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Catalyst & Catalyst Carrier Pore Size Distribution

Sample: DWTR-TN Fine
Operator: SMW
Submitter: SMW
File: C:\3Flex\data\Sam Wallace\210914_DWTRTN_vialC_port1.SMP

Started: 9/14/2021 2:25:18 PM
Completed: 9/15/2021 6:59:53 AM
Report time: 9/15/2021 10:24:38 AM
Sample mass: 0.2824 g
Analysis free space: 57.4076 cm³
Low pressure dose: 133.844 µmol/g
Automatic degas: No

Analysis adsorptive: N2
Analysis bath temp.: -195.937 °C
Thermal correction: No
Ambient free space: 16.8805 cm³ Measured
Equilibration interval: 10 to 20 s
Sample density: 1.000 g/cm³

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

Summary Report

Surface Area

Single point surface area at p/p° = 0.250713401: 6.9825 m²/g

BET Surface Area: 7.2342 m²/g

BJH Adsorption cumulative surface area of pores between 15.000 Å and 1,000.000 Å diameter: 6.3439 m²/g

BJH Desorption cumulative surface area of pores between 15.000 Å and 1,000.000 Å diameter: 7.0521 m²/g

Pore Volume

Single point adsorption total pore volume of pores less than 2,597.391 Å diameter at p/p° = 0.992578361: 0.018996 cm³/g

Single point desorption total pore volume of pores less than 3,215.993 Å diameter at p/p° = 0.994018391: 0.019662 cm³/g

BJH Adsorption cumulative volume of pores between 15.000 Å and 1,000.000 Å diameter: 0.013669 cm³/g

BJH Desorption cumulative volume of pores between 15.000 Å and 1,000.000 Å diameter: 0.016474 cm³/g

Pore Size

Adsorption average pore diameter (4V/A by BET): 105.036 Å

Desorption average pore diameter (4V/A by BET): 108.718 Å

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Automatic degas:	No		

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Pore Size

BJH Adsorption average pore diameter (4V/A):	86.190 Å
BJH Desorption average pore diameter (4V/A):	93.443 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)
			01:35	745.676025
0.004800370	3.583504	42.590	02:10	746.505920
0.011881402	8.869720	50.625	02:16	746.521362
0.019932624	14.880717	54.305	02:20	746.550842
0.029968451	22.370695	58.195	02:24	746.474854
0.040183766	30.003553	61.621	02:28	746.658569
0.050096615	37.407082	64.165	02:31	746.698792
0.100410007	74.982834	74.225	02:35	746.766541
0.150367261	112.295700	82.265	02:39	746.809509
0.200755905	149.915894	89.258	02:42	746.757080
0.250713401	187.235641	95.520	02:46	746.811462
0.300530182	224.447235	101.422	02:49	746.837585
0.399785023	298.596832	111.178	02:53	746.893494
0.499765193	373.289703	121.052	02:56	746.930176
0.600510100	448.521118	132.572	02:59	746.900208
0.700310418	523.123718	148.469	03:02	746.988342
0.720581951	538.297852	152.476	03:05	747.032104
0.740162914	553.000000	156.762	03:08	747.132813
0.760584525	568.227295	161.839	03:11	747.092896
0.780713353	583.217224	167.774	03:14	747.031189
0.800506081	598.050354	173.881	03:17	747.090332
0.820453636	613.039612	181.094	03:20	747.195923
0.840559963	628.069031	189.639	03:23	747.203125
0.860592672	643.025085	199.905	03:26	747.188660
0.880263970	657.758179	212.555	03:30	747.228333
0.900285632	672.723877	228.272	03:33	747.233826
0.910289384	680.228577	238.771	03:35	747.266296
0.920419795	687.803467	250.256	03:38	747.271484

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

Isotherm Tabular Report

Relative Pressure (p/p°)	Absolute Pressure (mmHg)	Quantity Adsorbed (µmol/g)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
0.929824388	694.818481	262.901	03:41	747.257751
0.939402223	702.024902	279.306	03:44	747.310242
0.949611247	709.667542	299.197	03:47	747.324280
0.959805562	717.403809	326.400	03:50	747.447021
0.969282662	724.472412	360.489	03:53	747.431519
0.979230156	731.925293	412.135	03:57	747.449707
0.988305781	738.667969	490.158	04:01	747.408325
0.994018391	742.947510	566.233	04:05	747.418274
0.991017145	740.728882	555.210	04:08	747.443054
0.981216204	733.389282	475.238	04:13	747.428833
0.969716799	724.772278	406.118	04:16	747.406128
0.960681156	718.020508	367.655	04:19	747.407715
0.950550783	710.540771	337.245	04:22	747.504272
0.940458469	702.918945	313.879	04:25	747.421570
0.930617261	695.522461	295.661	04:28	747.377563
0.920037233	687.674316	280.422	04:31	747.441833
0.910230608	680.298767	268.855	04:34	747.391663
0.900350869	672.964905	258.521	04:37	747.447388
0.880295705	658.007446	241.538	04:40	747.484558
0.860325199	643.138245	228.137	04:44	747.552490
0.840031641	628.005737	217.917	04:47	747.597717
0.820595119	613.478394	208.669	04:51	747.601807
0.800516967	598.489136	200.717	04:55	747.628296
0.780074899	583.291626	193.817	04:59	747.737976
0.760136611	568.448242	187.959	05:02	747.823792
0.740452888	553.782654	182.550	05:06	747.897217
0.720112273	538.590271	177.854	05:10	747.925415
0.699992476	523.565491	173.493	05:13	747.958740

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Sample density: 1.000 g/cm³

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

Isotherm Tabular Report

Relative Pressure (p/p°)	Absolute Pressure (mmHg)	Quantity Adsorbed (µmol/g)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
0.600982175	449.501801	155.939	05:17	747.945313
0.500343478	374.221558	140.450	05:21	747.929321
0.401217343	300.120270	107.086	05:25	748.024170
0.300041044	224.450974	94.224	05:29	748.067566
0.250496107	187.396912	87.693	05:33	748.103088
0.200066816	149.660370	81.397	05:36	748.051941
0.150052458	112.249908	75.381	05:40	748.071106
0.100204524	74.960892	68.600	05:45	748.078918
0.050122422	37.502193	60.208	05:50	748.211914

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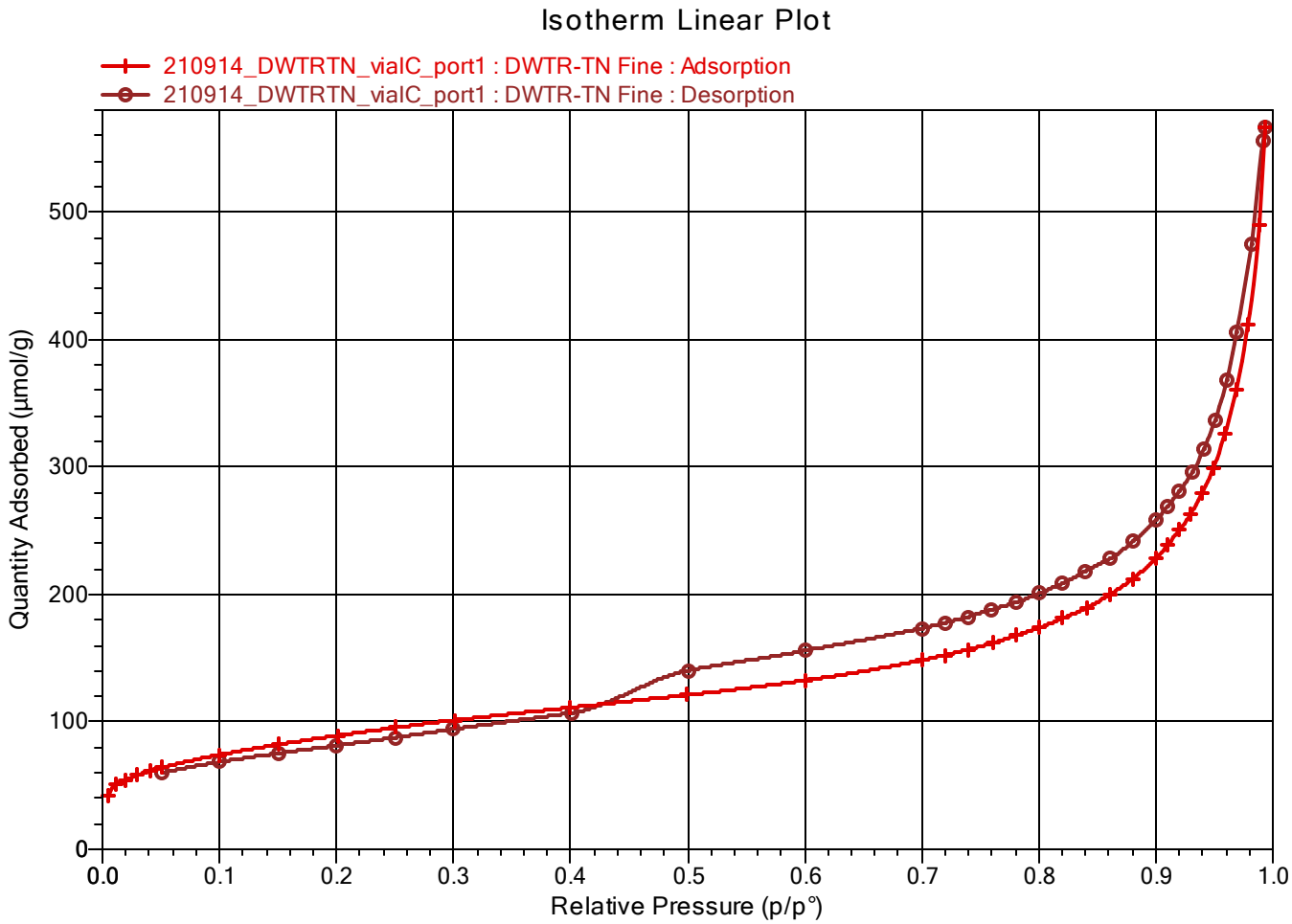

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Comments: Micropore analysis, BET surface area, and pore volume

BET Report

BET surface area: 7.2342 ± 0.0338 m²/g
Slope: 0.0133349 ± 0.0000623 g/µmol
Y-intercept: 0.0001509 ± 0.0000095 g/µmol
C: 89.377513
Qm: 74.152 µmol/g
Correlation coefficient: 0.9999564
Molecular cross-sectional area: 0.1620 nm²

Relative Pressure (p/p°)	Quantity Adsorbed (µmol/g)	1/[Q(p°/p - 1)]
0.040183766	61.621	0.0006794
0.050096615	64.165	0.0008219
0.100410007	74.225	0.0015038
0.150367261	82.265	0.0021513
0.200755905	89.258	0.0028141
0.250713401	95.520	0.0035030

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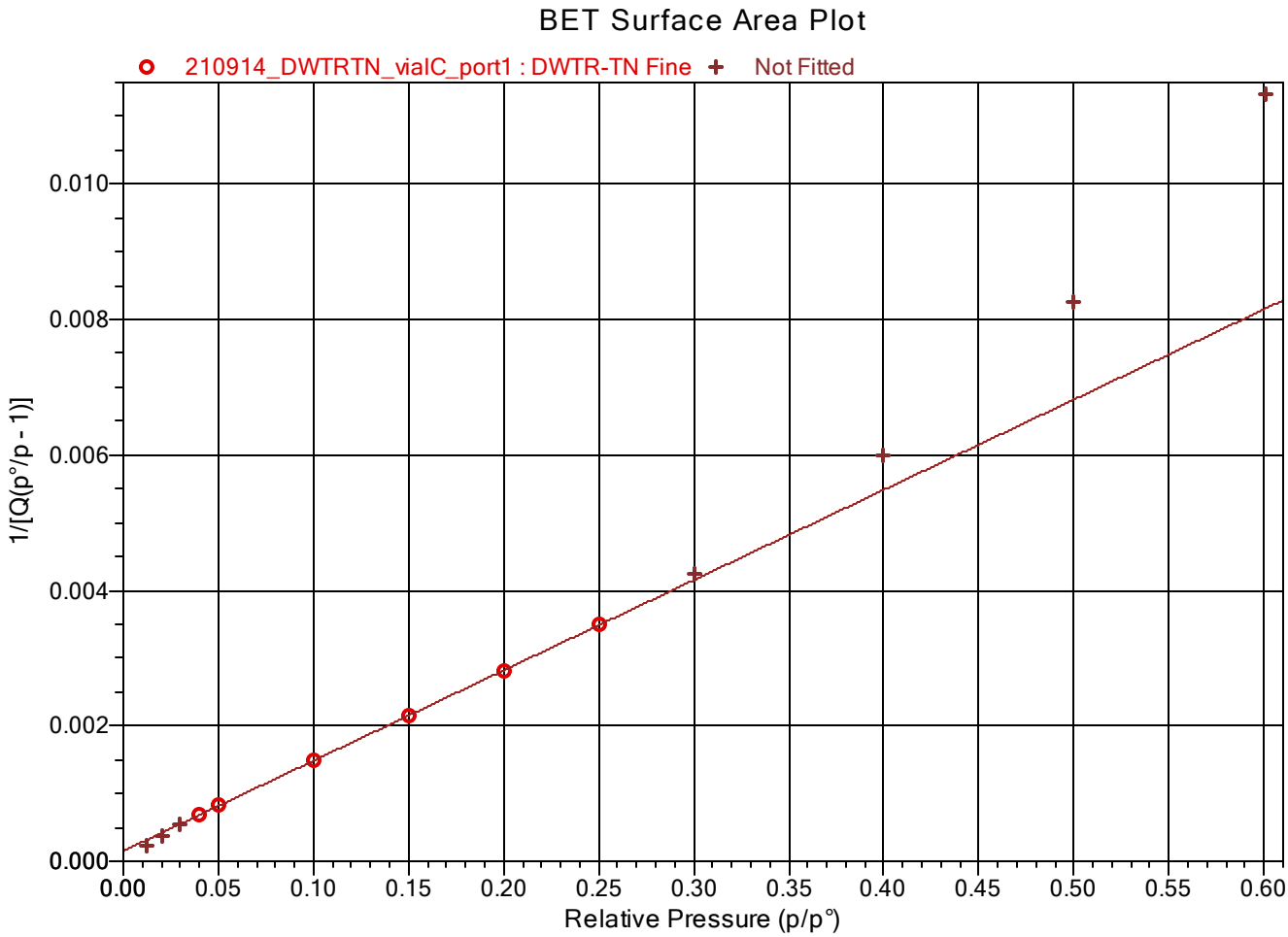

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BJH Desorption Pore Distribution Report

Standard
Harkins and Jura
$t = [13.99 / (0.034 - \log(p/p^\circ))]^{0.5}$

Diameter range: 15.000 to 1,000.000 Å
Adsorbate property factor: 9.53000 Å
Density conversion factor: 0.0015492
Fraction of pores open at both ends: 0.00

Pore Diameter Range (Å)	Average Diameter (Å)	Incremental Pore Volume (cm³/g)	Cumulative Pore Volume (cm³/g)	Incremental Pore Area (m²/g)	Cumulative Pore Area (m²/g)
1041.5 - 654.2	761.1	0.002627	0.002627	0.138	0.138
654.2 - 508.2	562.3	0.001493	0.004120	0.106	0.244
508.2 - 407.4	446.3	0.001200	0.005320	0.108	0.352
407.4 - 340.9	367.9	0.000935	0.006255	0.102	0.454
340.9 - 294.4	314.0	0.000737	0.006992	0.094	0.547
294.4 - 256.9	272.9	0.000621	0.007613	0.091	0.638
256.9 - 230.0	241.9	0.000473	0.008086	0.078	0.717
230.0 - 208.1	217.9	0.000426	0.008512	0.078	0.795
208.1 - 174.5	188.1	0.000707	0.009219	0.150	0.945
174.5 - 150.4	160.5	0.000559	0.009778	0.139	1.085
150.4 - 131.9	139.8	0.000419	0.010197	0.120	1.204
131.9 - 118.0	124.1	0.000388	0.010585	0.125	1.329
118.0 - 106.4	111.5	0.000330	0.010915	0.118	1.448
106.4 - 96.6	101.0	0.000283	0.011197	0.112	1.560
96.6 - 88.6	92.2	0.000237	0.011434	0.103	1.662
88.6 - 81.9	84.9	0.000221	0.011655	0.104	1.767
81.9 - 75.8	78.6	0.000184	0.011839	0.094	1.860
75.8 - 70.6	73.0	0.000172	0.012012	0.094	1.954
70.6 - 52.2	58.4	0.000724	0.012735	0.496	2.451

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Pore Diameter Range (Å)	Average Diameter (Å)	Incremental Pore Volume (cm³/g)	Cumulative Pore Volume (cm³/g)	Incremental Pore Area (m²/g)	Cumulative Pore Area (m²/g)
52.2 - 40.5	44.6	0.000675	0.013411	0.605	3.056
40.5 - 32.3	35.3	0.002178	0.015589	2.469	5.525
32.3 - 25.9	28.2	0.000350	0.015939	0.496	6.020
25.9 - 23.2	24.3	0.000191	0.016129	0.313	6.334
23.2 - 20.6	21.7	0.000147	0.016276	0.270	6.604
20.6 - 18.1	19.2	0.000089	0.016365	0.186	6.790
18.1 - 15.6	16.7	0.000109	0.016474	0.262	7.052

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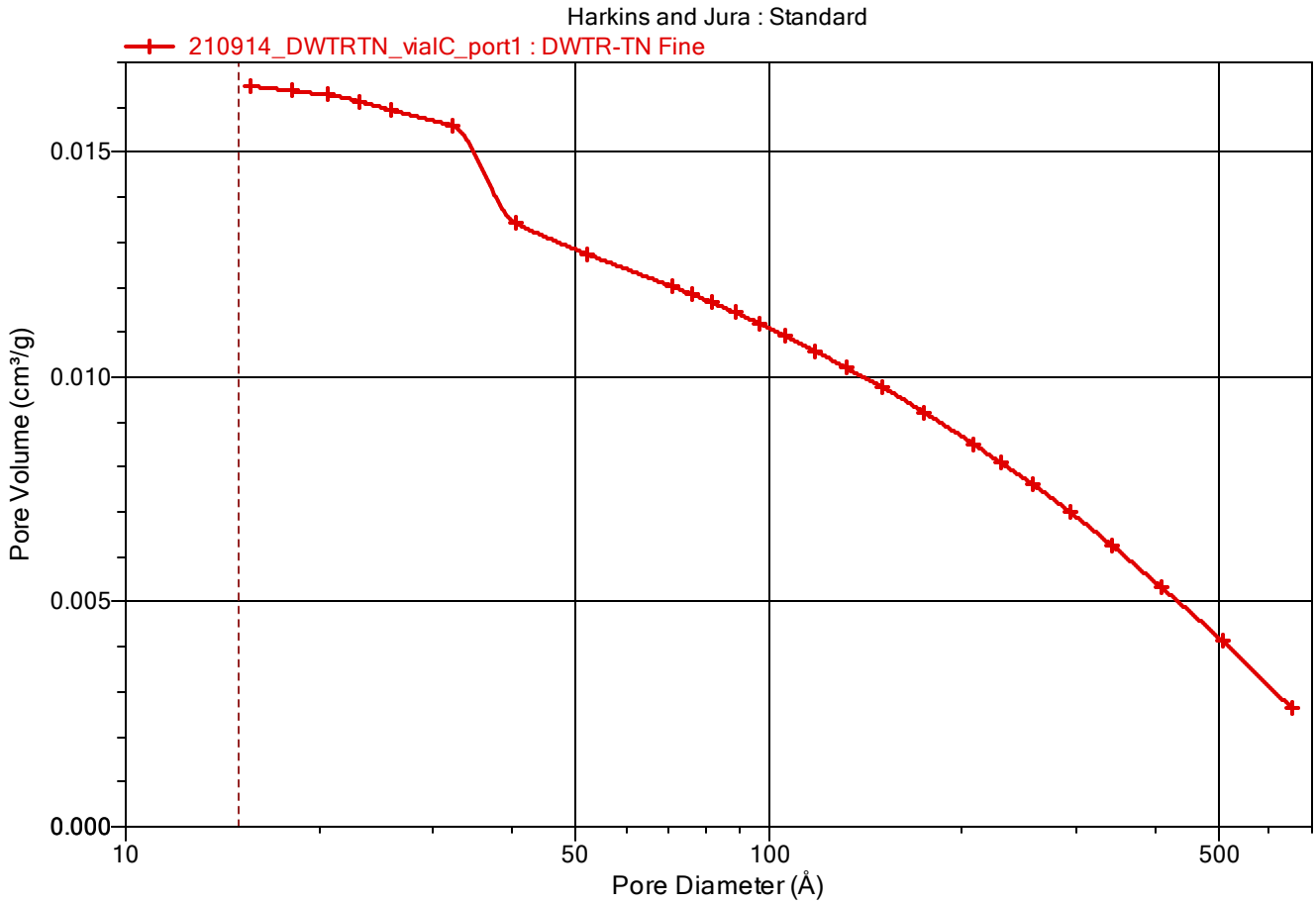
BJH Desorption Cumulative Pore Volume (Larger)



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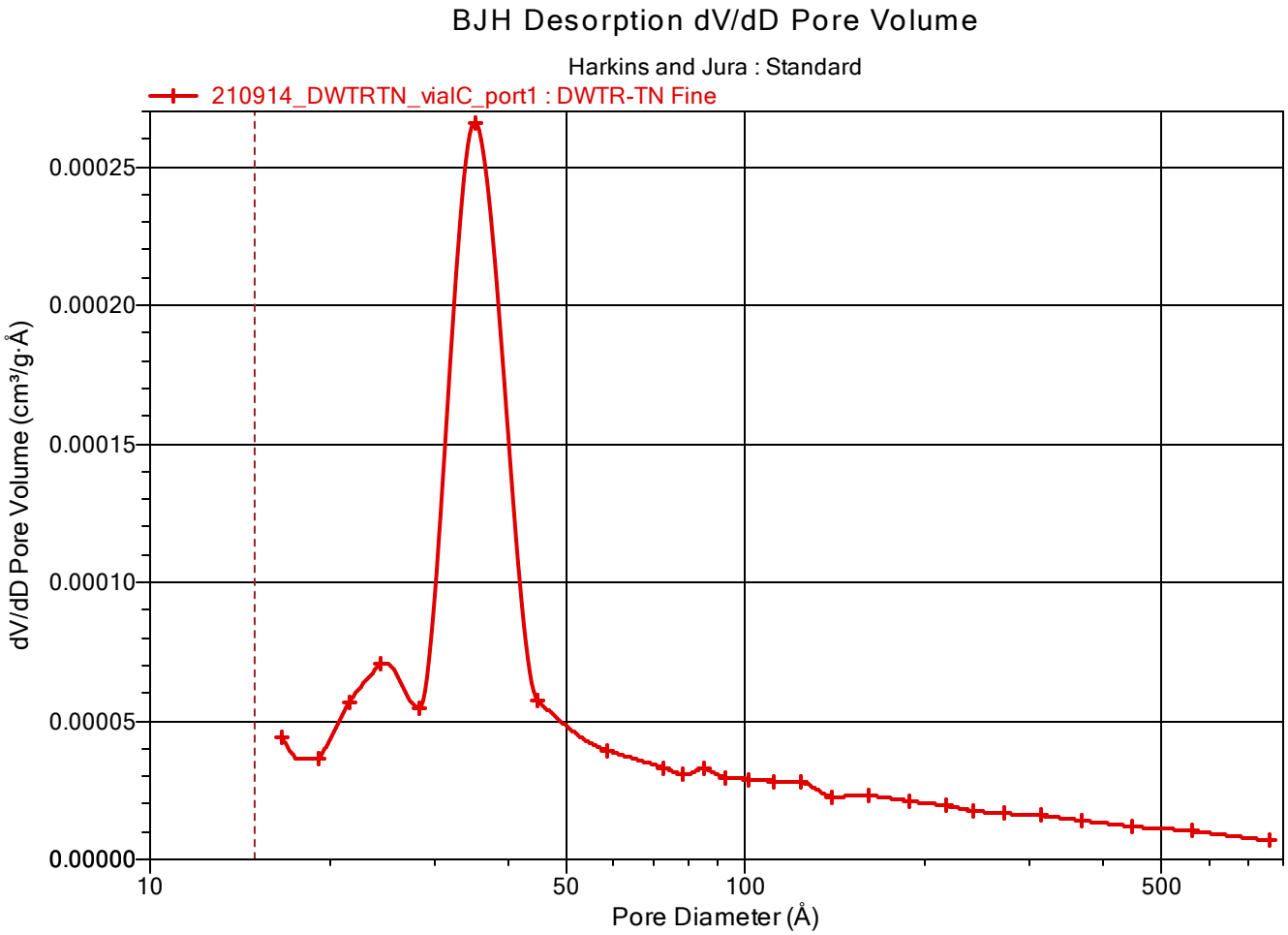

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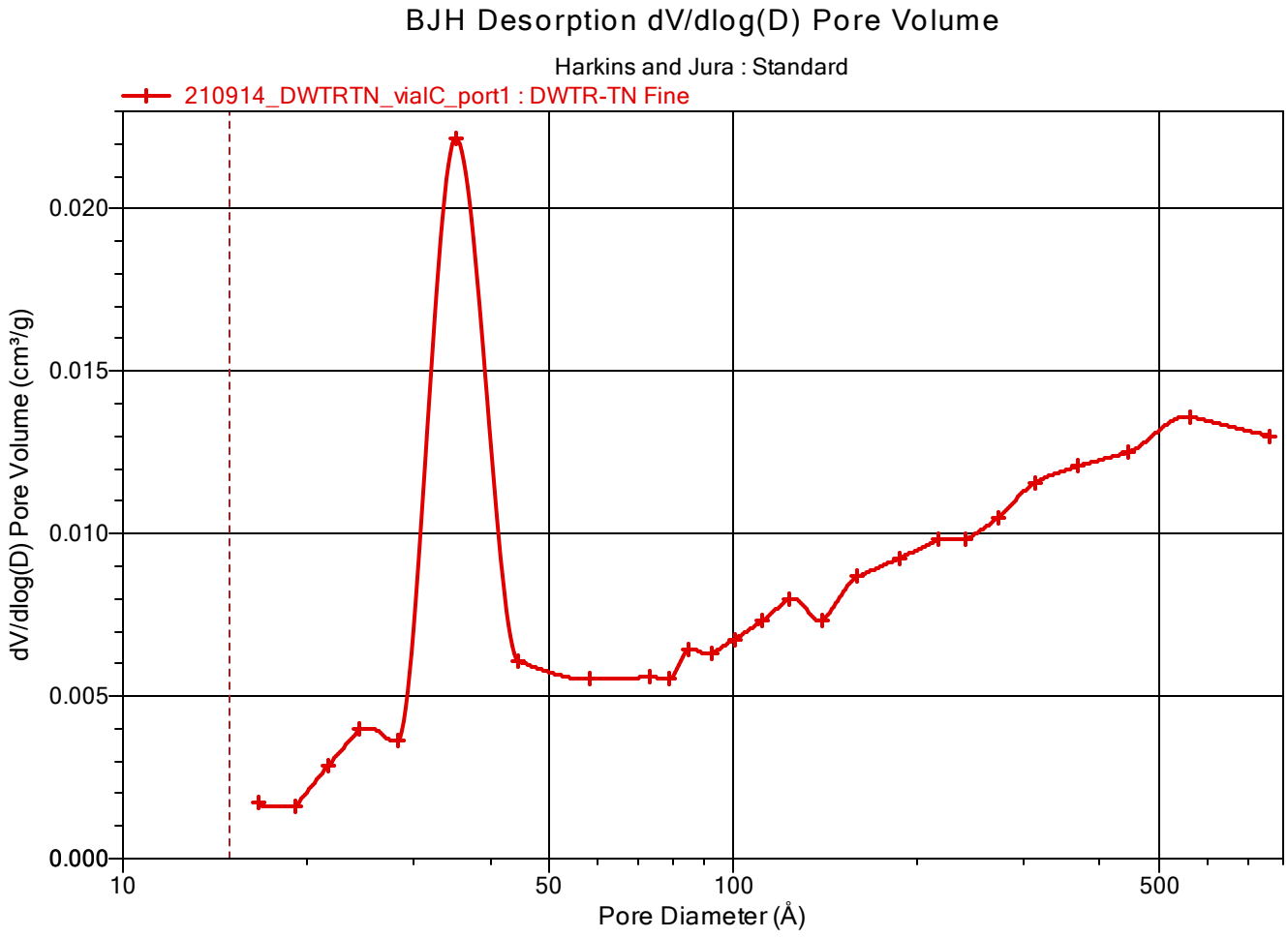

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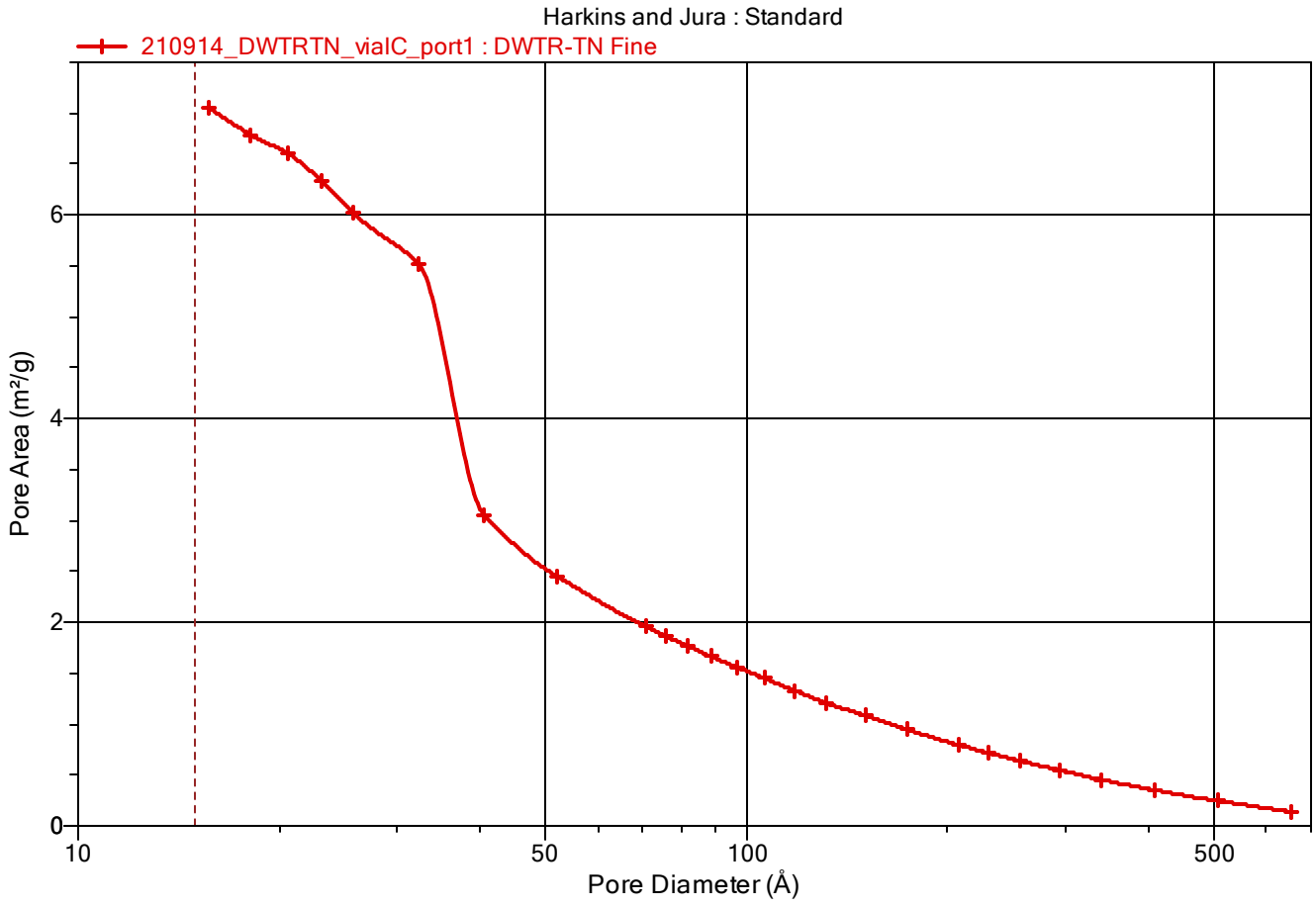
BJH Desorption Cumulative Pore Area (Larger)



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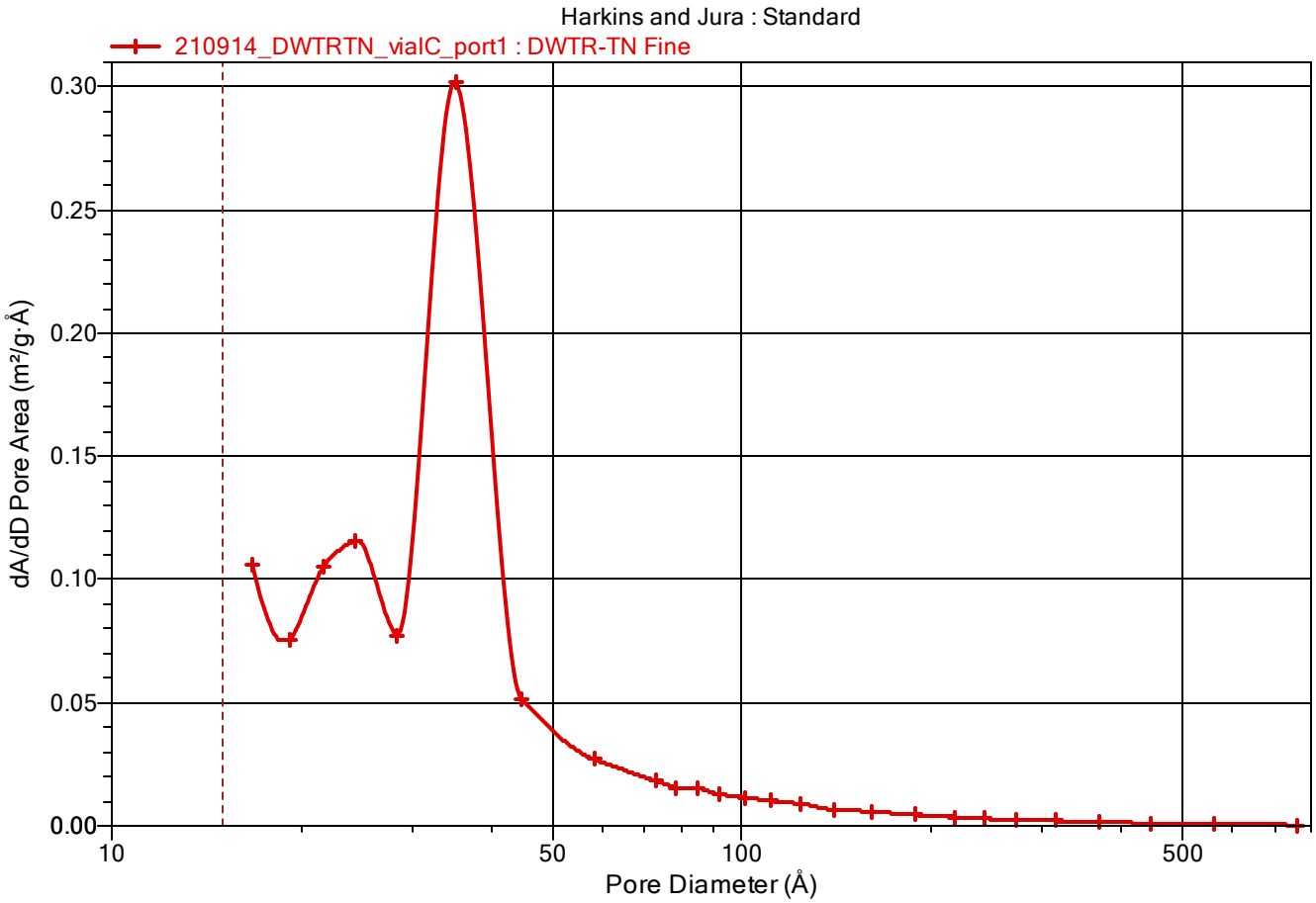
Automatic degas:	No		

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

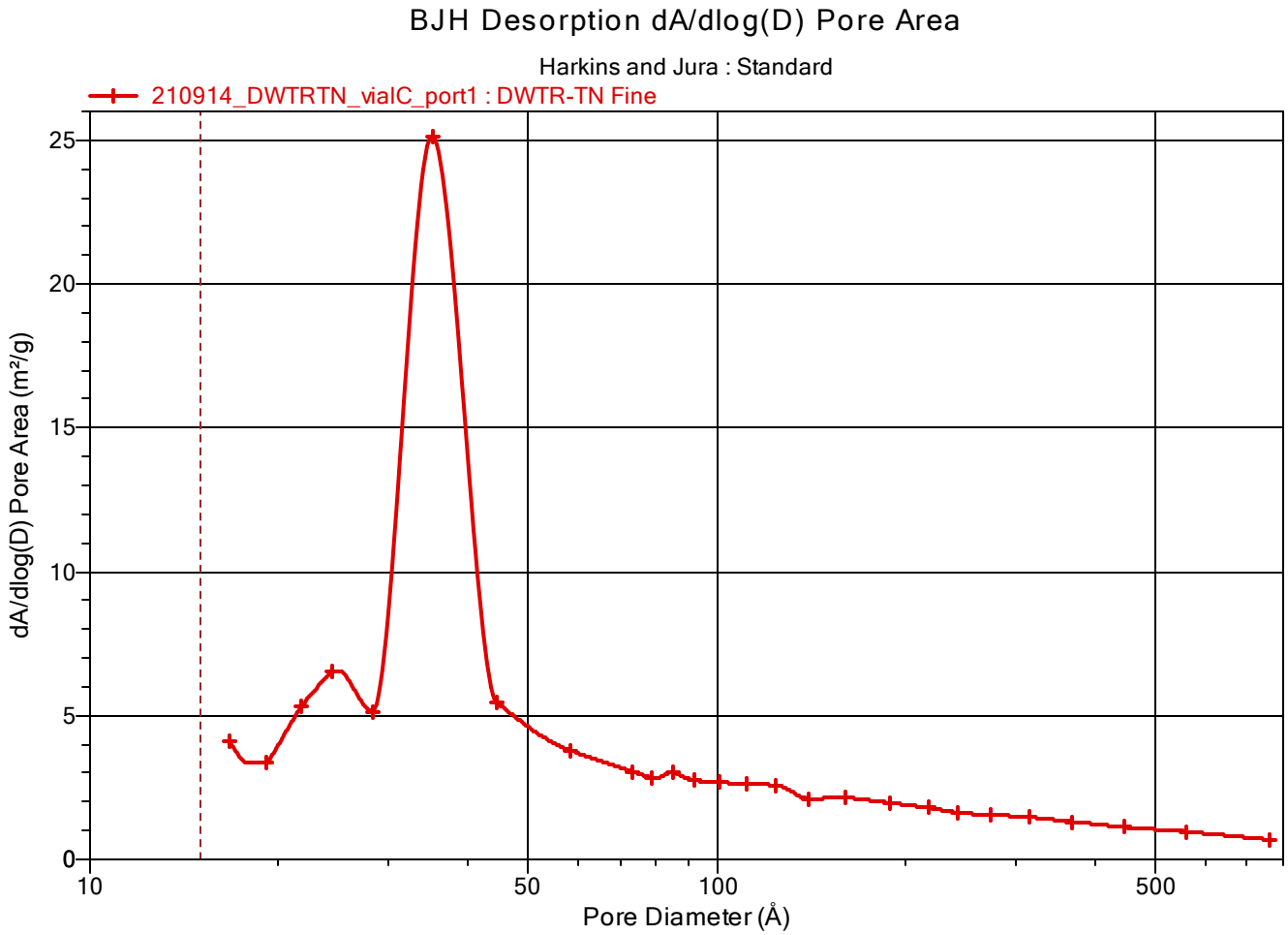
BJH Desorption dA/dD Pore Area



Sample: DWTR-TN Fine
Operator: SMW
Submitter: SMW
File: C:\3Flex\data\Sam Wallace\210914_DWTRTN_vialC_port1.SMP

Started:	9/14/2021 2:25:18 PM	Analysis adsorptive:	N2
Completed:	9/15/2021 6:59:53 AM	Analysis bath temp.:	-195.937 °C
Report time:	9/15/2021 10:24:38 AM	Thermal correction:	No
Sample mass:	0.2824 g	Ambient free space:	16.8805 cm³ Measured
Analysis free space:	57.4076 cm³	Equilibration interval:	10 to 20 s
Low pressure dose:	133.844 µmol/g	Sample density:	1.000 g/cm³
Automatic degas:	No		

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



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Horvath-Kawazoe Report

Cylinder Pore Geometry (Saito-Foley)

Maximum pore volume: 0.001758 cm³/g
at Relative Pressure: 0.011881402
Median pore width: 16.588 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·cm^4

Density conversion factor: 0.0015492

Absolute Pressure (mmHg)	Relative Pressure (p/p°)	Quantity Adsorbed (µmol/g)	Pore Width (Å)	Cumulative Pore Volume (cm³/g)	Differential Pore Volume (cm³/g·Å)
3.58350	0.004800370	42.59019	16.588	0.0015	0.0001
8.86972	0.011881402	50.62465	19.305	0.0018	0.0001

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Sample Information

Method:	Catalyst & Catalyst Carrier Pore Size - ASTM D4222
Sample:	DWTR-TN Fine
Operator:	SMW
Submitter:	SMW
Mass type:	Calculated
Empty tube:	46.7200 g
Sample + tube:	47.0024 g
Sample mass:	0.2824 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

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Operator: SMW
Submitter: SMW
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Analysis adsorptive: N2
Analysis bath temp.: -195.937 °C
Thermal correction: No
Ambient free space: 16.8805 cm³ Measured
Equilibration interval: 10 to 20 s
Sample density: 1.000 g/cm³

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

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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

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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\fpi\nitrogen.fpi
Dosing method:	Normal