

Catalyst & Catalyst Carrier Pore Size Distribution

3Flex 5.02

3Flex Version 5.02
Serial # 552 Unit 1 Port 2

Page 1 of 21

Sample: DWTR-WY Fine
Operator: SMW
Submitter: SMW
File: C:\3Flex\data\Sam Wallace\210914_DWTRWY_vialD_port2.SMP

Started: 9/14/2021 2:25:18 PM	Analysis adsorptive: N2
Completed: 9/15/2021 6:59:53 AM	Analysis bath temp.: -195.911 °C
Report time: 9/15/2021 10:24:42 AM	Thermal correction: No
Sample mass: 0.2430 g	Ambient free space: 16.7520 cm ³ Measured
Analysis free space: 56.9319 cm ³	Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g	Sample density: 1.000 g/cm ³
Automatic degas: No	

Comments: Micropore analysis, BET surface area, and pore volume

Summary Report

Surface Area

Single point surface area at $p/p^\circ = 0.150661398$: 23.4393 m²/gBET Surface Area: 24.0079 m²/g

BJH Adsorption cumulative surface area of pores
between 15.000 Å and 1,000.000 Å diameter: 15.3477 m²/g

BJH Desorption cumulative surface area of pores
between 15.000 Å and 1,000.000 Å diameter: 25.6392 m²/g

Pore Volume

Single point adsorption total pore volume of pores
less than 2,597.391 Å diameter at $p/p^\circ = 0.992578361$: 0.052348 cm³/g

Single point desorption total pore volume of pores
less than 3,354.456 Å diameter at $p/p^\circ = 0.994267390$: 0.054087 cm³/g

BJH Adsorption cumulative volume of pores
between 15.000 Å and 1,000.000 Å diameter: 0.036273 cm³/g

BJH Desorption cumulative volume of pores
between 15.000 Å and 1,000.000 Å diameter: 0.049364 cm³/g

Pore Size

Adsorption average pore diameter (4V/A by BET): 87.217 Å

Desorption average pore diameter (4V/A by BET): 90.115 Å

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Analysis adsorptive: N2

Analysis bath temp.: -195.911 °C

Thermal correction: No

Ambient free space: 16.7520 cm³ Measured

Equilibration interval: 10 to 20 s

Sample density: 1.000 g/cm³

Comments: Micropore analysis, BET surface area, and pore volume

Pore Size

BJH Adsorption average pore diameter (4V/A): 94.537 Å

BJH Desorption average pore diameter (4V/A): 77.013 Å

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Isotherm Tabular Report

Relative Pressure (p/p°)	Absolute Pressure (mmHg)	Quantity Adsorbed (μmol/g)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
0.000390970	0.292816	107.503	01:35	745.676025
0.003635199	2.725475	164.263	07:22	748.947693
0.008692918	6.515591	188.949	09:55	749.745544
0.014448758	10.829697	201.560	10:34	749.528564
0.019638804	14.719823	209.992	10:51	749.524414
0.030139817	22.589546	222.351	10:57	749.527466
0.040072991	30.036221	231.355	11:04	749.491821
0.050151624	37.591476	238.791	11:09	749.537781
0.099894655	74.865562	263.681	11:14	749.556519
0.150661398	112.942833	282.876	11:18	749.445129
0.200691391	150.420807	299.177	11:22	749.646790
0.250815775	187.989914	313.984	11:26	749.513000
0.300730461	225.398270	327.809	11:30	749.513916
0.400235490	299.979431	352.219	11:34	749.502625
0.500214798	374.885651	378.450	11:37	749.507324
0.600048869	449.732452	410.304	11:40	749.449341
0.699674446	524.387634	454.542	11:43	749.493042
0.719482991	539.288818	467.104	11:46	749.473755
0.740373693	554.917358	481.656	11:48	749.550476
0.760169258	569.731873	496.466	11:52	749.509827
0.780409286	584.931335	513.368	11:55	749.480286
0.799871664	599.451965	532.263	11:58	749.518677
0.820147049	614.741211	554.296	12:02	749.435181
0.840422126	629.868530	579.956	12:05	749.549988
0.860135727	644.671570	610.240	12:08	749.466858
0.880014762	659.607910	646.508	12:12	749.499817
0.899821854	674.477661	692.946	12:15	749.541870
			12:18	749.567993

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0.910078967	682.207336	722.932	12:21	749.613342
0.919568701	689.337524	755.489	12:24	749.631348
0.929936016	697.122925	794.689	12:26	749.646118
0.939039048	703.952881	838.890	12:30	749.652405
0.949039079	711.507874	895.054	12:33	749.713989
0.958617738	718.787659	963.876	12:37	749.816772
0.967921642	725.663391	1051.816	12:41	749.712952
0.977590829	732.849915	1172.862	12:45	749.648926
0.988561817	741.192444	1388.181	12:53	749.768433
0.994267390	745.390259	1557.349	13:00	749.687927
0.991457309	743.284241	1539.543	13:03	749.688599
0.980590812	735.143677	1402.208	13:09	749.694641
0.969915710	727.271973	1295.032	13:14	749.830078
0.960949640	720.476685	1220.408	13:17	749.754883
0.950870177	713.030640	1153.526	13:21	749.871704
0.940972704	705.562744	1097.832	13:25	749.822754
0.930442688	697.728943	1049.577	13:28	749.889221
0.920638596	690.255249	1010.974	13:31	749.757019
0.910900796	682.935974	976.962	13:33	749.736938
0.900057305	674.882019	944.360	13:37	749.821167
0.881412715	660.946777	896.042	13:41	749.872070
0.860163641	645.058838	850.497	13:45	749.925720
0.840661771	630.449585	815.955	13:48	749.944397
0.820513476	615.390015	785.339	13:52	750.005981
0.800595866	600.413818	759.265	13:56	749.958679
0.780004781	584.966309	734.462	13:59	749.952209
0.760457892	570.341980	714.293	14:03	749.998108
0.740684181	555.509338	695.416	14:07	749.994873

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Isotherm Tabular Report

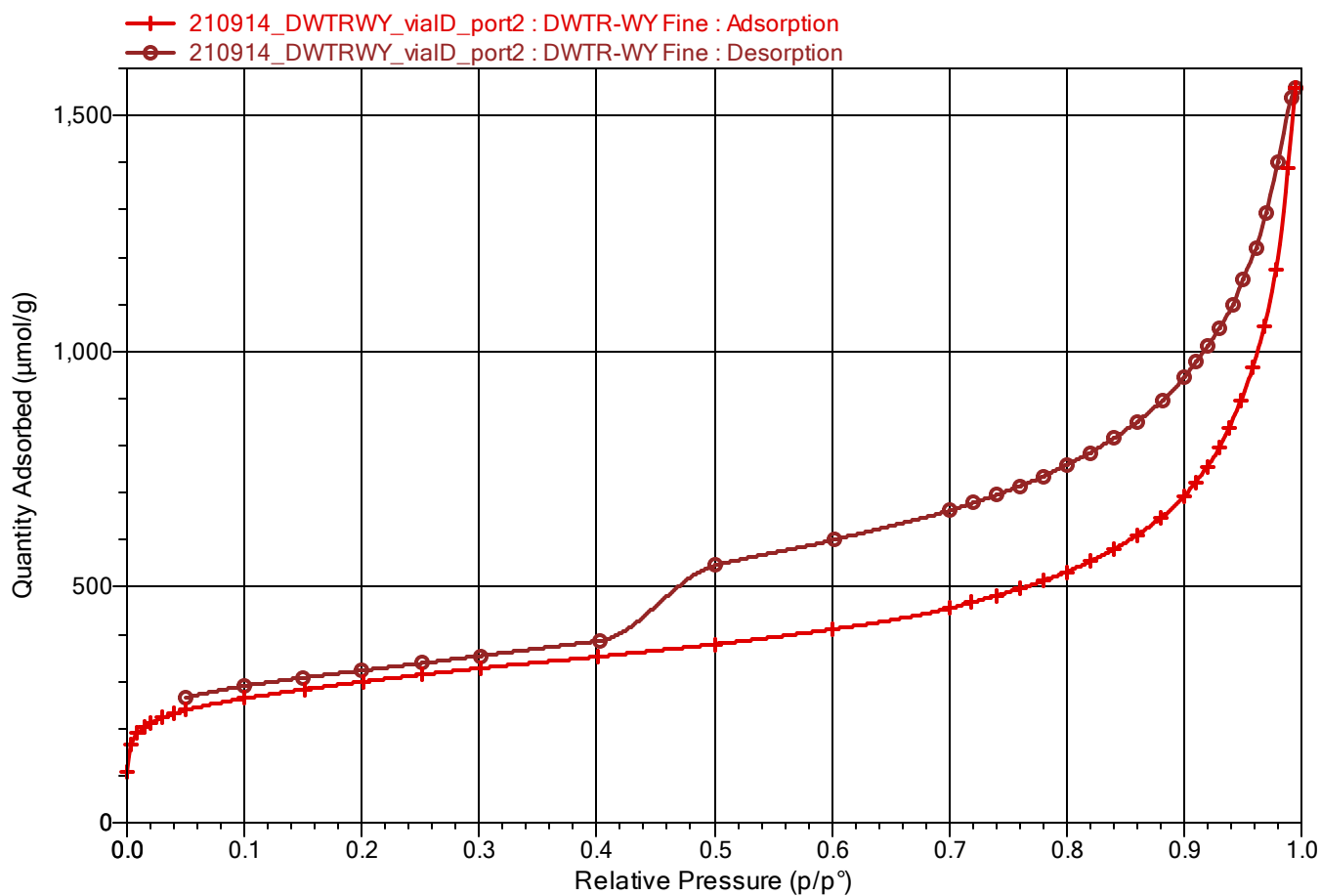
Relative Pressure (p/p°)	Absolute Pressure (mmHg)	Quantity Adsorbed (µmol/g)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
0.720408265	540.301758	678.027	14:11	749.993835
0.700564818	525.394409	662.146	14:14	749.958313
0.602036964	451.514862	600.221	14:18	749.978638
0.500911474	375.693756	545.948	14:23	750.020264
0.402008757	301.506470	386.035	14:28	749.999756
0.301515201	226.140228	354.051	14:33	750.012695
0.250896956	188.218918	338.324	14:37	750.184143
0.200027336	150.060974	322.788	14:41	750.202332
0.150140645	112.615463	307.468	14:44	750.066467
0.100272882	75.209686	289.685	14:50	750.050110
0.050307491	37.728920	265.458	14:57	749.966248

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Isotherm Linear Plot



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BET Report

BET surface area: 24.0079 ± 0.0543 m²/g

Slope: 0.0040462 ± 0.0000092 g/µmol

Y-intercept: 0.0000174 ± 0.0000007 g/µmol

C: 233.550067

Qm: 246.086 µmol/g

Correlation coefficient: 0.9999898

Molecular cross-sectional area: 0.1620 nm²

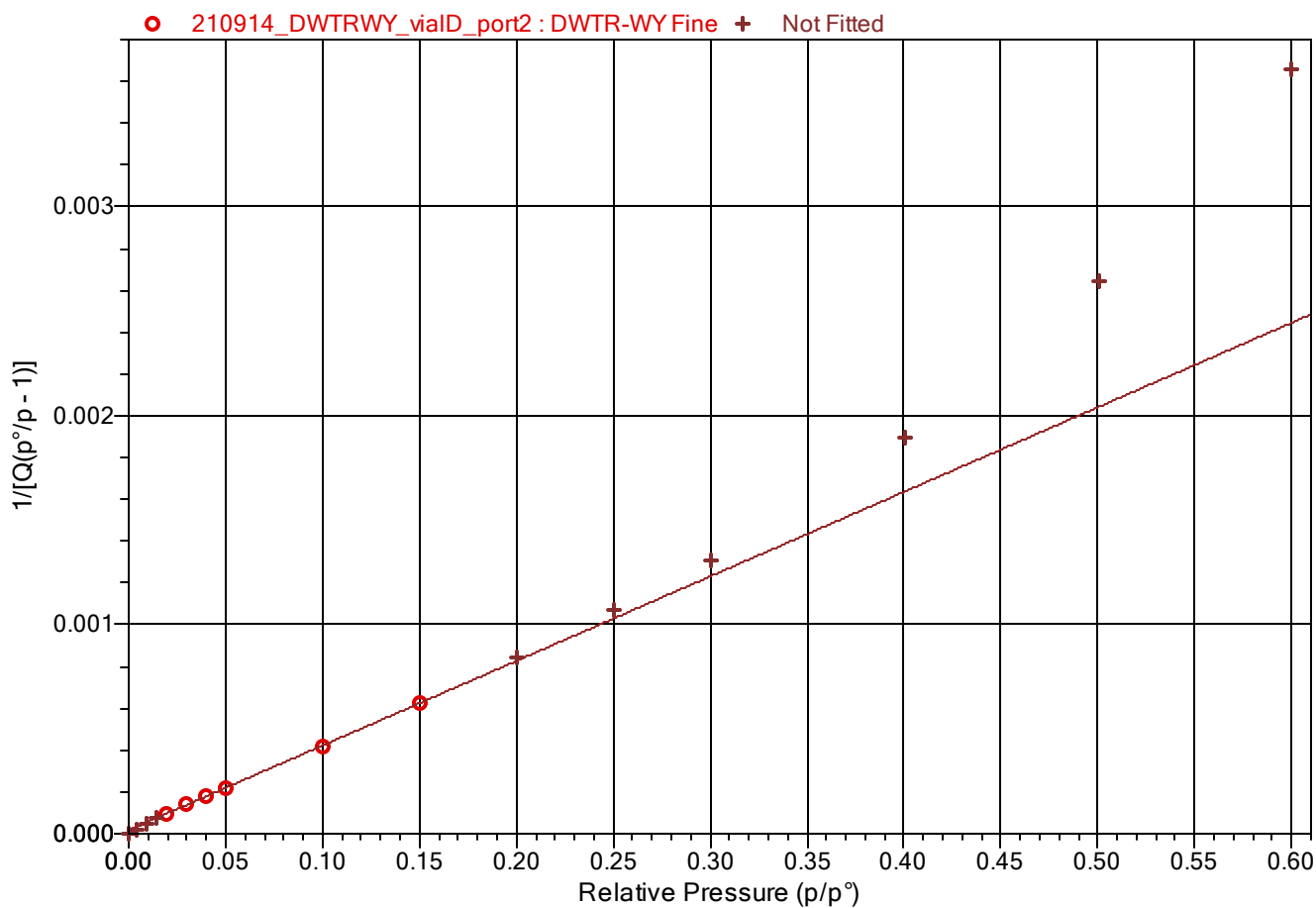
Relative Pressure (p/p°)	Quantity Adsorbed (µmol/g)	1/[Q(p°/p - 1)]
0.019638804	209.992	0.0000954
0.030139817	222.351	0.0001398
0.040072991	231.355	0.0001804
0.050151624	238.791	0.0002211
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0.150661398	282.876	0.0006271

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BET Surface Area Plot



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BJH Desorption Pore Distribution Report

Standard

Halsey

$$t = 3.54 [-5 / \ln(p/p^\circ)]^{0.333}$$

Diameter range: 15.000 to 1,000.000 Å

Adsorbate property factor: 9.53000 Å

Density conversion factor: 0.0015495

Fraction of pores open at both ends: 0.00

Pore Diameter Range (Å)	Average Diameter (Å)	Incremental Pore Volume (cm ³ /g)	Cumulative Pore Volume (cm ³ /g)	Incremental Pore Area (m ² /g)	Cumulative Pore Area (m ² /g)
1017.3 - 662.6	766.3	0.004092	0.004092	0.214	0.214
662.6 - 513.9	569.0	0.002891	0.006982	0.203	0.417
513.9 - 411.1	450.7	0.002626	0.009609	0.233	0.650
411.1 - 344.0	371.3	0.002217	0.011825	0.239	0.889
344.0 - 293.4	314.5	0.001941	0.013766	0.247	1.136
293.4 - 258.3	273.5	0.001569	0.015335	0.229	1.365
258.3 - 230.9	242.9	0.001397	0.016731	0.230	1.595
230.9 - 206.6	217.3	0.001350	0.018081	0.248	1.843
206.6 - 175.1	188.1	0.002038	0.020119	0.433	2.277
175.1 - 149.3	159.9	0.001953	0.022073	0.489	2.765
149.3 - 131.5	139.1	0.001497	0.023569	0.430	3.196
131.5 - 117.1	123.4	0.001342	0.024911	0.435	3.631
117.1 - 105.7	110.7	0.001153	0.026064	0.417	4.047
105.7 - 96.0	100.3	0.001117	0.027182	0.446	4.493
96.0 - 88.2	91.7	0.000908	0.028090	0.396	4.889
88.2 - 81.6	84.6	0.000862	0.028952	0.408	5.297
81.6 - 75.7	78.4	0.000798	0.029749	0.407	5.704
75.7 - 70.6	72.9	0.000738	0.030487	0.404	6.108
70.6 - 52.7	58.7	0.003045	0.033532	2.076	8.184

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Ambient free space: 16.7520 cm³ Measured

Equilibration interval: 10 to 20 s

Sample density: 1.000 g/cm³

Comments: Micropore analysis, BET surface area, and pore volume

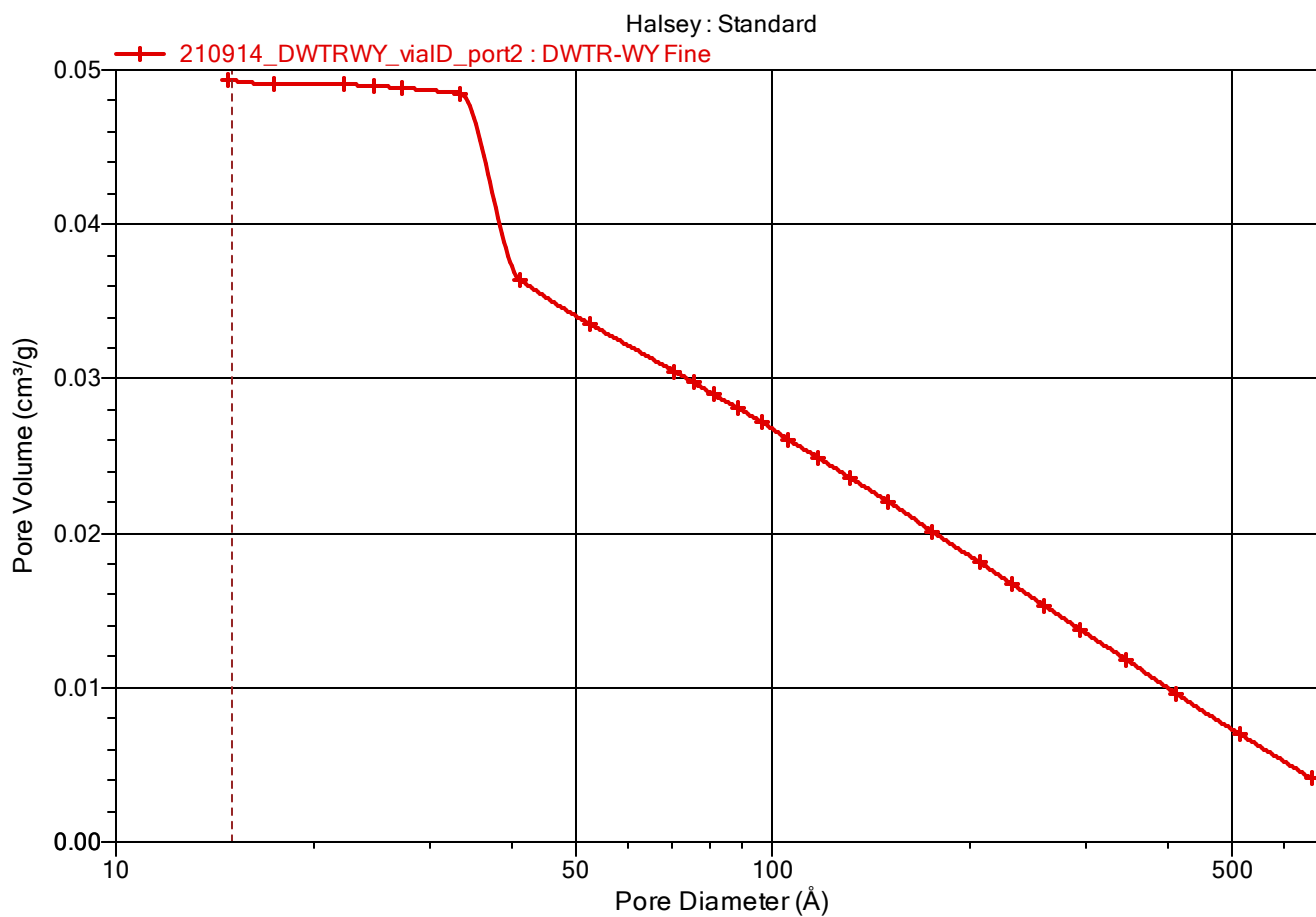
Pore Diameter Range (Å)	Average Diameter (Å)	Incremental Pore Volume (cm ³ /g)	Cumulative Pore Volume (cm ³ /g)	Incremental Pore Area (m ² /g)	Cumulative Pore Area (m ² /g)
52.7 - 41.3	45.3	0.002873	0.036405	2.537	10.721
41.3 - 33.4	36.3	0.012098	0.048503	13.334	24.054
33.4 - 27.3	29.5	0.000329	0.048832	0.446	24.500
27.3 - 24.6	25.8	0.000145	0.048977	0.225	24.725
24.6 - 22.2	23.2	0.000077	0.049054	0.132	24.857
22.2 - 17.5	19.0	0.000007	0.049061	0.015	24.872
17.5 - 14.8	15.8	0.000303	0.049364	0.767	25.639

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BJH Desorption Cumulative Pore Volume (Larger)



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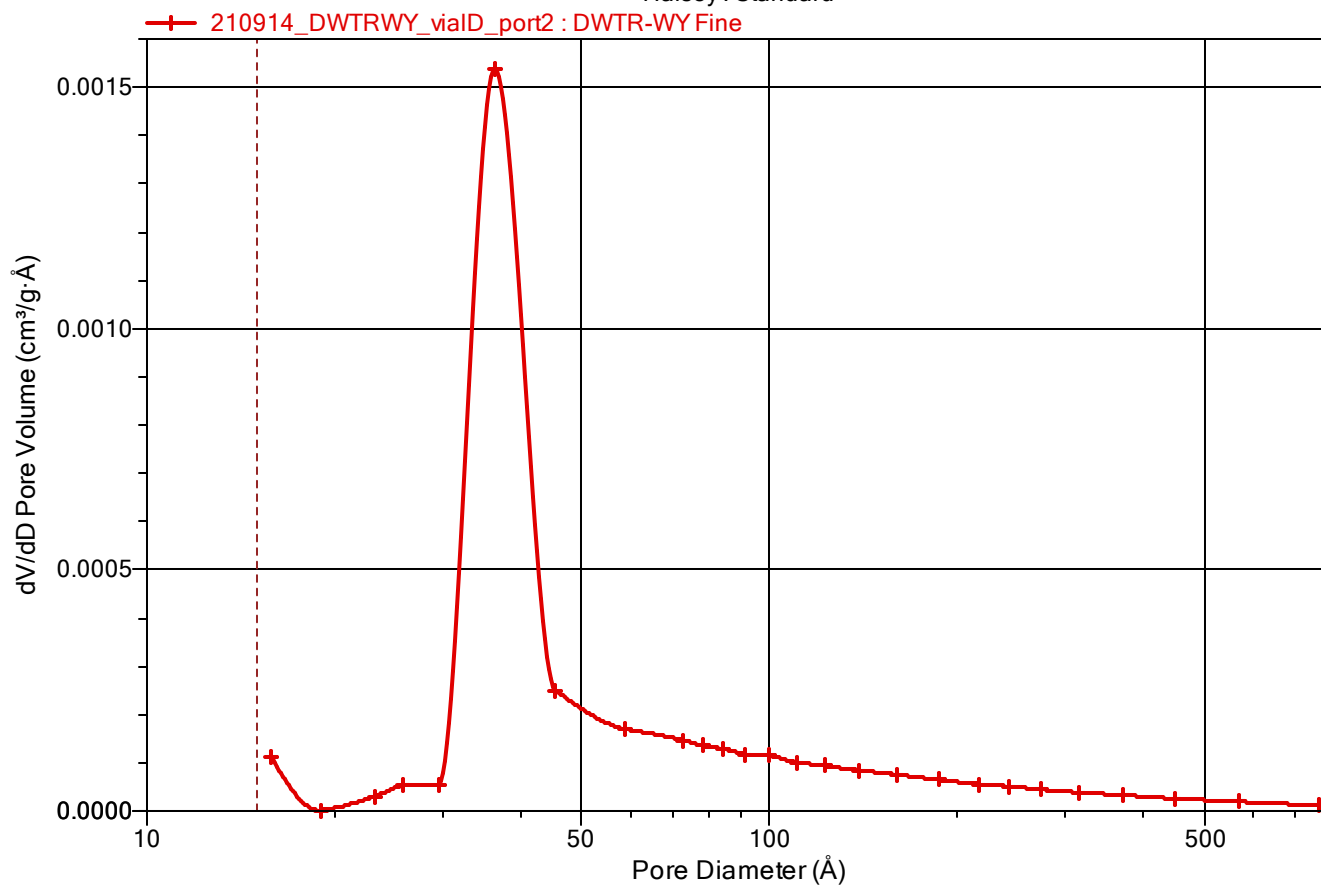
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Sample density: 1.000 g/cm³

Comments: Micropore analysis, BET surface area, and pore volume

BJH Desorption dV/dD Pore Volume

Halsey : Standard



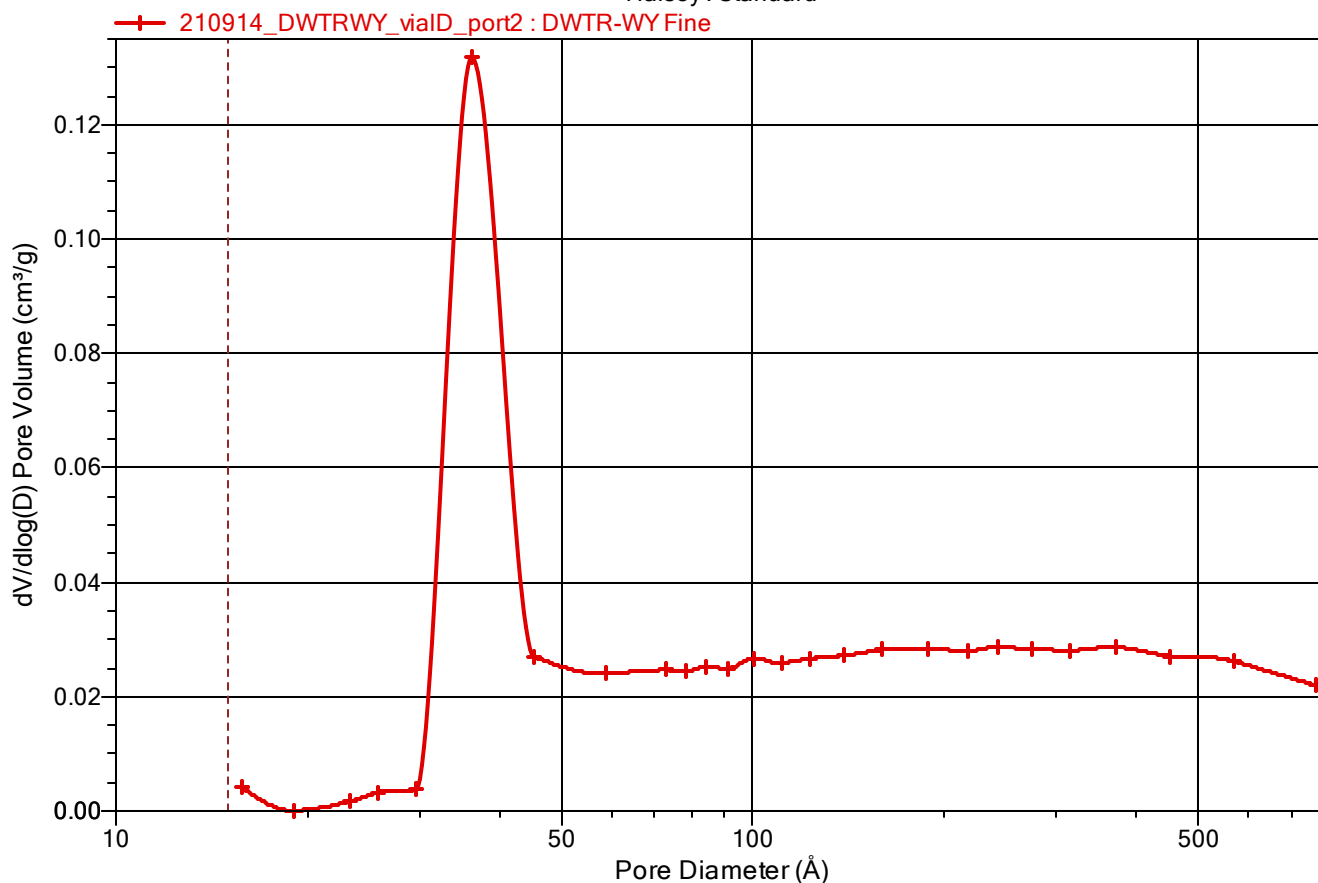
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BJH Desorption dV/dlog(D) Pore Volume

Halsey : Standard

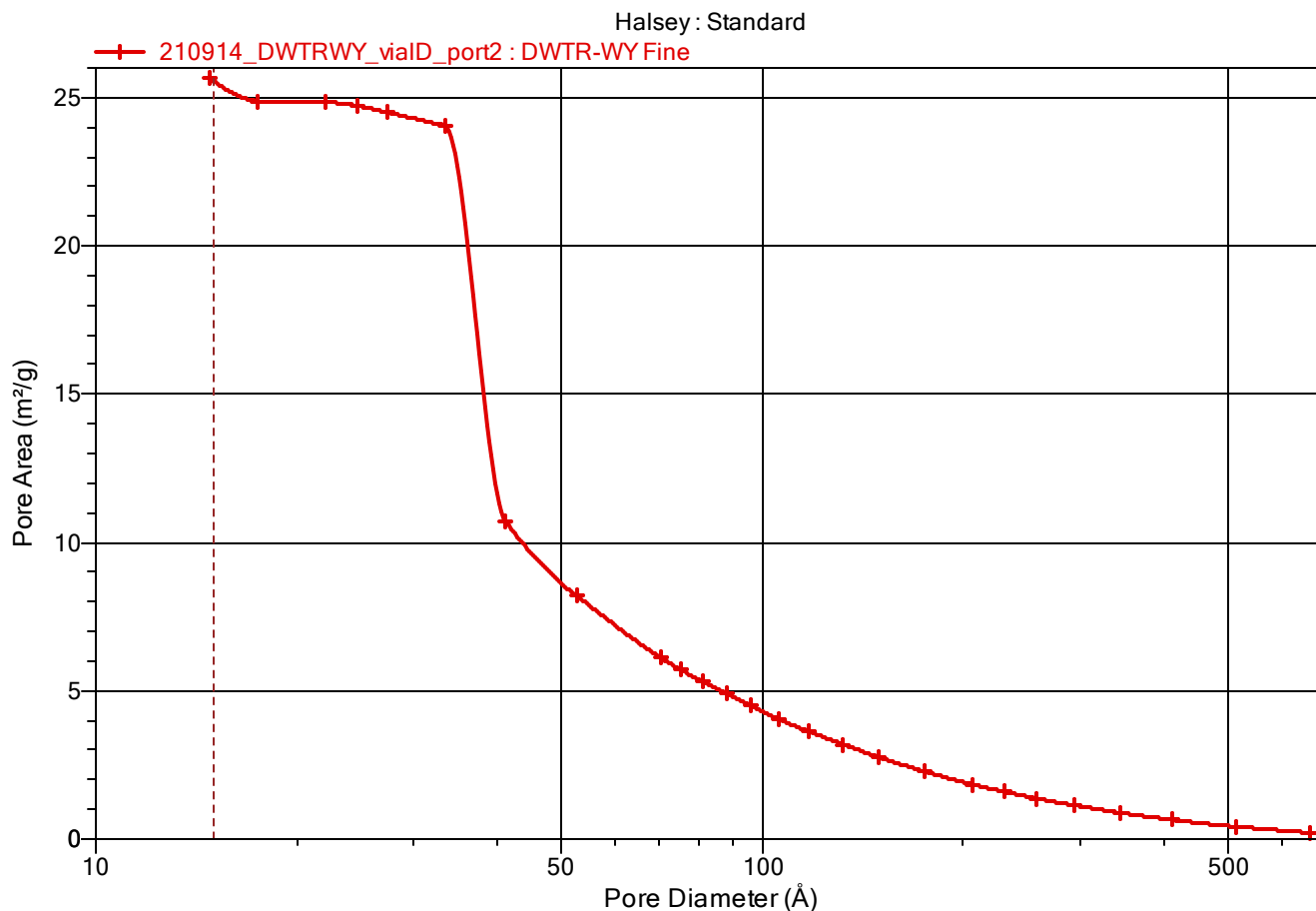


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BJH Desorption Cumulative Pore Area (Larger)



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Thermal correction: No

Ambient free space: 16.7520 cm³ Measured

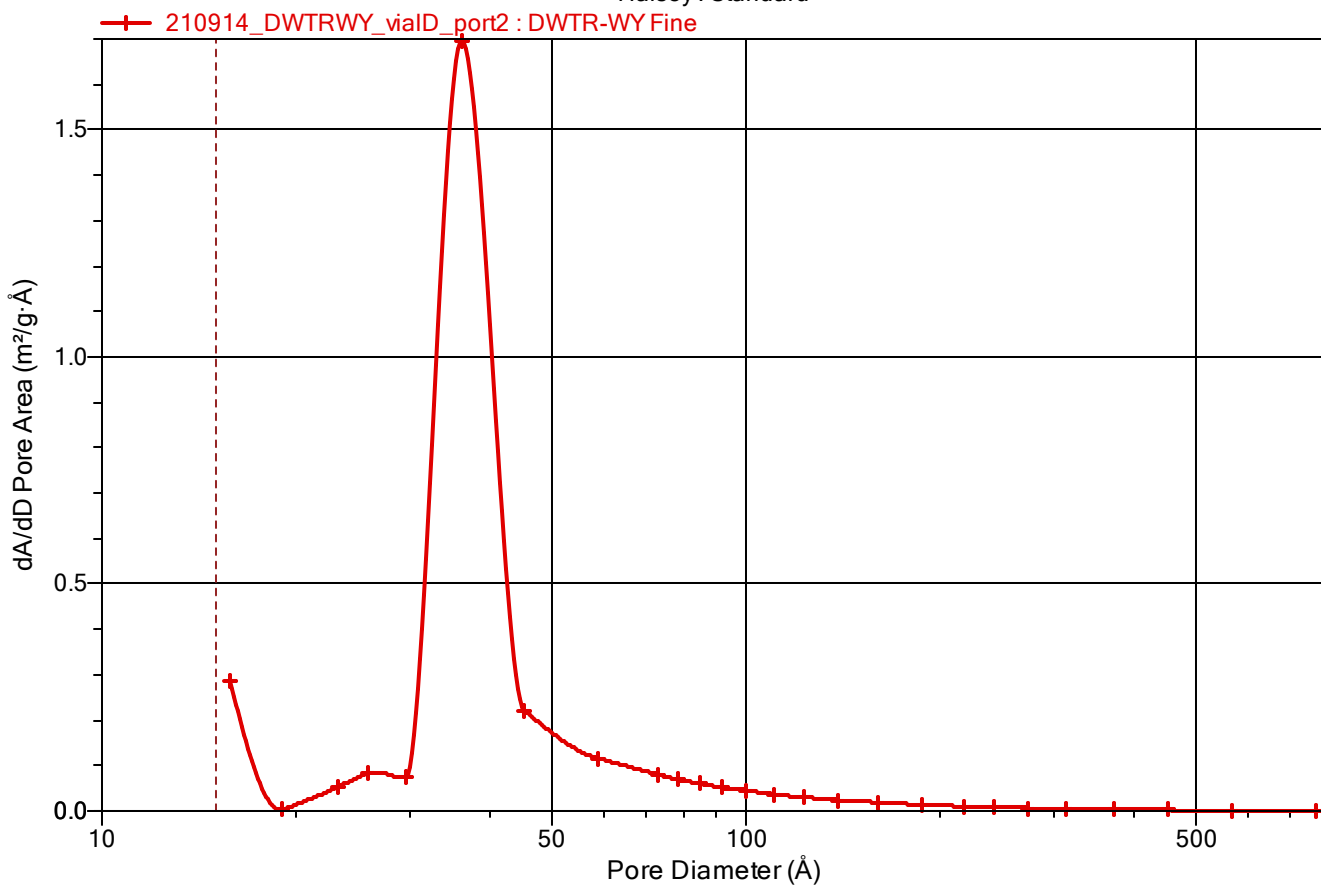
Equilibration interval: 10 to 20 s

Sample density: 1.000 g/cm³

Comments: Micropore analysis, BET surface area, and pore volume

BJH Desorption dA/dD Pore Area

Halsey : Standard



Catalyst & Catalyst Carrier Pore Size Distribution

3Flex 5.02

3Flex Version 5.02
Serial # 552 Unit 1 Port 2

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Sample: DWTR-WY Fine

Operator: SMW

Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914_DWTRWY_vialD_port2.SMP

Started: 9/14/2021 2:25:18 PM

Completed: 9/15/2021 6:59:53 AM

Report time: 9/15/2021 10:24:42 AM

Sample mass: 0.2430 g

Analysis free space: 56.9319 cm³

Low pressure dose: 133.844 μmol/g

Automatic degas: No

Analysis adsorptive: N2

Analysis bath temp.: -195.911 °C

Thermal correction: No

Ambient free space: 16.7520 cm³ Measured

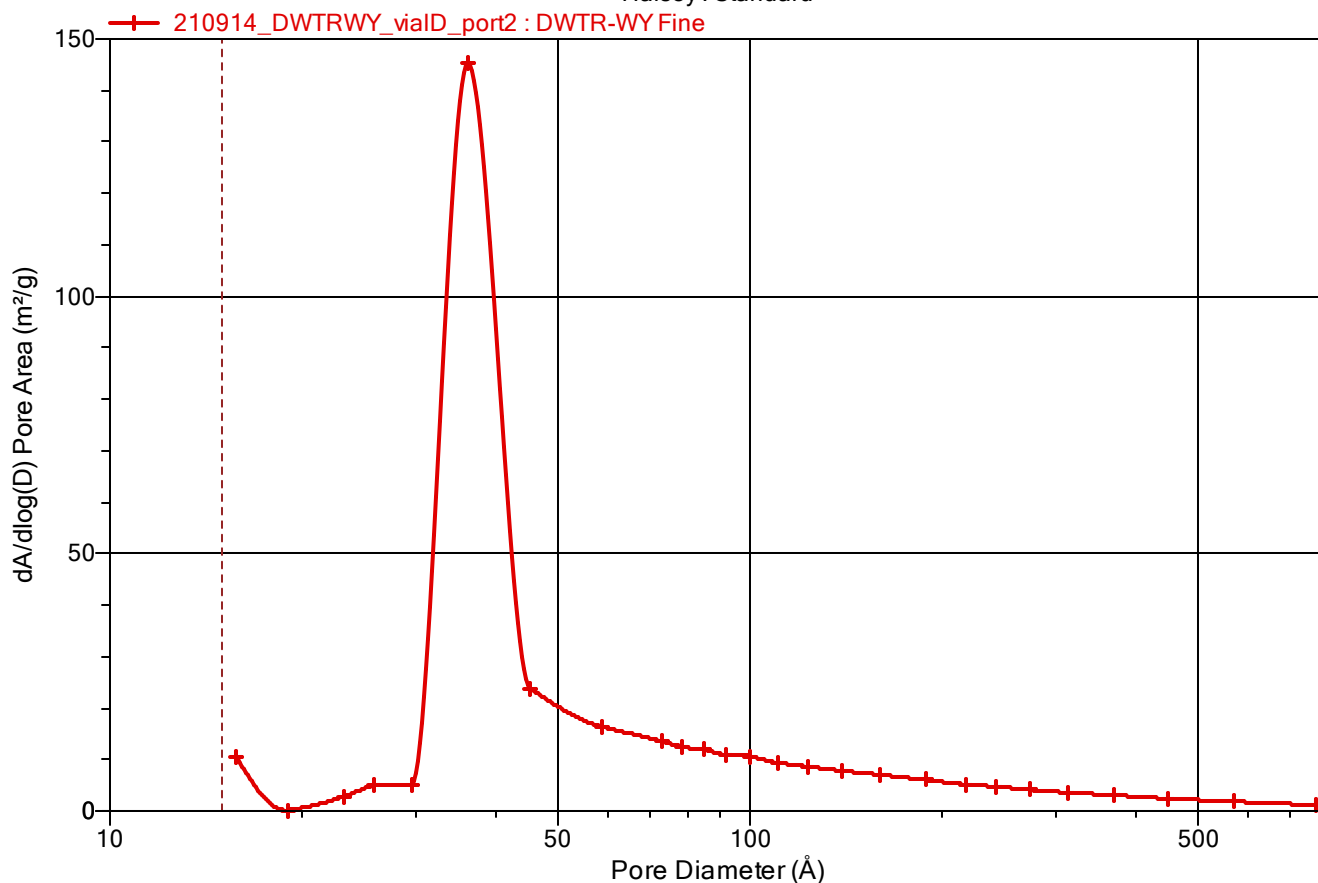
Equilibration interval: 10 to 20 s

Sample density: 1.000 g/cm³

Comments: Micropore analysis, BET surface area, and pore volume

BJH Desorption dA/dlog(D) Pore Area

Halsey : Standard



Catalyst & Catalyst Carrier Pore Size Distribution

3Flex 5.02

3Flex Version 5.02
Serial # 552 Unit 1 Port 2

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Sample: DWTR-WY Fine
Operator: SMW
Submitter: SMW
File: C:\3Flex\data\Sam Wallace\210914_DWTRWY_vialD_port2.SMP

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Completed: 9/15/2021 6:59:53 AM	Analysis bath temp.: -195.911 °C
Report time: 9/15/2021 10:24:42 AM	Thermal correction: No
Sample mass: 0.2430 g	Ambient free space: 16.7520 cm ³ Measured
Analysis free space: 56.9319 cm ³	Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g	Sample density: 1.000 g/cm ³
Automatic degas: No	

Comments: Micropore analysis, BET surface area, and pore volume

Horvath-Kawazoe Report Cylinder Pore Geometry (Saito-Foley)

Maximum pore volume: 0.007000 cm³/g
at Relative Pressure: 0.014448758
Median pore width: 12.262 Å
Relative pressure range: 1e-09 to 0.0157326

Diameter of adsorptive molecule: 3.000 Å
Diameter of sample atom: 3.040 Å
Interaction parameter: 3.49e-43 erg·cm⁴

Density conversion factor: 0.0015495

Absolute Pressure (mmHg)	Relative Pressure (p/p°)	Quantity Adsorbed (µmol/g)	Pore Width (Å)	Cumulative Pore Volume (cm ³ /g)	Differential Pore Volume (cm ³ /g·Å)
0.29282	0.000390970	107.50330	12.262	0.0037	0.0003
2.72547	0.003635199	164.26334	15.920	0.0057	0.0005
6.51559	0.008692918	188.94909	18.250	0.0066	0.0004
10.82970	0.014448758	201.55998	20.034	0.0070	0.0002

Catalyst & Catalyst Carrier Pore Size Distribution

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Serial # 552 Unit 1 Port 2

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Sample: DWTR-WY Fine
Operator: SMW
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File: C:\3Flex\data\Sam Wallace\210914_DWTRWY_vialD_port2.SMP

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Low pressure dose: 133.844 µmol/g	Sample density: 1.000 g/cm ³
Automatic degas: No	

Comments: Micropore analysis, BET surface area, and pore volume

Sample Information

Method: Catalyst & Catalyst Carrier Pore Size - ASTM D4222
Sample: DWTR-WY Fine
Operator: SMW
Submitter: SMW
Mass type: Calculated
Empty tube: 47.1657 g
Sample + tube: 47.4087 g
Sample mass: 0.2430 g
Density: 1.000 g/cm³
Type of data: Automatically collected
Instrument type: 3500
Original instrument type: 3500
Comments: Micropore analysis, BET surface area, and pore volume

Sample Tube

Sample tube: Sample Tube
Ambient free space: 1.0000 cm³
Analysis free space: 1.0000 cm³
Use isothermal jacket: No
Use filler rod: No
Vacuum seal type: None

Degas Conditions

Degas conditions: According to ASTM Test Method D4222

Smart VacPrep evacuation
Backfill sample tube: No
Evacuation rate: 5.0 mmHg/s

Catalyst & Catalyst Carrier Pore Size Distribution

3Flex 5.02

3Flex Version 5.02
Serial # 552 Unit 1 Port 2

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Sample: DWTR-WY Fine
Operator: SMW
Submitter: SMW
File: C:\3Flex\data\Sam Wallace\210914_DWTRWY_vialD_port2.SMP

Started: 9/14/2021 2:25:18 PM	Analysis adsorptive: N2
Completed: 9/15/2021 6:59:53 AM	Analysis bath temp.: -195.911 °C
Report time: 9/15/2021 10:24:42 AM	Thermal correction: No
Sample mass: 0.2430 g	Ambient free space: 16.7520 cm ³ Measured
Analysis free space: 56.9319 cm ³	Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g	Sample density: 1.000 g/cm ³
Automatic degas: No	

Comments: Micropore analysis, BET surface area, and pore volume

Smart VacPrep evacuation			
Unrest. evacuation from: 5.0 mmHg			
Vacuum level: 1.000000e-02 mmHg			
Evacuation time: 10 min			
Temperature ramp rate: 10.0 °C/min			
Target temperature: 30 °C			
Hold pressure: 100 mmHg			
Heating Phase			
Sample prep: Stage	Temperature (°C)	Ramp Rate (°C/min)	Time (min)
1	30	10	10

Analysis Conditions

Analysis conditions: According to ASTM Test Method D4222-03
Absolute pressure dosing: No
Set external trigger: No

Pressure Table				
Starting Pressure (p/p°)	Pressure Increment (p/p°)	Dose Amount (µmol/g)	Equilibration Interval (s)	Ending Pressure (p/p°)
0.000000000		133.844	20	0.010000000
0.010000000	0.010000000		15	0.050000000
0.050000000	0.050000000		15	0.300000000
0.300000000	0.100000000		10	0.700000000
0.700000000	0.020000000		10	0.900000000
0.900000000	0.010000000		10	0.990000000
0.990000000			10	0.995000000
0.995000000			10	0.990000000
0.990000000	0.010000000		10	0.900000000

Catalyst & Catalyst Carrier Pore Size Distribution

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3Flex Version 5.02
Serial # 552 Unit 1 Port 2

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Sample: DWTR-WY Fine
Operator: SMW
Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914_DWTRWY_vialD_port2.SMP

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Low pressure dose: 133.844 µmol/g	Sample density: 1.000 g/cm ³
Automatic degas: No	

Comments: Micropore analysis, BET surface area, and pore volume

Pressure Table				
Starting Pressure (p/p°)	Pressure Increment (p/p°)	Dose Amount (µmol/g)	Equilibration Interval (s)	Ending Pressure (p/p°)
0.900000000	0.020000000		15	0.700000000
0.700000000	0.100000000		15	0.300000000
0.300000000	0.050000000		15	0.050000000

Preparation

Match transducer: Yes
Backfill gas: Nitrogen
Evacuation rate: 5.0 mmHg/s
Unrestricted evacuation from: 5.0 mmHg
Vacuum level: 1.0e-03 mmHg
Evacuation time: 0.10 h
Degas in situ: No

Leak test: No
Elevator operation: Automatic

Free Space

Measured before analysis
Lower Dewar for evacuation: Yes
Evacuation time: 0.50 h
Outgas test: Yes
Outgas test duration: 120 s

p° and Temperature

p° type: Measured in Psat tube for each point
Temperature type: Calculated from p° or Psat

Catalyst & Catalyst Carrier Pore Size Distribution

3Flex 5.02

3Flex Version 5.02
Serial # 552 Unit 1 Port 2

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Sample: DWTR-WY Fine
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Analysis free space: 56.9319 cm ³	Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g	Sample density: 1.000 g/cm ³
Automatic degas: No	

Comments: Micropore analysis, BET surface area, and pore volume

Dosing

Target tolerance: 2.0% or 2.000 mmHg
Minimum equilibration delay at p/p° >= 0.995: 600 s
Minimum equilibration delay: 0.00 h
Maximum equilibration delay: 999.00 h

Termination

Backfill at end of analysis: Yes
Backfill gas: Nitrogen

Adsorptive Properties

Adsorptive: Nitrogen (N2)
Maximum manifold pressure: 925.00 mmHg
Therm. tran. hard-sphere diameter: 3.6810 Å
Molecular cross-sectional area: 0.162 nm²
Adsorbate molecular weight: 28.01
Mass flow constant: 1.000
Thermal conductivity: 1.00
Gas blend: No
Adsorbed-phase free-space correction: Yes
Fluid properties: H:\3500\files\fp\nitrogen.fpi
Dosing method: Normal