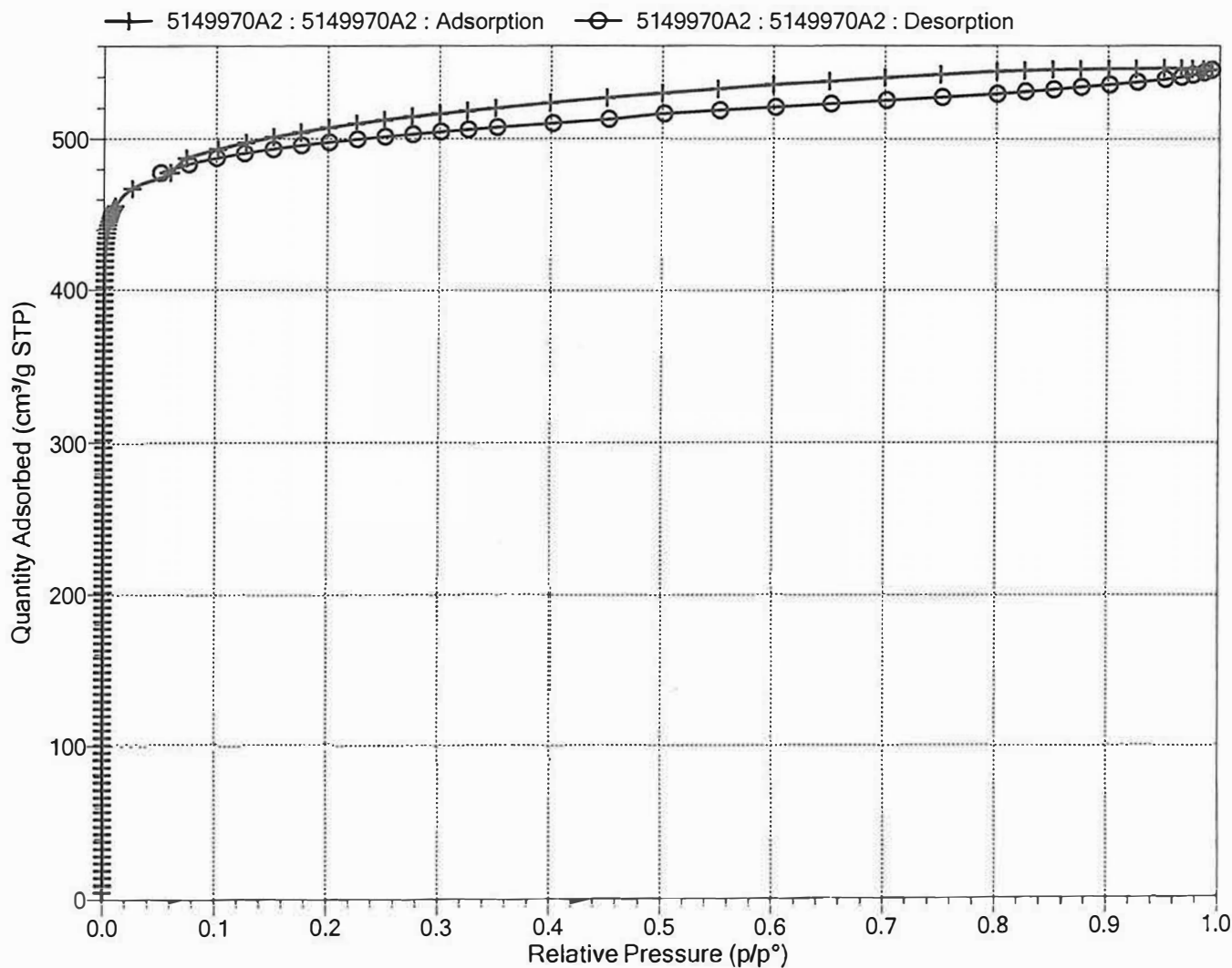
3Flex Version 5.02
Serial # 862 Unit 1 Port 1

Sample: 5149970A2
Operator: JF
Submitter: Particle Technology Labs
File: C:\3Flex\data\51499-70\5149970A2.SMP

Started: 6/7/2021 1:28:13 PM	Analysis adsorptive: N2
Completed: 6/9/2021 3:38:58 PM	Analysis bath temp.: 77.206 K
Report time: 6/9/2021 3:52:46 PM	Thermal correction: No
Sample mass: 0.0316 g	Ambient free space: 20.9316 cm ³ Measured
Analysis free space: 63.6329 cm ³	Equilibration interval: 20 to 30 s
Low pressure dose: 5.0000 cm ³ /g STP	Sample density: 1.000 g/cm ³
Automatic degas: No	

Comments: HKUST-1 MOF HK PTL Project#51499-70 PTL ID: 486157-70

Isotherm Linear Plot





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3Flex 5.02

3Flex Version 5.02
Serial # 862 Unit 1 Port 1

20210609

Sample: 5149970A2
Operator: JF
Submitter: Particle Technology Labs
File: C:\3Flex\data\51499-70\5149970A2.SMP

Started: 6/7/2021 1:28:13 PM	Analysis adsorptive: N2
Completed: 6/9/2021 3:38:58 PM	Analysis bath temp.: 77.206 K
Report time: 6/9/2021 3:52:46 PM	Thermal correction: No
Sample mass: 0.0316 g	Ambient free space: 20.9316 cm ³ Measured
Analysis free space: 63.6329 cm ³	Equilibration interval: 20 to 30 s
Low pressure dose: 5.0000 cm ³ /g STP	Sample density: 1.000 g/cm ³
Automatic degas: No	

Comments: HKUST-1 MOF HK PTL Project#51499-70 PTL ID: 486157-70

BET Report

BET surface area: 1,993.0809 ± 1.3464 m²/g
Slope: 0.002184 ± 0.000001 g/cm³ STP
Y-intercept: 0.000000 ± 0.000000 g/cm³ STP
C: 7,537.777322
Qm: 457.9081 cm³/g STP
Correlation coefficient: 0.9999979
Molecular cross-sectional area: 0.1620 nm²

Relative Pressure (p/p°)	Quantity Adsorbed (cm ³ /g STP)	1/[Q(p°/p - 1)]
0.002256651	438.0128	0.000005
0.002819007	440.8257	0.000006
0.003462227	443.3873	0.000008
0.004176871	445.6883	0.000009
0.004950738	447.7374	0.000011
0.005788288	449.6296	0.000013
0.006679110	451.3510	0.000015
0.007624450	452.9148	0.000017
0.008585101	454.3199	0.000019
0.009604457	455.6602	0.000021
0.024760796	467.3299	0.000054



Particle Technology Labs

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3Flex 5.02

3Flex Version 5.02
Serial # 862 Unit 1 Port 1

Sample: 5149970A2
Operator: JF
Submitter: Particle Technology Labs
File: C:\3Flex\data\51499-70\5149970A2.SMP

Started: 6/7/2021 1:28:13 PM
Completed: 6/9/2021 3:38:58 PM
Report time: 6/9/2021 3:52:46 PM
Sample mass: 0.0316 g
Analysis free space: 63.6329 cm³
Low pressure dose: 5.0000 cm³/g STP
Automatic degas: No

Analysis adsorptive: N2
Analysis bath temp.: 77.206 K
Thermal correction: No
Ambient free space: 20.9316 cm³ Measured
Equilibration interval: 20 to 30 s
Sample density: 1.000 g/cm³

Comments: HKUST-1 MOF HK PTL Project#51499-70 PTL ID: 486157-70

BET Surface Area Plot

