Sample: 240607-5Mo.5FeACcal-IWI-mk-020
Operator: Bryce
Submitter:
File: D:\Flex\data\Bryce\000-050 240607 5Mo.5FeAC_MK020 H2 TPR.SMP

Started: 6/7/2024 11:06:43 AM   Sample mass: 0.1125 g
Completed: 6/7/2024 3:38:27 PM   Report time: 6/12/2024 4:07:57 PM

Comments: Cold trap in LN2/IPA slurry
TPR with 10% H2
5Mo.5FeAC IWI MK020

Summary Report

Experiment 1: AgO TPR with H2Ar

Analysis type: Temperature Programmed
Calibration: None
Measured flow rate: 2,230.7 µmol/min
Signal offset: 0.00000
Signal inverted: No

Peak Number	Temperature at Maximum (°C)	Area	Peak Height
1	477.7	0.85950	-6.624e-02
2	748.6	8.081e-06	-1.068e-04
3	777.9	1.684e-04	-2.419e-04

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Signal (a.u.) vs. Time

Sample: 240607-5Mo.5FeACcal-IWl-mk-020
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Temperature vs. Time

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Sample Information

Method: $ AgO TPR with H2Ar
Sample: 240607-5Mo.5FeACcal-IWI-mk-020
Operator: Bryce
Submitter:
Mass type: Calculated
Empty tube: 31.5548 g
Sample + tube: 31.6673 g
Sample mass: 0.1125 g
Density: 1.000 g/cm³
Type of data: Automatically collected
Instrument type: 3500 Dynamic Chemi
Original instrument type: 3500 Dynamic Chemi
Comments: Cold trap in LN2/IPA slurry
TPR with 10% H2
5Mo.5FeAC IWI MK020

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	5.000	100.00	1	0

	Stoichiometry
Adsorptive Hydrogen	2.000
Oxygen	2.000
Carbon Monoxide	1.000

Element	Atomic Weight	Atomic Cross Sect. Area (nm²)	Density (g/cm³)	Percent of Sample Mass (%)	Percent Reduced (%)	MxOy X	MxOy Y
Iron	55.847	0.0613	7.890	0.500	100.00	1	0

Analysis Conditions

Analysis conditions: 10% H2
View conditions for:

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

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Baseline Options
Duration: 1.00 min

Tasks

	Description	Details
1.01	Experiment	AgO TPR with H2Ar
		Type: Temperature Programmed
1.02	Gas Flow	Carrier gas: Nitrogen
		Loop or injection gas:
1.03	Temperature Ramp	Type: Sample
		Temperature: 150.0 °C
		Ramp rate: 10.0 °C/min
		Hold time: 45.00 min
1.04	Temperature Ramp	Type: Sample
		Temperature: 40.0 °C
		Ramp rate: 10.0 °C/min
		Hold time: 30.00 min
1.05	Gas Flow	Carrier gas: Hydrogen-Argon
		Loop or injection gas:
1.06	Set Detector	Enable detector: Yes
		Filament temperature: 175.0 °C
1.07	Wait	Wait until baseline is stable.
1.08	Start Recording	One measurement every 0.10 s
1.09	Temperature Ramp	Type: Sample
		Temperature: 950.0 °C
		Ramp rate: 10.0 °C/min
		Hold time: 0.00 min
1.10	Stop Recording	Stop Recording
	Termination	Return to ambient: Yes
		Carrier gas:
		Loop gas:

Adsorptive Properties

Adsorptive: Hydrogen-Argon (H2Ar)
Maximum manifold pressure: 925.00 mmHg
Therm. tran. hard-sphere diameter: 0.31480 nm
Molecular cross-sectional area: 0.143 nm²
Adsorbate molecular weight: 39.95
Mass flow constant: 1.000
Relative thermal conductivity: 1.40
Gas blend: Yes
Inert gas: Argon
Active gas: Hydrogen
% Active Concentration 10.000 %
Fluid properties: H:\FPI\fpiv6\argon.fpi
Dosing method: Normal

Sample: 240607-5Mo.5FeACcal-IWI-mk-020
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Submitter:
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Adsorptive: Nitrogen (N2)
Maximum manifold pressure: 925.00 mmHg
Therm. tran. hard-sphere diameter: 0.36810 nm
Molecular cross-sectional area: 0.162 nm²
Adsorbate molecular weight: 28.01
Mass flow constant: 1.000
Relative thermal conductivity: 1.00
Gas blend: No
Fluid properties: H:\FPI\fpiv6\nitrogen.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

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Sample Log

Date	Time	Log Message
6/7/2024	11:06:44 AM	1.01 Experiment started. Type: Temperature Programmed
6/7/2024	11:06:44 AM	1.02 Set gas flow. Carrier gas: N2 Flow rate: 50.00 cm³ STP/min Loop gas:
6/7/2024	11:06:45 AM	1.03 Ramping Sample temperature at 10.0 °C/min to 150.0 °C for 45 minutes.
6/7/2024	12:07:49 PM	1.04 Ramping Sample temperature at 10.0 °C/min to 40.0 °C for 30 minutes.
6/7/2024	12:52:11 PM	1.05 Set gas flow. Carrier gas: H2Ar Flow rate: 50.00 cm³ STP/min Loop gas:
6/7/2024	12:52:12 PM	1.06 Set detector. Detector enabled: Yes Filament temperature: 175.0 °C
6/7/2024	12:52:12 PM	1.07 Wait for baseline stable. Time: 300 s
6/7/2024	1:13:42 PM	1.08 Recording started. Carrier gas: H2Ar Flow rate: 50.00 cm³ STP/min Loop gas: Recording period: 0.10 s
6/7/2024	1:13:42 PM	1.09 Ramping Sample temperature at 10.0 °C/min to 950.0 °C for 0 minutes.
6/7/2024	2:59:37 PM	1.10 Recording ended.
6/7/2024	2:59:37 PM	2.01 Analysis terminated. Detector enabled: No Return to ambient temperature: Yes
6/7/2024	3:38:27 PM	Finished a sample analysis for D:\Flex\d...\000-050 240607 5Mo.5FeAC_MK020 H2 TPR.SMP.