Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

Started: 6/3/2025 5:16:57 PM
Completed: 6/3/2025 9:48:28 PM
Sample mass: 0.1181 g
Report time: 1/19/2026 6:05:24 PM

Summary Report

Experiment 1: CoHe pulse chemisorption

Analysis type: Pulse Chemisorption
Calibration: None
Measured flow rate: 2,230.8 µmol/min
Signal offset: 0.00000
Signal inverted: Yes

Peak Number	Temperature at Maximum (°C)	Area	Peak Height
1	35.1	7.8932e-04	-2.2144e-04
2	35.0	1.0282e-03	-6.0473e-04
3	34.9	1.6133e-03	-9.8460e-04
4	35.1	2.2524e-03	-1.2832e-03
5	34.9	3.1544e-03	-1.5101e-03
6	35.0	3.1113e-03	-1.8503e-03
7	34.9	3.4999e-03	-1.8961e-03

Injection Number	Injection Type	Injection Volume (mL)
1	Loop	0.49810
2	Loop	0.49810
3	Loop	0.49810
4	Loop	0.49810
5	Loop	0.49810
6	Loop	0.49810
7	Loop	0.49810

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

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Sample mass: 0.1181 g
Report time: 1/19/2026 6:05:24 PM

Pulse Chemisorption Report

Experiment 1 CoHe pulse chemisorption
Analysis type: Pulse Chemisorption
Calibration: None
Measured flow rate: 2,230.8 µmol/min
Signal offset: 0.00000
Signal inverted: Yes
Number of Peaks Used for Saturation: 1

Peak Table

Peak Number	Temperature at Maximum (°C)	Quantity Adsorbed (µmol/g)	Cumulative Quantity (µmol/g)
1	35.1	10.52351	10.52351
2	35.0	9.59626	20.11978
3	34.9	7.32438	27.44416
4	35.1	4.84336	32.28752
5	34.9	1.34157	33.62909
6	35.0	1.50881	35.13790
7	34.9	0.00000	35.13790

Pulse Chemisorption Analysis Summary

Element	Percent of Sample Mass (%)	Percent Reduced (%)	MxOy X	MxOy Y	AMU	Stoichiometry Factor	Atomic Cross-Sectional Area (nm²)	Density (g/cm³)
molybdenum	19.500	100.00	1	0	95.940	1.000	0.0730	10.220

2640- The Active Metal Table does not specify a stoichiometry factor for the adsorptive Carbon Monoxide of the element molybdenum. One (1.0) was substituted for this value in the calculations.

Active loop volume at 110.0 °C: 1.6047 µmol
Cumulative quantity: 35.13790 µmol/g
Metal dispersion: 1.7288 %
Fractional coverage: 0.017288
Metallic surface area: 1.5447 m²/g sample
Metallic surface area: 7.9217 m²/g metal
Crystallite size (hemisphere): 741.1112 Å
Crystallite size (cube): 617.5927 Å

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
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Started: 6/3/2025 5:16:57 PM
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Report time: 1/19/2026 6:05:24 PM

Active Surface Area Report

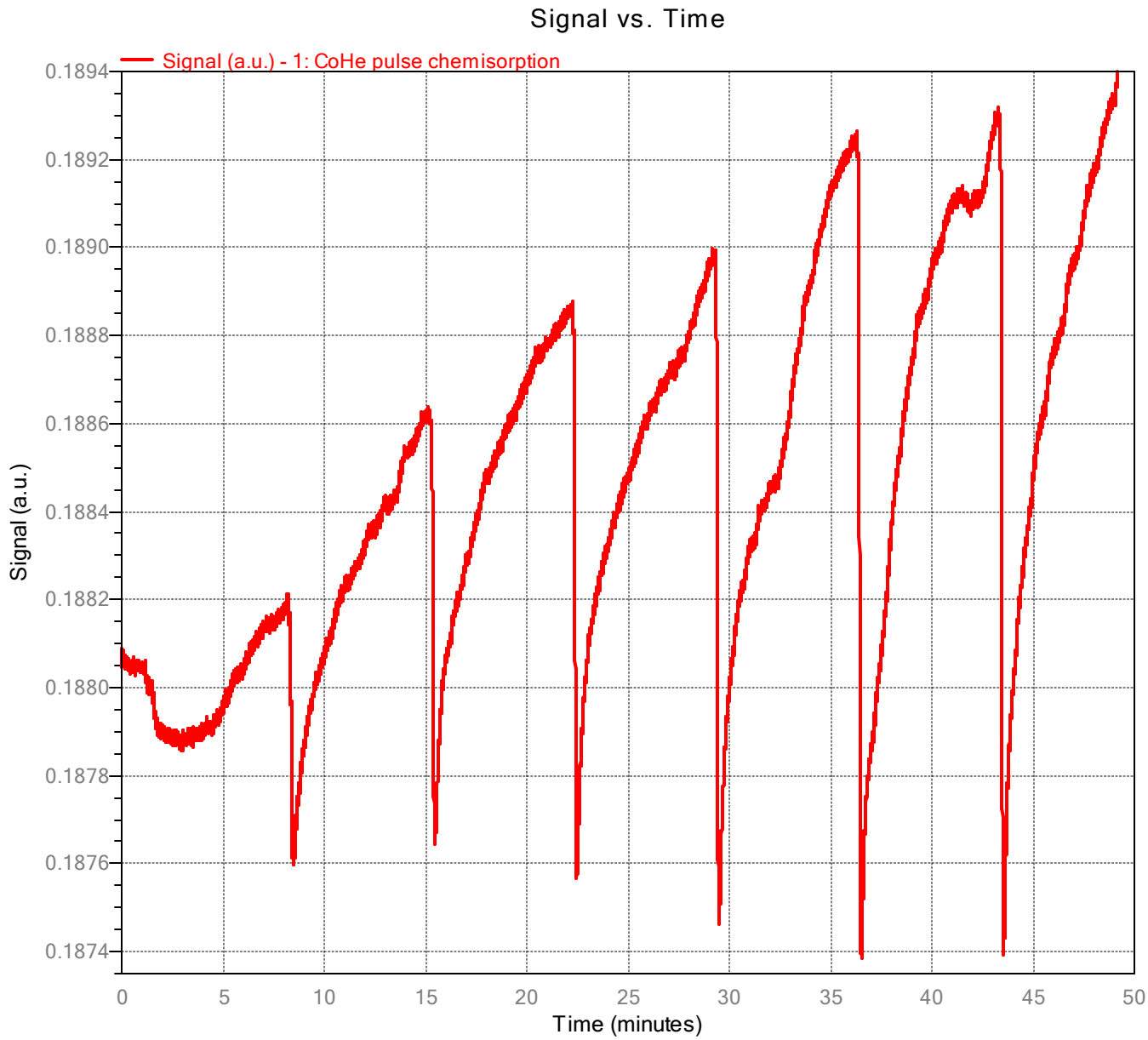
Active Surface Area

4615- No experiments were selected for inclusion in this report.

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

Started: 6/3/2025 5:16:57 PM
Completed: 6/3/2025 9:48:28 PM

Sample mass: 0.1181 g
Report time: 1/19/2026 6:05:24 PM



Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

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Sample mass: 0.1181 g
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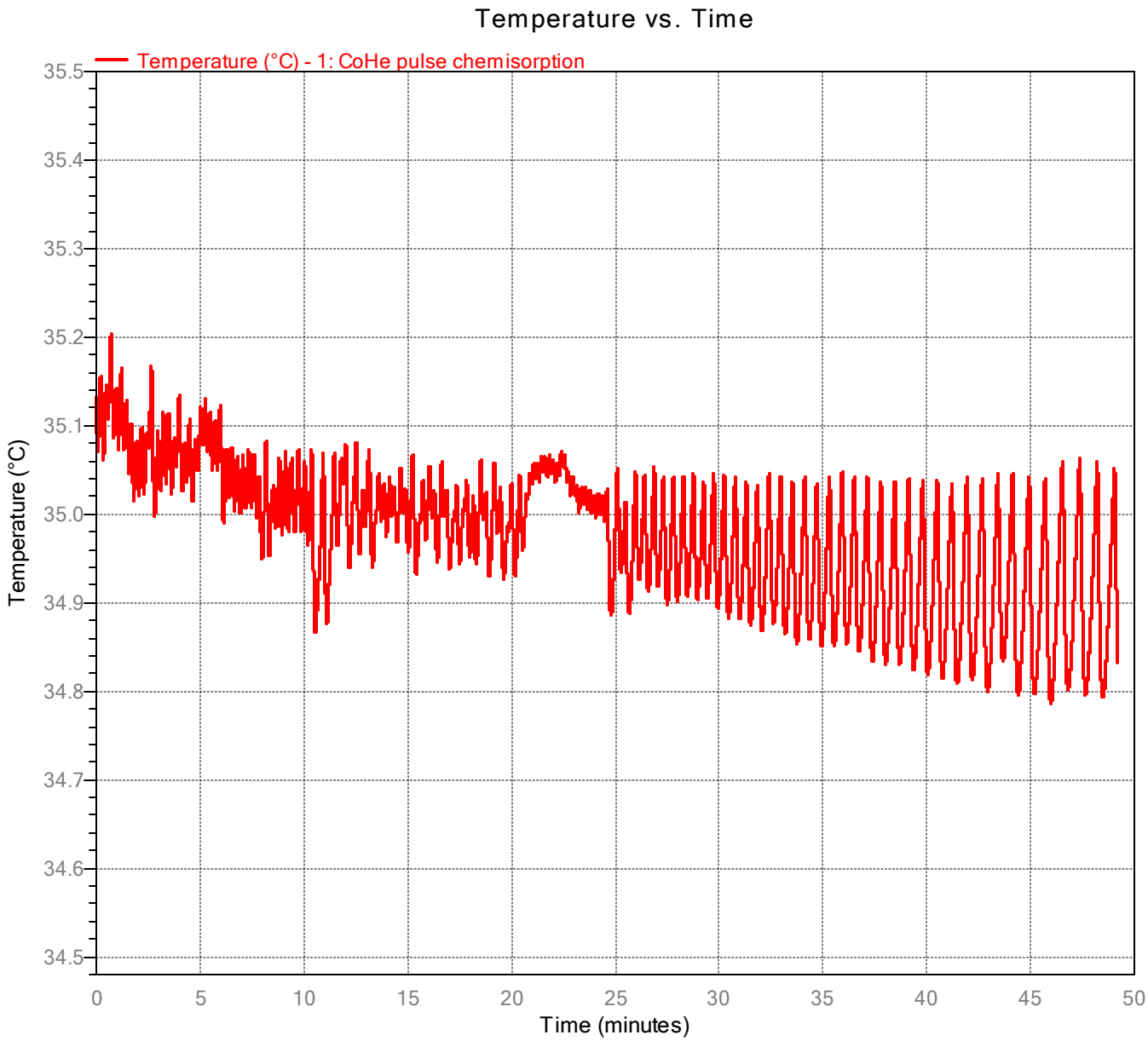

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

Started: 6/3/2025 5:16:57 PM
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Sample mass: 0.1181 g
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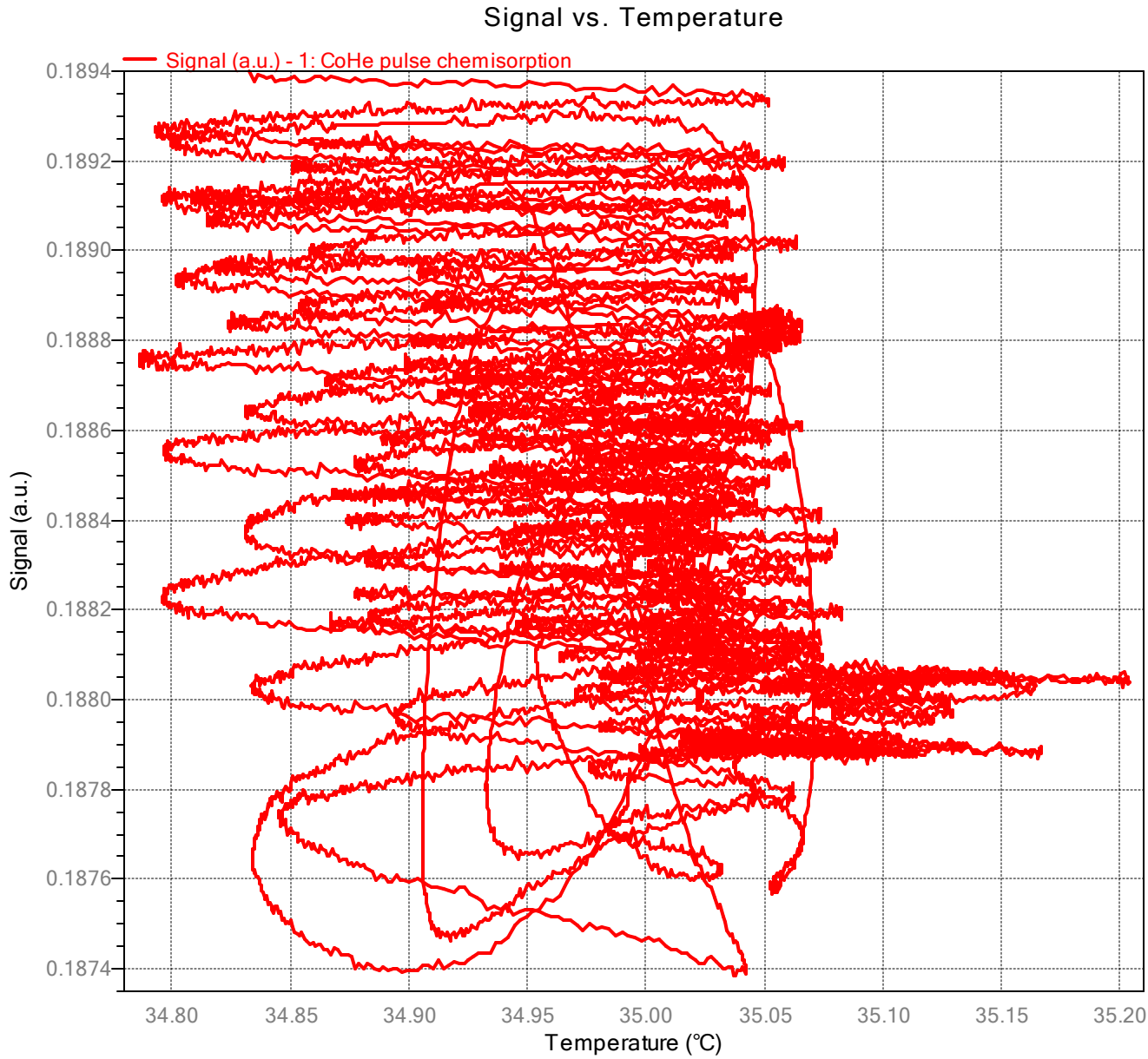

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

Started: 6/3/2025 5:16:57 PM
Completed: 6/3/2025 9:48:28 PM
Sample mass: 0.1181 g
Report time: 1/19/2026 6:05:24 PM

Sample Information

Method: Default
Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
Mass type: Entered
Sample mass: 0.1181 g
Density: 1.000 g/cm³
Type of data: Automatically collected
Instrument type: 2930
Original instrument type: 2930
Comments:

Active Metals Table

Element	Atomic Weight	Atomic Cross Sect. Area (nm²)	Density (g/cm³)	Percent of Sample Mass (%)	Percent Reduced (%)	MxOy X	MxOy Y
molybdenum	95.940	0.0730	10.220	19.500	100.00	1	0
	Adsorptive	Stoichiometry					
	Carbon Monoxide-Helium	1.000					

Analysis Conditions

Analysis conditions: Analysis Conditions
View conditions for: AutoChem III 2930

Baseline Options

Stable Baseline
Slope threshold: 0.010 %/min
Duration: 5.00 min
Change from Baseline
Acceleration threshold: 0.200 %/min²
Duration: 0.10 min
Return to Baseline
Acceleration threshold: 0.050 %/min²
Duration: 1.00 min

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

Started: 6/3/2025 5:16:57 PM
Completed: 6/3/2025 9:48:28 PM
Sample mass: 0.1181 g
Report time: 1/19/2026 6:05:24 PM

Tasks

	Description	Details
1.01	Experiment	--- CoHe pulse chemisorption --- Pulse
1.02	Instrument Settings	--- Instrument Settings --- Carrier: H2Ar @ 50.00 (None @ 100.00) (Bypass) (Bypass) (Fill) (Analyze) Trap
1.03	Temperature Ramp	--- Temperature Ramp --- Type: Sample Temperature: 500.0 °C Ramp rate: 10.0 °C/min Hold time: 90.00 min
1.04	Instrument Settings	--- Instrument Settings --- Carrier: He @ 50.00 (H2Ar @ 50.00) (Bypass) (Bypass) (Fill) (Analyze) Bypass
1.05	Wait	--- Wait --- Wait 60.00 min.
1.06	Instrument Settings	--- Instrument Settings --- Filaments:245.0 °C (Disabled)
1.07	Temperature Ramp	--- Temperature Ramp --- Type: Sample Temperature: 35.0 °C Ramp rate: 90.0 °C/min Hold time: 5.00 min
1.08	Instrument Settings	--- Instrument Settings --- Loop: COHe @ 50.00 (None @ 100.00) Reflux: 20.0 °C (Disabled) Flask: 20.0 °C (Disabled)
1.09	Wait	--- Wait --- Wait for return to baseline.
1.10	Start Recording	--- Start Recording --- One measurement every 0.10 s Set external trigger: No
1.11	Start Repeat	--- Start Repeat --- Repeat until peaks are equal or 25 times.
1.12	Dose	--- Dose --- Inject loop gas Wait for change in baseline or 5.00 min, then wait for a return to baseline.
1.13	Stop Repeat	--- Stop Repeat ---
1.14	Stop Recording	--- Stop Recording ---

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

Started: 6/3/2025 5:16:57 PM
Completed: 6/3/2025 9:48:28 PM
Sample mass: 0.1181 g
Report time: 1/19/2026 6:05:24 PM

Tasks

	Description	Details
1.15	Instrument Settings	--- Instrument Settings --- Loop: None @ 50.00 (COHe @ 50.00) Filaments:Disabled (245.0 °C)
1.16	Wait	--- Wait --- Wait 5.00 min.
	Termination	--- Termination --- Carrier: None @ 100.00 (He @ 50.00) Loop: None @ 100.00 (None @ 50.00) Reflux: Disabled (20.0 °C) Flask: Disabled (20.0 °C) Sample: Ambient (35.0 °C) Rate: Ambient (90.0 °C/min)

Stoichiometry Factors for Experiment 1

Element	Adsorptive	Stoichiometry
chromium	Carbon Monoxide-Helium	1.000

Adsorptive Properties

Adsorptive: Helium (He)
Maximum manifold pressure: 123.323 kPa
Therm. tran. hard-sphere diameter: 2.6300 Å
Molecular cross-sectional area: 0.123 nm²
Adsorbate molecular weight: 4.00
Mass flow constant: 1.000
Relative thermal conductivity: 5.84
Gas blend: No
Adsorbed-phase free-space correction: No
Fluid properties: C:\dev\product\2930\example-data\helium.FPI
Dosing method: Normal

Adsorptive: Carbon Monoxide-Helium (COHe)
Maximum manifold pressure: 123.323 kPa
Therm. tran. hard-sphere diameter: 3.5900 Å
Molecular cross-sectional area: 0.125 nm²
Adsorbate molecular weight: 28.01
Mass flow constant: 1.000
Relative thermal conductivity: 5.29
Gas blend: Yes
Inert gas: Helium
Active gas: Carbon Monoxide
% Active Concentration 10.320 %
Adsorbed-phase free-space correction: Yes
Fluid properties: H:\FPI\fpiv7\carbon monoxide.fpi
Dosing method: Normal

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

Started: 6/3/2025 5:16:57 PM
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Sample mass: 0.1181 g
Report time: 1/19/2026 6:05:24 PM

Adsorptive:	Hydrogen-Argon (H2Ar)
Maximum manifold pressure:	123.323 kPa
Therm. tran. hard-sphere diameter:	2.9680 Å
Molecular cross-sectional area:	0.123 nm²
Adsorbate molecular weight:	2.02
Mass flow constant:	1.000
Relative thermal conductivity:	1.40
Gas blend:	Yes
Inert gas:	Argon
Active gas:	Hydrogen
% Active Concentration	10.000 %
Adsorbed-phase free-space correction:	Yes
Fluid properties:	H:\FPI\fpiv7\hydrogen.fpi
Dosing method:	Normal

Report Options

Peak Detection/Integration Options

Baseline mode:	Best fit baseline
Minimum peak height:	0.25 % F.S.
Peak smoothing:	0 points
Sensitivity:	1.0e-02 % F.S.
Maximum shoulder ratio:	33%
Maximum group separation:	33%
Minimum peak area:	1.0 % F.S.·min
Maximum baseline slope:	0.1 % F.S./sec

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

Started: 6/3/2025 5:16:57 PM
Completed: 6/3/2025 9:48:28 PM
Sample mass: 0.1181 g
Report time: 1/19/2026 6:05:24 PM

Sample Log

Date	Time	Log Message
6/3/2025	5:16:57 PM	Starting a sample analysis for C:\Users\b22...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP on port 1.
6/3/2025	5:16:58 PM	1.01 Experiment started. Type: Pulse
6/3/2025	5:16:58 PM	1.02 Set carrier gas: H2Ar Loop gas: N2He Trap valve: Trap Analysis valve: Analysis Sample temperature: 20.0 °C Detector enabled: No
6/3/2025	5:17:05 PM	1.03 Ramping Sample temperature at 10.0 °C/min to 500.0 °C for 90 minutes.
6/3/2025	7:35:30 PM	1.04 Set carrier gas: He Loop gas: N2He Trap valve: Bypass Analysis valve: Analysis Sample temperature: 500.0 °C Detector enabled: No
6/3/2025	7:35:35 PM	1.05 Wait for time. Time: 3600 s
6/3/2025	8:35:35 PM	1.06 Set carrier gas: He Loop gas: N2He Trap valve: Bypass Analysis valve: Analysis Sample temperature: 500.0 °C Detector enabled: Yes
6/3/2025	8:35:36 PM	1.07 Ramping Sample temperature at 90.0 °C/min to 35.0 °C for 5 minutes.
6/3/2025	8:53:12 PM	1.08 Set carrier gas: He Loop gas: COHe Trap valve: Bypass Analysis valve: Analysis Sample temperature: 35.0 °C Detector enabled: Yes
6/3/2025	8:53:13 PM	1.09 Wait for return to baseline. Time: 60 s
6/3/2025	8:54:14 PM	1.10 Recording started. Carrier gas: He Flow rate: 50.00 cm³ STP/min Loop gas: COHe Recording period: 0.10 s External trigger: No
6/3/2025	8:54:14 PM	1.11 Start repeat sequence. Repeat until peaks are equal 25 times.
6/3/2025	8:54:14 PM	1.12 Dose: Inject loop gas. Wait for change from baseline or time, then return to baseline. Time: 5 min
6/3/2025	8:55:15 PM	Inject loop gas Injection volume: 0.4981 mL. Atmospheric pressure: 745.97 mmHg. Ambient temperature: 24.9 °C
6/3/2025	9:01:15 PM	1.13 Check for end of repeat sequence after 1 times. Continue repeating: Yes
6/3/2025	9:01:15 PM	1.12 Dose: Inject loop gas. Wait for change from baseline or time, then return to baseline. Time: 5 min
6/3/2025	9:02:16 PM	Inject loop gas Injection volume: 0.4981 mL. Atmospheric pressure: 746.02 mmHg. Ambient temperature: 24.8 °C
6/3/2025	9:08:17 PM	1.13 Check for end of repeat sequence after 2 times. Continue repeating: Yes
6/3/2025	9:08:17 PM	1.12 Dose: Inject loop gas. Wait for change from baseline or time, then return to baseline. Time: 5 min
6/3/2025	9:09:18 PM	Inject loop gas Injection volume: 0.4981 mL. Atmospheric pressure: 746.06 mmHg. Ambient temperature: 24.7 °C
6/3/2025	9:15:18 PM	1.13 Check for end of repeat sequence after 3 times. Continue repeating: Yes
6/3/2025	9:15:18 PM	1.12 Dose: Inject loop gas. Wait for change from baseline or time, then return to baseline. Time: 5 min
6/3/2025	9:16:19 PM	Inject loop gas Injection volume: 0.4981 mL. Atmospheric pressure: 746.06 mmHg. Ambient temperature: 24.6 °C
6/3/2025	9:22:20 PM	1.13 Check for end of repeat sequence after 4 times. Continue repeating: Yes
6/3/2025	9:22:20 PM	1.12 Dose: Inject loop gas. Wait for change from baseline or time, then return to baseline. Time: 5 min
6/3/2025	9:23:21 PM	Inject loop gas Injection volume: 0.4981 mL. Atmospheric pressure: 746.17 mmHg. Ambient temperature: 24.5 °C
6/3/2025	9:29:22 PM	1.13 Check for end of repeat sequence after 5 times. Continue repeating: Yes
6/3/2025	9:29:22 PM	1.12 Dose: Inject loop gas. Wait for change from baseline or time, then return to baseline. Time: 5 min
6/3/2025	9:30:22 PM	Inject loop gas Injection volume: 0.4981 mL. Atmospheric pressure: 746.28 mmHg. Ambient temperature: 24.4 °C
6/3/2025	9:36:24 PM	1.13 Check for end of repeat sequence after 6 times. Continue repeating: Yes

Sample: 000-163 Mo3Fe1-C_B-CO pulse 110 mg
Operator: Mihir
Submitter:
File: C:\Users\kulka133\OneDrive - Michigan State University\CMS...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP

Started: 6/3/2025 5:16:57 PM
Completed: 6/3/2025 9:48:28 PM
Sample mass: 0.1181 g
Report time: 1/19/2026 6:05:24 PM

Sample Log

Date	Time	Log Message
6/3/2025	9:36:24 PM	1.12 Dose: Inject loop gas. Wait for change from baseline or time, then return to baseline. Time: 5 min
6/3/2025	9:37:24 PM	Inject loop gas Injection volume: 0.4981 mL. Atmospheric pressure: 746.25 mmHg. Ambient temperature: 24.3 °C
6/3/2025	9:43:25 PM	1.13 Check for end of repeat sequence after 7 times. Continue repeating: No
6/3/2025	9:43:25 PM	1.14 Recording ended.
6/3/2025	9:43:25 PM	1.15 Set carrier gas: He Loop gas: N2He Trap valve: Bypass Analysis valve: Analysis Sample temperature: 35.0 °C Detector enabled: No
6/3/2025	9:43:27 PM	1.16 Wait for time. Time: 300 s
6/3/2025	9:48:27 PM	2.01 Analysis terminated. Carrier gas: N2He Detector enabled: No Return to ambient temperature: Yes
6/3/2025	9:48:28 PM	Finished a sample analysis for C:\Users\b22...\000-163 Mo3Fe1-C_B-CO pulse 110 mg.SMP on port 1.