Sample: 240610-5Mo1.5FeACcal-IWI-mk-021
Operator: Bryce
Submitter:
File: D:\Flex\data\Bryce\000-051 240610 5Mo1.5FeAC_MK021 H2 TPR.SMP

Started: 6/10/2024 11:46:32 AM
Completed: 6/10/2024 4:21:08 PM
Sample mass: 0.1080 g
Report time: 6/12/2024 4:08:33 PM

Comments: Cold trap in LN2/IPA slurry
TPR with 10% H2
5Mo1.5FeAC IWI MK021

## Summary Report

### Experiment 1: AgO TPR with H2Ar

Analysis type: Temperature Programmed
Calibration: None
Measured flow rate: 2,230.8 µmol/min
Signal offset: 0.00000
Signal inverted: No

| Peak Number | Temperature at Maximum (°C) | Area | Peak Height |
|---|---|---|---|
| 1 | 201.6 | 1.398e-03 | 2.242e-04 |
| 2 | 488.7 | 0.95791 | -6.900e-02 |

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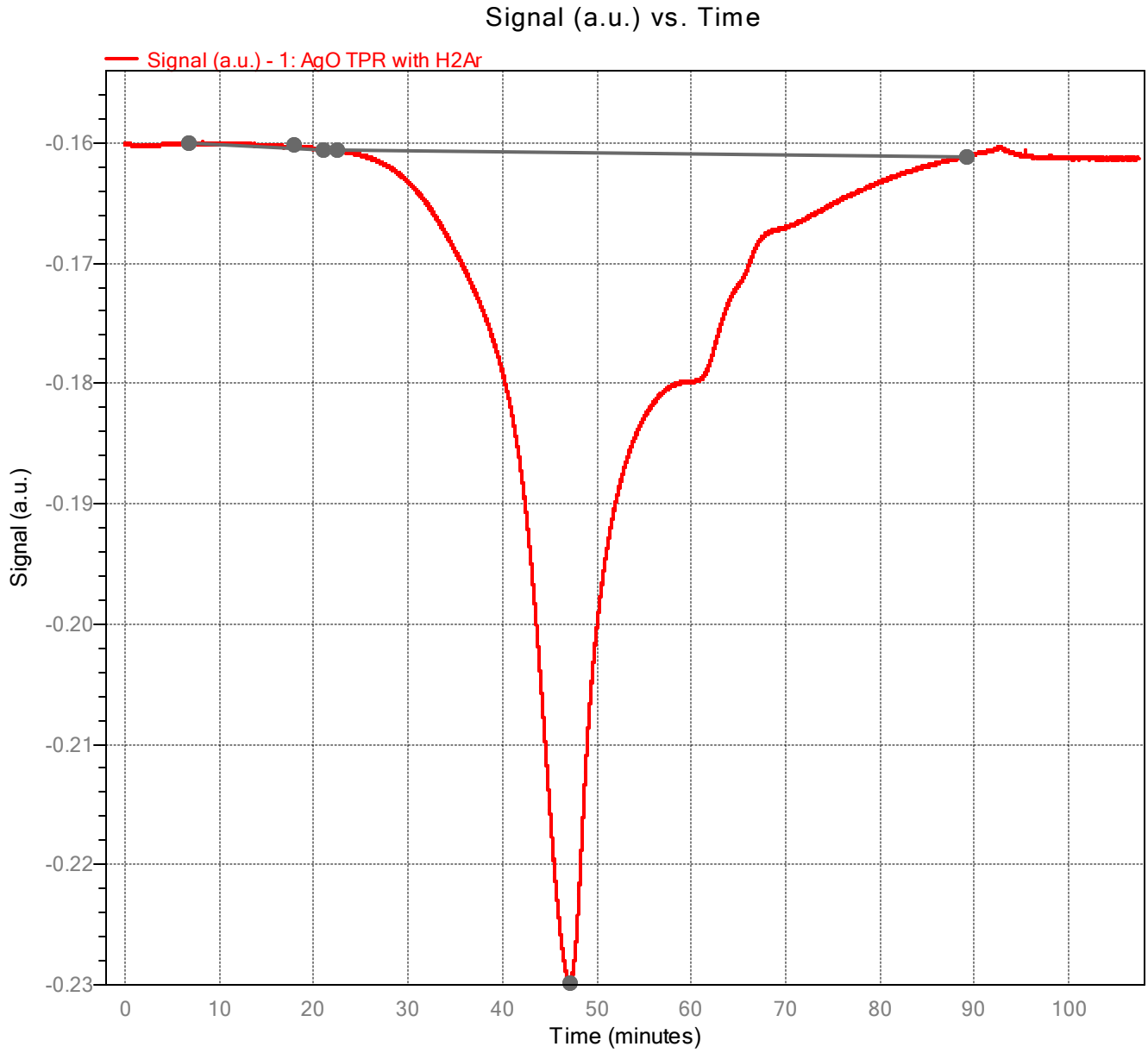

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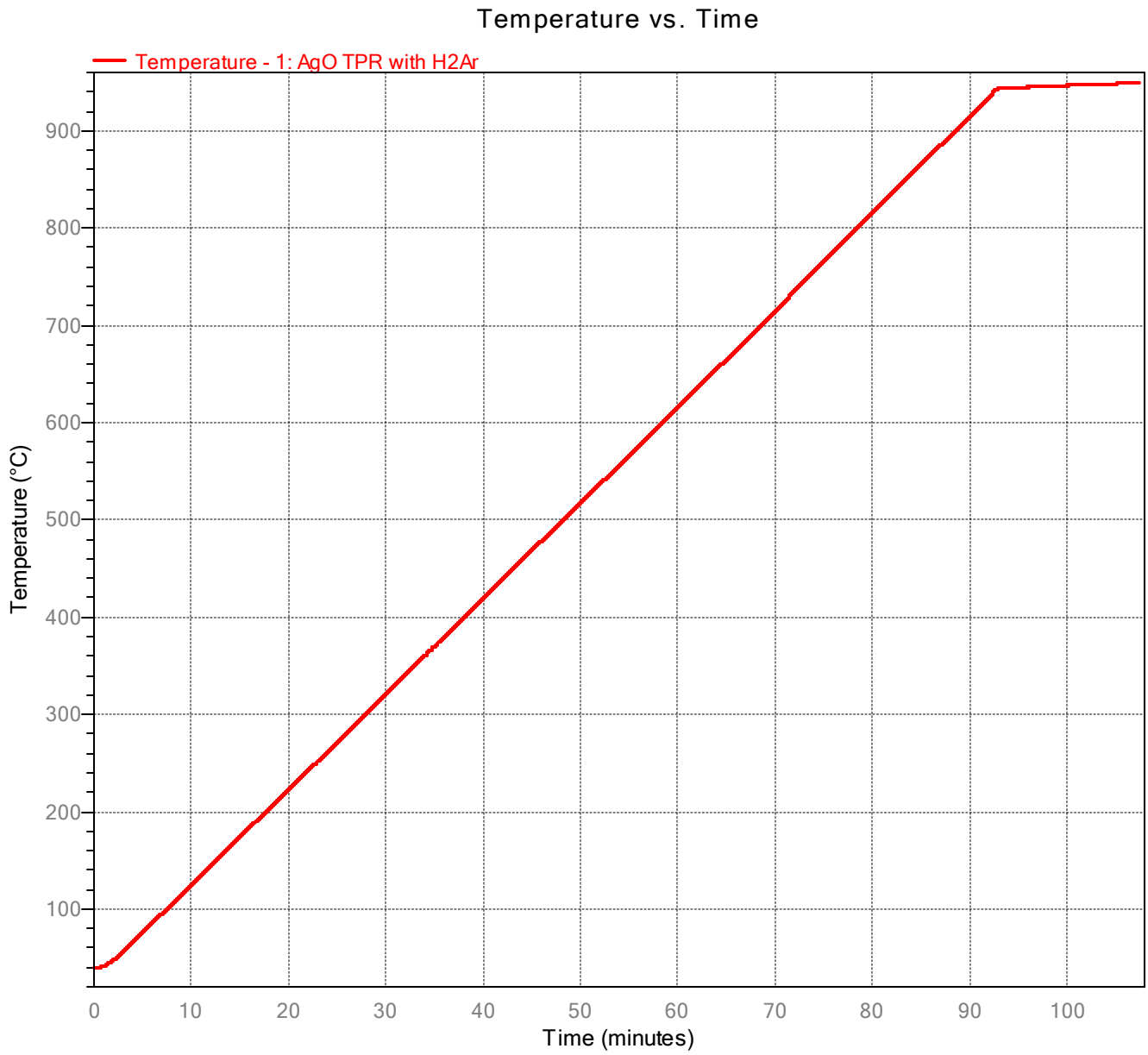

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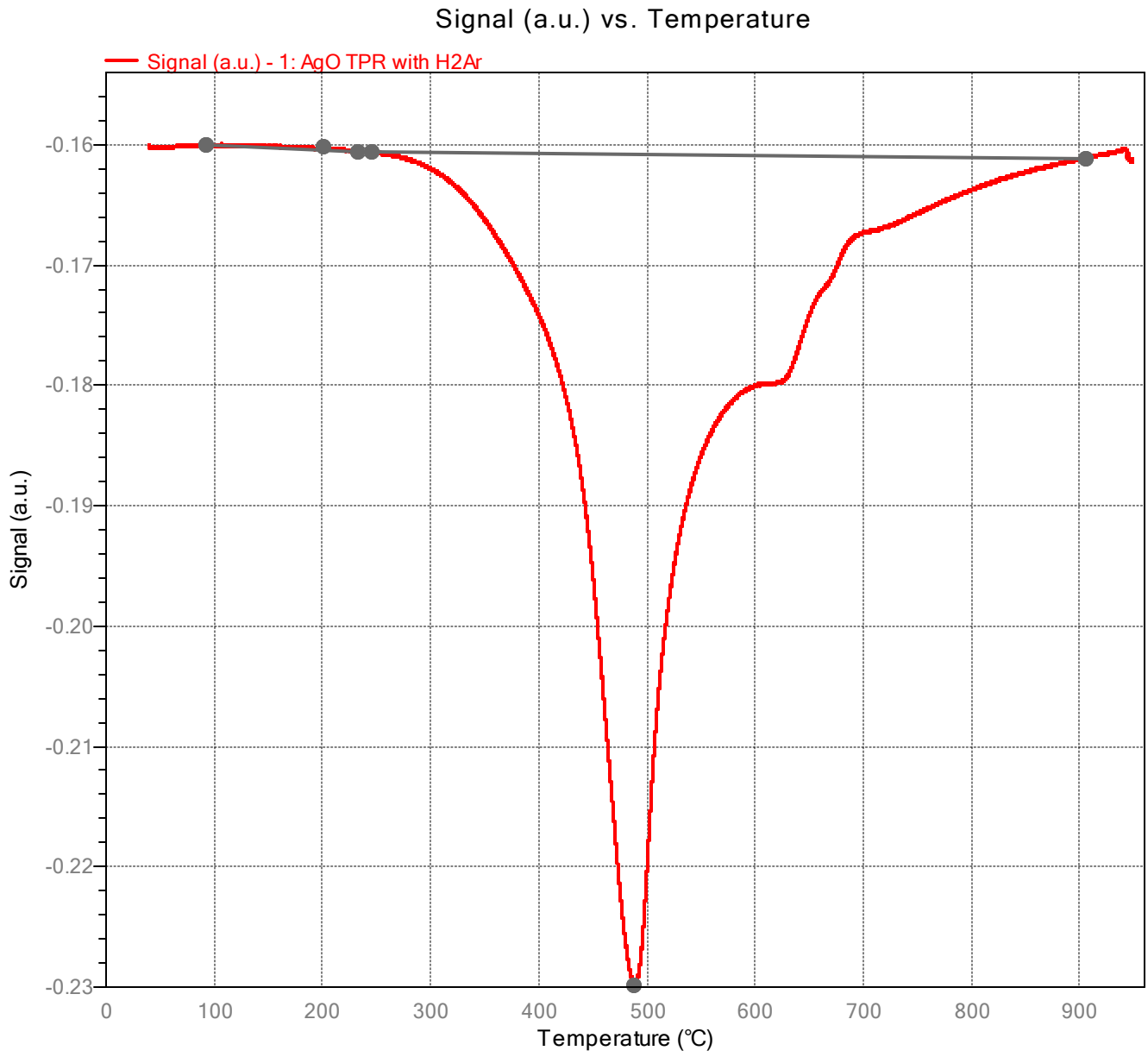

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## Sample Information

Method: $ AgO TPR with H2Ar
Sample: 240610-5Mo1.5FeACcal-IWI-mk-021
Operator: Bryce
Submitter:
Mass type: Calculated
Empty tube: 32.3797 g
Sample + tube: 32.4877 g
Sample mass: 0.1080 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
5Mo1.5FeAC IWI MK021

### 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 |
| | Adsorptive | Stoichiometry | | | | | |
| | Hydrogen | 2.000 | | | | | |
| | Oxygen | 2.000 | | | | | |
| | Carbon Monoxide | 1.000 | | | | | |
| Iron | 55.847 | 0.0613 | 7.890 | 1.500 | 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<br>Type: Temperature Programmed |
| 1.02 | Gas Flow | Carrier gas: Nitrogen<br>Loop or injection gas: |
| 1.03 | Temperature Ramp | Type: Sample<br>Temperature: 150.0 °C<br>Ramp rate: 10.0 °C/min<br>Hold time: 45.00 min |
| 1.04 | Temperature Ramp | Type: Sample<br>Temperature: 40.0 °C<br>Ramp rate: 10.0 °C/min<br>Hold time: 30.00 min |
| 1.05 | Gas Flow | Carrier gas: Hydrogen-Argon<br>Loop or injection gas: |
| 1.06 | Set Detector | Enable detector: Yes<br>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<br>Temperature: 950.0 °C<br>Ramp rate: 10.0 °C/min<br>Hold time: 0.00 min |
| 1.10 | Stop Recording<br>Termination | Stop Recording<br>Return to ambient: Yes<br>Carrier gas:<br>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

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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 |
|---|---|---|
| 6/10/2024 | 11:46:32 AM | 1.01 Experiment started. Type: Temperature Programmed |
| 6/10/2024 | 11:46:32 AM | 1.02 Set gas flow. Carrier gas: N2 Flow rate: 50.00 cm³ STP/min Loop gas: |
| 6/10/2024 | 11:47:22 AM | 1.03 Ramping Sample temperature at 10.0 °C/min to 150.0 °C for 45 minutes. |
| 6/10/2024 | 12:48:58 PM | 1.04 Ramping Sample temperature at 10.0 °C/min to 40.0 °C for 30 minutes. |
| 6/10/2024 | 1:33:08 PM | 1.05 Set gas flow. Carrier gas: H2Ar Flow rate: 50.00 cm³ STP/min Loop gas: |
| 6/10/2024 | 1:33:08 PM | 1.06 Set detector. Detector enabled: Yes Filament temperature: 175.0 °C |
| 6/10/2024 | 1:33:08 PM | 1.07 Wait for baseline stable. Time: 300 s |
| 6/10/2024 | 1:54:59 PM | 1.08 Recording started. Carrier gas: H2Ar Flow rate: 50.00 cm³ STP/min Loop gas: Recording period: 0.10 s |
| 6/10/2024 | 1:54:59 PM | 1.09 Ramping Sample temperature at 10.0 °C/min to 950.0 °C for 0 minutes. |
| 6/10/2024 | 3:42:24 PM | 1.10 Recording ended. |
| 6/10/2024 | 3:42:24 PM | 2.01 Analysis terminated. Detector enabled: No Return to ambient temperature: Yes |
| 6/10/2024 | 4:21:08 PM | Finished a sample analysis for D:\Flex\...\000-051 240610 5Mo1.5FeAC_MK021 H2 TPR.SMP. |