Appendix C – Reactivity Testing Results and Analysis

Fatal Runaway Reaction and Explosion at Givaudan Sense Colour / D.D. Williamson

No. 2024-06-I-KY

TABLE OF CONTENTS

OVERVIEW

This appendix contains laboratory calorimetry reports used to evaluate the chemical reactivity, heat release, and pressure behavior of the Reactor 6 (Cooker 6) recipe. These results are followed by gas analysis reports that identify the gases produced during the reactions. The appendix also includes solids analysis of the black char material formed during calorimetry testing, with comparison to black samples retrieved from remnants inside Reactor 6 (Cooker 6).

LABORATORY CALORIMETRY REPORTS

The following reports detail the calorimetry testing conducted on the Reactor 6 (Cooker 6) recipe and invert sugar alone. Both Automatic Pressure-Tracking Adiabatic Calorimeter (APTAC) and Accelerating Rate Calorimeter (ARC) tests were conducted. Vent Sizing Package 2 (VSP2) tesing was also conducted.

Automatic Pressure-Tracking Adiabatic Calorimeter (APTAC™) Report

Chemical Reactivity Evaluation

Invert, Phosphoric Acid, Sodium Hydroxide and Antifoam Reactions

Report to:
U.S. Chemical Safety and Hazard Investigation Board
470 L'Enfant Plaza SW
Suite 604 #23278
Washington, DC 20026

Date: September 15, 2025

This report was prepared by ioKinetic for the account of CSB. This report represents ioKinetic's best judgment in light of information made available to us. Opinions in this report are based in part upon data and information (Sample Identification) provided by CSB and / or CSB's advisors and affiliates. This report relates only to the sample as received unless otherwise noted. The reader is advised that ioKinetic has not independently verified the data or the information contained therein. This report must be read in its entirety. The reader understands that no assurances can be made that all liabilities have been identified. This report does not constitute a legal opinion. The results provided are apparatus dependent and should not be used for direct scale-up. They apply to the samples as tested and are useful as a comparison tool only.

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Report No.: ioK#: 25099 Rev.1

AT-1922

95 Stiles Road | Salem, New Hampshire 03079
www.ioKinetic.com | P: 603.893.7009 | F: 603.386.6522

Revision History

Rev.	Date	List of Changes	Prepared by	Approved by
0	5/30/2025	Draft Final Review Copy	E. Shaaban, PhD	A. Iskandar, PhD
1	09/15/2025	Final Report	E. Shaaban, PhD	A. Iskandar, PhD

Table of Contents

List of Tables

Appendices

1 Study Overview

This report presents the results of the Automatic Pressure-Tracking Adiabatic Calorimeter (APTAC™) testing for invert, phosphoric acid, sodium hydroxide, and antifoam.

Two tests were completed: one titled 'APTAC-CSB03132025 Test 1' used invert, phosphoric acid, and sodium hydroxide sourced from food and chemical suppliers, and the other, 'APTAC-CSB-03192025 Test 2' used chemicals from the Givaudan site. Both test recipes were based on the materials added to the cooker prior to the runaway event. These materials and their quantities are summarized in Table 1 and referenced in the files “Cooker 6 484 Batch Sequence Day of Incident” and “Summary of Information Provided by CSB.”

Table 1: Quantities of Materials Added to Cooker 6 Before Incident

Material	Original Recipe (Pounds)	Percent
Invert	[redacted]	[redacted]
Phosphoric Acid [redacted]	[redacted]	[redacted]
Sodium Hydroxide [redacted]	[redacted]	[redacted]
Water	[redacted]	[redacted]
Antifoam	[redacted]	[redacted]
Total	[redacted]	100.00

To facilitate adiabatic measurements and feasible lab-scale testing with the instrument configuration, the multiple caustic addition steps were consolidated into a single injection at room temperature.

The composition of the two tests is summarized in Table 2 below.

Table 2: Composition Information for the Two APTAC Tests

Components (g)	APTAC - CSB 03132025 Test1		APTAC-CSB-03192025 Test 2	
	Source	Weight (g)	Soure	Weight (g)
Invert	Domino Foods Inc.	[redacted]	Givaudan	[redacted]
Phosphoric Acid [redacted]	Sigma-Aldrich	[redacted]	Givaudan	[redacted]
Sodium Hydroxide [redacted]	Sigma-Aldrich	[redacted]	Givaudan, item #328	[redacted]
Water	ioKinetic	[redacted]	ioKinetic	[redacted]
Antifoam	-	[redacted]	Givaudan	[redacted]
	Total:	49.812	50.118	

1.1 APTAC Test Setup and Procedure

1. APTAC - CSB 03132025 Test 1

Invert sugar was charged into a stainless steel APTAC test cell under an air atmosphere. A Heat-Wait-Search (HWS) program was initiated, starting at 40 °C and ramping up to 400 °C in 5 °C increments, with a 0.03 °C/min exotherm sensitivity and a 1500 psia pressure limit. Once equilibrium was reached at 40 °C during search mode, phosphoric acid was injected. Ten minutes later, sodium hydroxide solution was added. Water was then injected, and the main valve was closed. No antifoam was injected.

2. APTAC - CSB-03192025 Test 2

In an air atmosphere, invert sugar was charged into a stainless steel APTAC test cell. A Heat-Wait-Search (HWS) program was initiated, starting at 40 °C and ramping up to 400 °C in 5 °C increments, with an exotherm sensitivity of 0.03 °C/min and a pressure limit of 1500 psia. Once equilibrium was reached at 40 °C during the search mode, phosphoric acid was injected. Ten minutes later, sodium hydroxide solution was added. Water and antifoam were premixed at a 96:4 ratio, and the required amount of this mixture was then injected before closing the main valve.

Information about the test setup is summarized in Table 3. Additional test details relative to samples can be found in the APTAC test reports in Appendix B. The detailed APTAC test description is provided in Appendix A.

Table 3: APTAC™ Experiment Information

APTAC Test Name	Cell Material / Mass (g) / Volume (mL)	Total Sample Mass (g)	Φ
APTAC - CSB 03132025 Test1	Stainless Steel / 93.22 / 110.00	49.812	1.65
APTAC-CSB-03192025 Test 2	Stainless Steel / 91.48 / 130.36	50.118	1.63

2 Test Results and Discussion

The APTAC test results are summarized in Table 4. Complete data reports generated by Process Safety Office® SuperChems® are included in Appendix B.

Table 4: Summary of APTAC™ Test Results

Test Name	Mass Loss (%)	Observed Result	Onset T (°C)	T Rise (°C)	Adiabatic T Rise (°C)	ΔHr (cal/g)	Max. T (°C)	Max. dT/dt (°C/min)	Max. P (psia)	Max. dP/dt (psi/min)
APTAC-CSB 03132025 Test1	12.622	Exotherm Exotherm Exotherm	40.03 63.82 111.64	16.45 1.61 154.4	27.09 2.65 254.18	-8.48 -0.83 -79.54	275.7	22.56	1447	34.61
APTAC-CSB-03192025 Test 2	10.934	Exotherm Exotherm Exotherm	40.16 73.12 117.35	20.5 2.77 157.8	33.47 4.52 257.11	-10.49 -1.42 -80.60	275.3	192.13	1523.8	43.81

The following observations were noted with respect to the data presented:

1. After cooldown, the 'APTAC-CSB03132025 Test 1' cell contained 370.5 psia of non-condensable gas at 38 °C. Upon venting, 6.287 g of sample mass was lost, accounting for both released gas and residue in the pressure transfer tube. The initial reactant mass was 49.812 g. After the test, 43.525 g remained—approximately 32.9 g of black solid and 10.6 g of pale yellow liquid.
2. After the cooldown, the “APTAC-CSB-03192025 Test 2” test cell contained 406 psia of non-condensable gas at 44 °C. Upon venting, 5.48 g of the sample was lost, accounting for both the released gas and material remaining in the pressure transfer tube. The initial mass of the reactants was 50.118 g. After the test, 44.638 g remained—consisting of approximately 32.64 g of black solid and 12.00 g of pale yellow liquid.

Appendix A: Test Description

An Automatic Pressure-Tracking Adiabatic Calorimeter (APTAC™) measures the time-dependent adiabatic pressure and temperature response of a reactive chemical or chemical mixture. Due to its unique pressure balancing technology and larger sample size, the APTAC™ has a low thermal inertia (~1.10), similar to that of a full-scale reactor or storage vessel. During an exothermic event, the system will achieve more realistic adiabatic and temperature rise rates. Typically, APTAC™ data can be directly applied to larger vessels with minor scale-up corrections.

Building on the calorimetry expertise developed through the original (APTAC™), the advanced APTAC™ instrument has additional capabilities to perform experiments requiring low self-heat rate detection, reactant injection, vented operation, isothermal aging, and gas/solid phase reaction analysis. Data can be used to complete pressure relief and flare systems design, simulate batch and semi-batch reaction processes, and define physical properties.

The data generated from the APTAC™ is listed in Table A1 below.

Table A1: APTAC™ Data Summary

Results	Description	Unit
Thermal inertia	Thermal inertia of test cell with sample	N/A
T_{onset}	The onset temperature of exotherm	°C
$(dT/dt)_{max}$	Maximum self-heat rate of exotherm	°C/min
$(dP/dt)_{max}$	Maximum pressure rise rate of exotherm	psi/min
T_{max}	Temperature at maximum self-heat rate	°C
P_{max}	Maximum pressure generated from exotherm	psi
ΔT	Temperature rise measured	°C
ΔT adiabatic	Adiabatic temperature rise calculated	°C
ΔH	Enthalpy of reaction	cal/g mix

To conduct a test, the reaction mixture is introduced into a spherical test cell whose volume is approximately 130 ml. The cell is equipped with a thermocouple mounted inside the sample fluid. The pressure is recorded by means of a pressure transducer. The APTAC™ has an exothermic onset detectability as low as 0.04°C/min.

The APTAC™ can track temperatures up to approximately 400°C /min. Operator skill ensures proper calibration. The instrument is fully automated and once operating, needs minimal to no operator intervention.

Some details on the APTAC™ 264 include:

- Operating test cell temperature range: room temperature to 400°C
- Temperature Accuracy: +/-0.1°C
- Operating test cell pressure range: 0 to 140 bar (2,000 psia)
- Pressure accuracy: 0.1% of full scale
- Sample size: 5-100 ml standard
- Tracking rate at adiabatic operation up to 400 °C /min
- Test cell material options include Hastelloy- C, Titanium, Stainless Steel, Glass
- Stirring, injection, and venting capability
- ASTM standard: E1981

Definitions

Adiabatic Calorimeter – an instrument designed to make calorimetric measurements while maintaining a minimal heat loss or gain between the sample and its environment.

HWS – Heat, Wait, Search. The system heats the sample to a temperature, then waits to allow thermal stabilization, and finally search if there is any adiabatic increase in the sample temperature (self-heating).

Thermal Inertia (Φ factor) – the ability of a system (vessel plus reactants) to store heat.

According to ASTM E1981:

$$\text{Thermal inertia } (\Phi\text{-factor}) = 1 + \frac{m_c C_{p.c}}{m_s C_{p.s}}$$

m_c = container mass
$C_{p,c}$= container heat capacity
m_s = sample mass
$C_{p,s}$= sample heat capacity

The heat of Reaction (ΔH_r) – the net calculated heat liberated during an exotherm.

Weight loss (%)- the loss in the sample's weight after the reaction due to the release of non-condensable gases.

Total pressure change (ΔP) - the difference between the initial and final pressure after cooling down to ambient temperature.

Observed Temperature Rise – the temperature difference between the final temperature and the onset temperature of an exotherm.

Adiabatic Temperature Rise – the temperature rise that would be observed in an exothermic reaction if all of the heat liberated were used to increase the temperature of only the sample, calculated as the product of the observed adiabatic temperature rise and the thermal inertia factor.

Onset Temperature – the temperature at which the exothermic self-heating starts.

Figure 1: APTAC™ Calorimeter

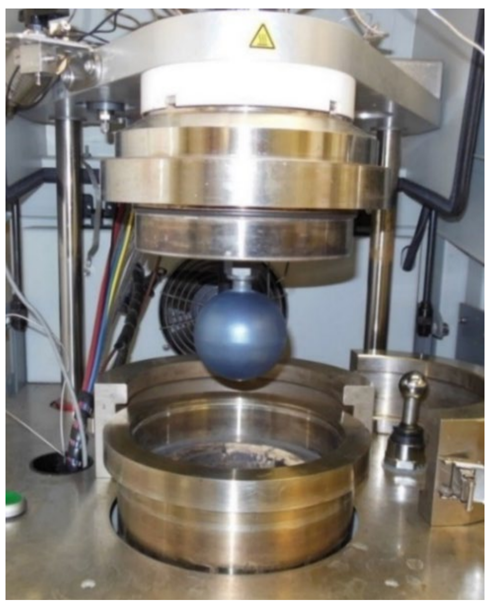

Photo Courtesy of ioKinetic, LLC

Appendix B: Test Data Reports

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Today's Time and Date	12:41:43 PM, Thu May 29 2025
Test Date	March 17, 2025
Test Location	Salem, NH
Author	E.Shaaban
Operator	A.Iskandar
Test Description	Invert, Phosphoric Acid, and Sodium Hydroxide Test Number APTAC-Citrine-03132025 Test 1
Lab Notebook Reference	Page no.147
Comments	In an air atmosphere, the invert sugar was charged into a stainless steel APTAC test cell. A Heat-Wait-Search (HWS) program was initiated, starting at 40 C and increasing up to 400 C with 5 C heat steps, a 0.03 C/min exotherm sensitivity, and a 1500 psia pressure limit. Once the instrument reached equilibrium at 40 C and during the search mode, phosphoric acid was injected. Ten minutes after the phosphoric acid addition, the sodium hydroxide solution was introduced. Water was then injected, and the main valve was closed. The 1st exotherm was observed following the water injection. The test was terminated upon reaching the pressure limit. After cooldown, the test chamber contained 370.5 psia of non-condensable gas at 38C. Upon venting the non-condensable gas, a total of 6.287 g of the sample was lost. This weight loss accounts for both vented gas and material remaining within the pressure transfer tube. The initial mass of the reactants was 49.812 g, while the final remaining mass was 43.525 g, consisting of approximately 32.9 g of black solid and 10.6 g of pale yellow liquid.
Ambient Conditions	P: 1006 mbar, T: 20.5C, RH: 18.5%, tested under Air
Sample Description	

Maximum test temperature	275.71 C
Maximum value of dT/dt	22.56 C/min
Maximum test pressure	1447.03 psia
Maximum value of dP/dt	34.61 psi/min

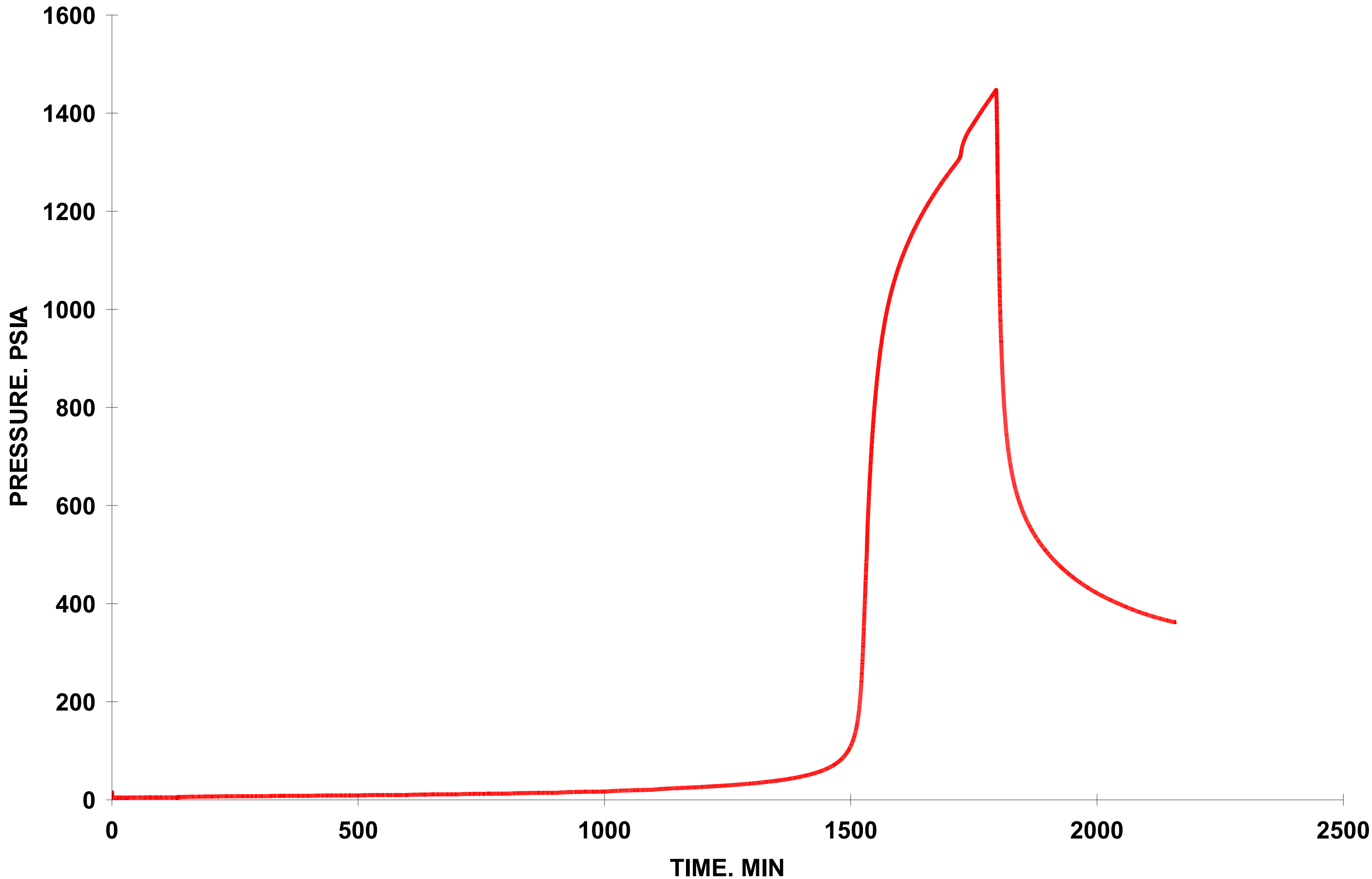
Data File Name C:\USERS\SHAABAN.E.NH\ONEDRIVE - IOMOSAIC CORP\COMPANIES\CITRINE\TEST 1\APTAC-CITRINE-03132025 TEST 1.TXT

Data Type APTAC Instrument ID = APTAC1

Chemical Component Name and/or Description	Mass g	Heat Capacity cal/g	Volume ml	Molecular Weight	Mass Fraction. %	Supplied By	Date Acquired
SUCROSE / $C_{12}H_{22}O_{11}$ / Invert Sugar, Nulomoline, Tl	[redacted]	[redacted]	[redacted]	342.300	[redacted]	Domino Foods Inc.	03102025
PHOSPHORIC ACID / H_3O_4P / Phosphoric acid [redacted]	[redacted]	[redacted]	[redacted]	97.995	[redacted]	Sigma	03102025
SODIUM HYDROXIDE / HNaO / sodium hydroxide [redacted]	[redacted]	[redacted]	[redacted]	39.997	[redacted]	Sigma	03102025
WATER / H_2O / Water	[redacted]	1.000	[redacted]	18.015	[redacted]	ioKinetic	-
Initial	49.812		[redacted]				
Final after cooldown	43.525						
Lost	6.287	12.622	% Lost				

Thermal Inertia Without Fittings	1.65
Thermal Inertia With Fittings	1.94

	Exotherm 1	Exotherm 2	Exotherm 3	Exotherm 4	Total
Onset Temperature. C	40.03	63.82	111.64	274.92	
End Temperature. C	56.49	65.43	265.99	275.53	
Temperature Rise. C	16.45	1.61	154.35	0.61	
Adiabatic Temperature Rise Without Fittings. C	27.09	2.65	254.18	1.00	
Heat of Reaction Without Fittings. cal/g mix	8.48	0.83	79.54	0.31	89.17
Adiabatic Temperature Rise With Fittings. C	31.96	3.13	299.79	1.18	
Heat of Reaction With Fittings. cal/g mix	10.00	0.98	93.82	0.37	105.17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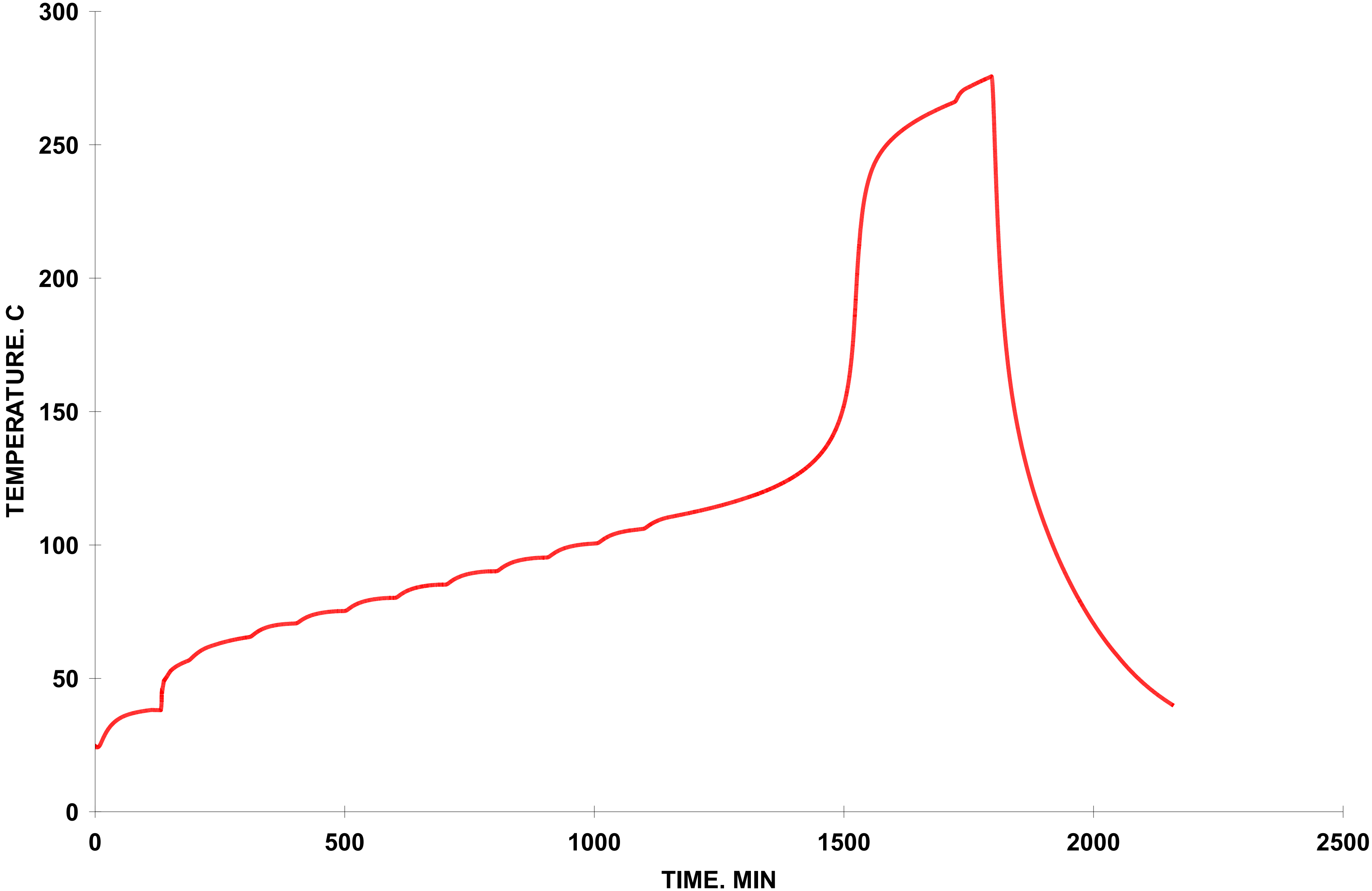
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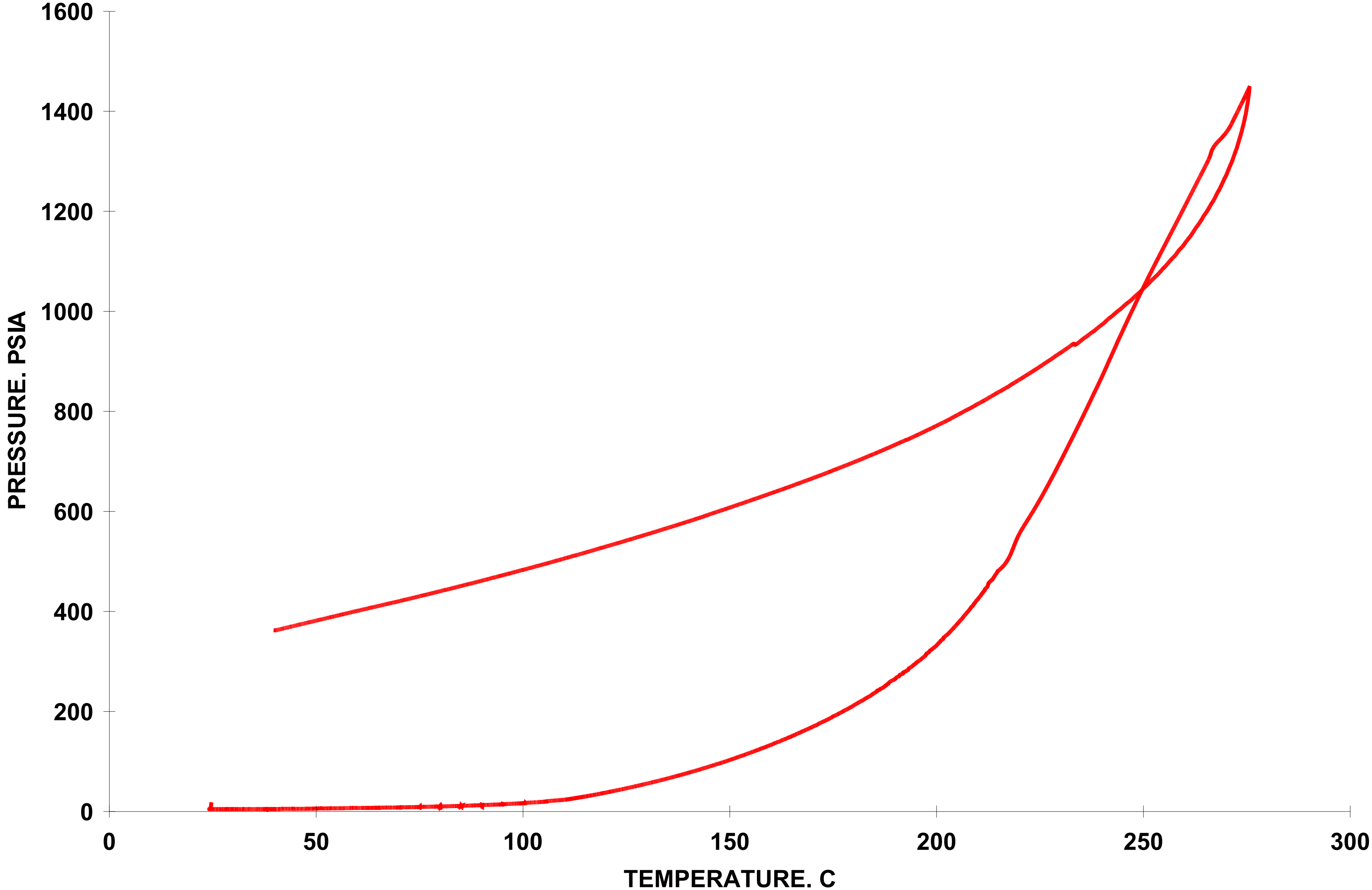
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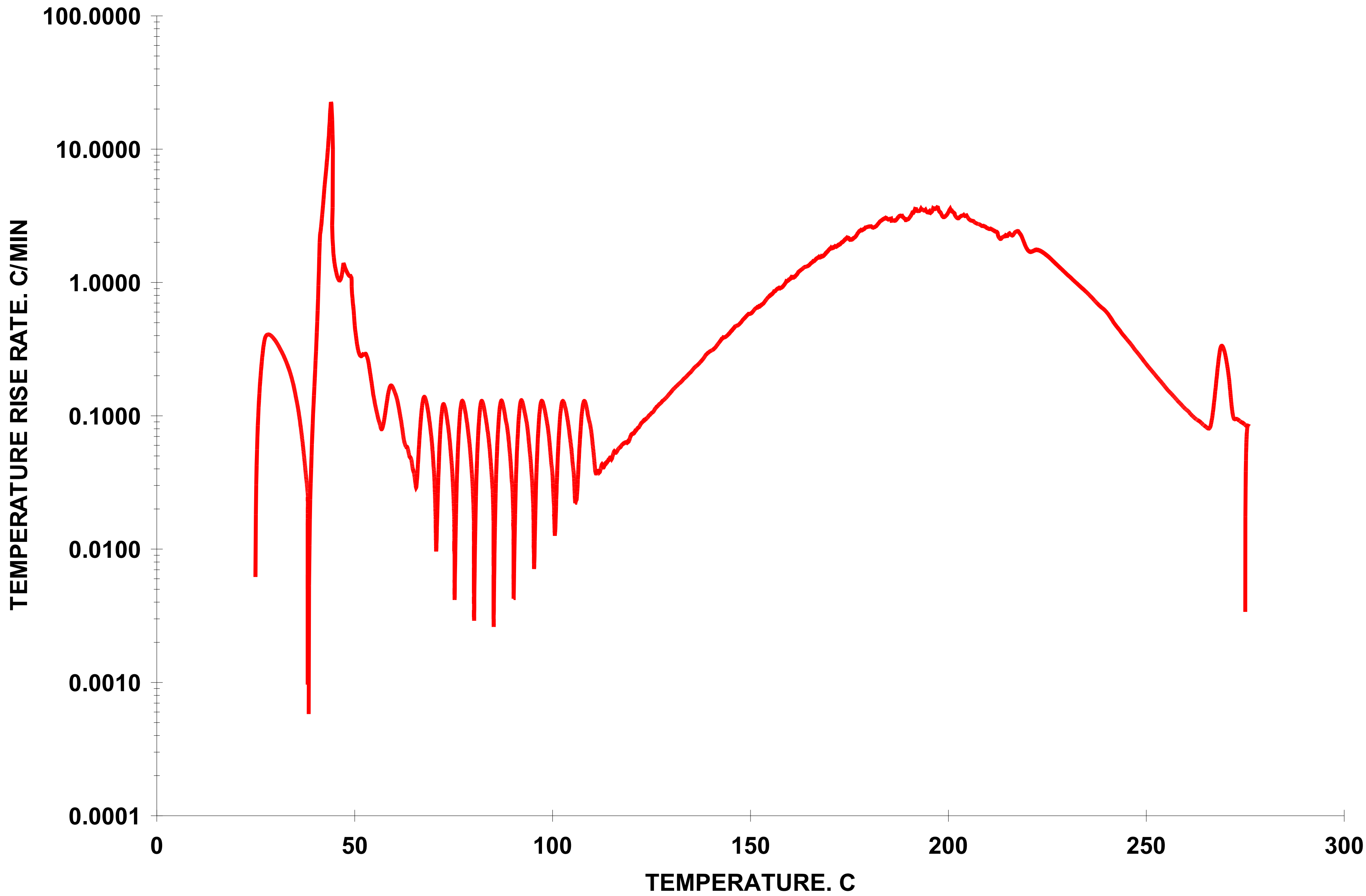
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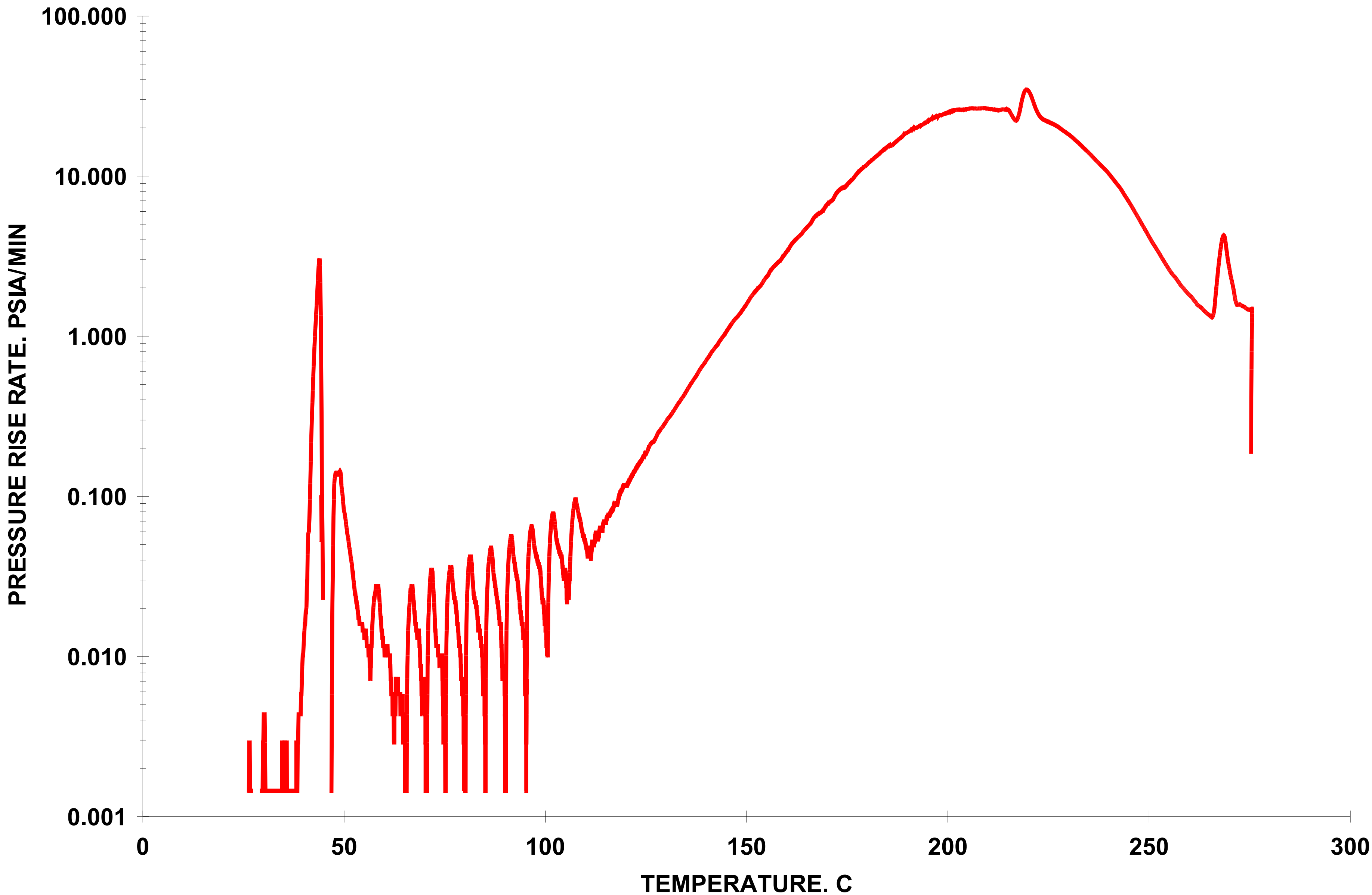
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Test Cell Part Number	00000000	
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Test Cell Mass. gms	93.22	
Test Cell Volume. ml	110	
Test Cell Heat Capacity. cal/g/C	0.1081545786	
Fittings Material of Construction	User Specified, Titanium, or TITAN	
Fittings Mass. gms	14.8639	
Fittings Heat Capacity. cal/g/C	0.1242037143	
Foil Material of Construction	User Specified, METHANE, or METHYI	
Foil Mass. gms	0	
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dP/dt column	8	Bara/min
Stirrer speed column. RPM	7	
Instrument mode column	5	
Use all data points		
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Instrument wait mode	2	
Instrument search mode	3	
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Instrument manual mode	-1	
Instrument idle mode	-1	

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Today's Time and Date	05:04:10 PM, Thu Mar 20 2025
Test Date	March 19, 2025
Test Location	Salem, NH
Author	E.Shaaban
Operator	A.Iskandar
Test Description	Invert, Phosphoric Acid, Sodium Hydroxide, Water and Antifoam-Givaudan Test Number APTAC-CSB-03192025 Test 2
Lab Notebook Reference	Page no.149
Comments	In an air atmosphere, the invert sugar was charged into a stainless steel APTAC test cell. A Heat-Wait-Search (HWS) program was initiated, starting at 40 C and increasing up to 400 C with 5 C heat steps, a 0.03 C/min exotherm sensitivity, and a 1500 psia pressure limit. Once the instrument reached equilibrium at 40 C and during the search mode, phosphoric acid was injected. Ten minutes after the phosphoric acid addition, the sodium hydroxide solution was introduced. Water + Antifoam was mixed (96 to 4 %) first then the required amount from the mixture was injected, and the main valve was closed. The test was terminated upon reaching the pressure limit. After cooldown, the test chamber contained 406 psia of non-condensable gas at 44C. Upon venting the non-condensable gas, a total of 5.48 g of the sample was lost. This weight loss accounts for both vented gas and material remaining within the pressure transfer tube. The initial mass of the reactants was 50.118 g, while the final remaining mass was 44.638 g, consisting of approximately 32.64 g of black solid and 12.00 g of pale yellow liquid.
Ambient Conditions	P: 1014 mbar, T: 19.6C, RH: 18.0%, tested under Air
Sample Description	

Maximum test temperature	275.26 C
Maximum value of dT/dt	192.13 C/min
Maximum test pressure	1523.78 psia
Maximum value of dP/dt	43.81 psi/min

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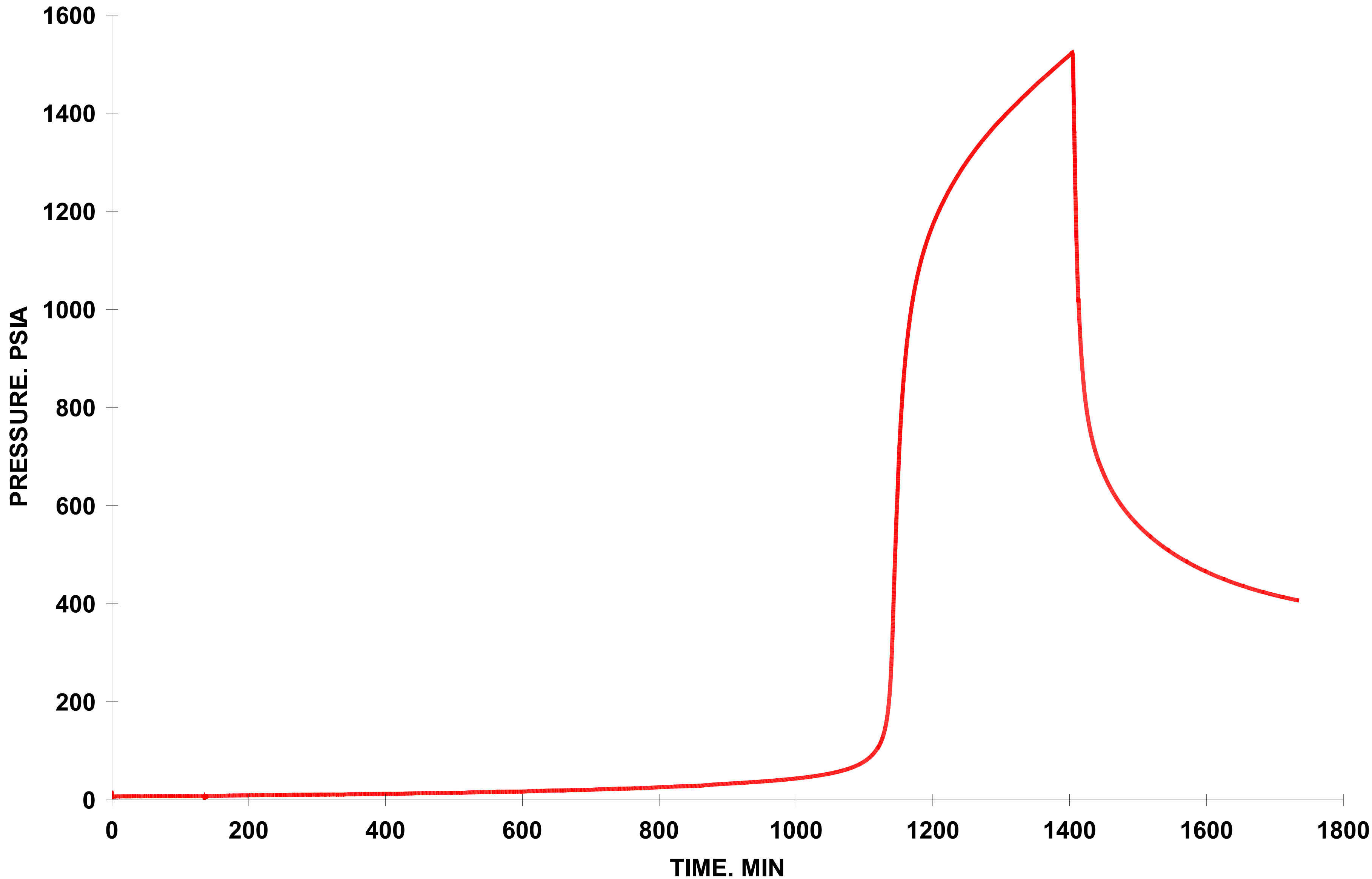
Data Type APTAC Instrument ID = APTAC1

Chemical Component Name and/or Description	Mass g	Heat Capacity cal/g	Volume ml	Molecular Weight	Mass Fraction. %	Supplied By	Date Acquired
SUCROSE / $C_{12}H_{22}O_{11}$ / R0026 invert	[redacted]	[redacted]	[redacted]	342.300	[redacted]	Givaudan	02242025
PHOSPHORIC ACID / H_3O_4P / Phosphoric acid [redacted]	[redacted]	[redacted]	[redacted]	97.995	[redacted]	Givaudan	02242025
SODIUM HYDROXIDE / HNaO / sodium hydroxide [redacted]	[redacted]	[redacted]	[redacted]	39.997	[redacted]	Givaudan	02242025
User Component 4 / Antifoam	[redacted]	[redacted]	[redacted]	0.000	[redacted]	Givaudan	02242025
WATER / H_2O / Water	[redacted]	1.000	[redacted]	18.015	[redacted]	ioKinetic	-
Initial	50.118		34.646				
Final after cooldown	44.638						
Lost	5.480	10.934	% Lost				

Thermal Inertia Without Fittings	1.63
Thermal Inertia With Fittings	1.76

	Exotherm 1	Exotherm 2	Exotherm 3	Total
Onset Temperature. C	40.16	73.12	117.35	
End Temperature. C	60.70	75.89	275.11	
Temperature Rise. C	20.54	2.77	157.76	
Adiabatic Temperature Rise Without Fittings. C	33.47	4.52	257.11	
Heat of Reaction Without Fittings. cal/g mix	10.49	1.42	80.60	92.51
Adiabatic Temperature Rise With Fittings. C	36.22	4.89	278.26	
Heat of Reaction With Fittings. cal/g mix	11.36	1.53	87.23	100.12



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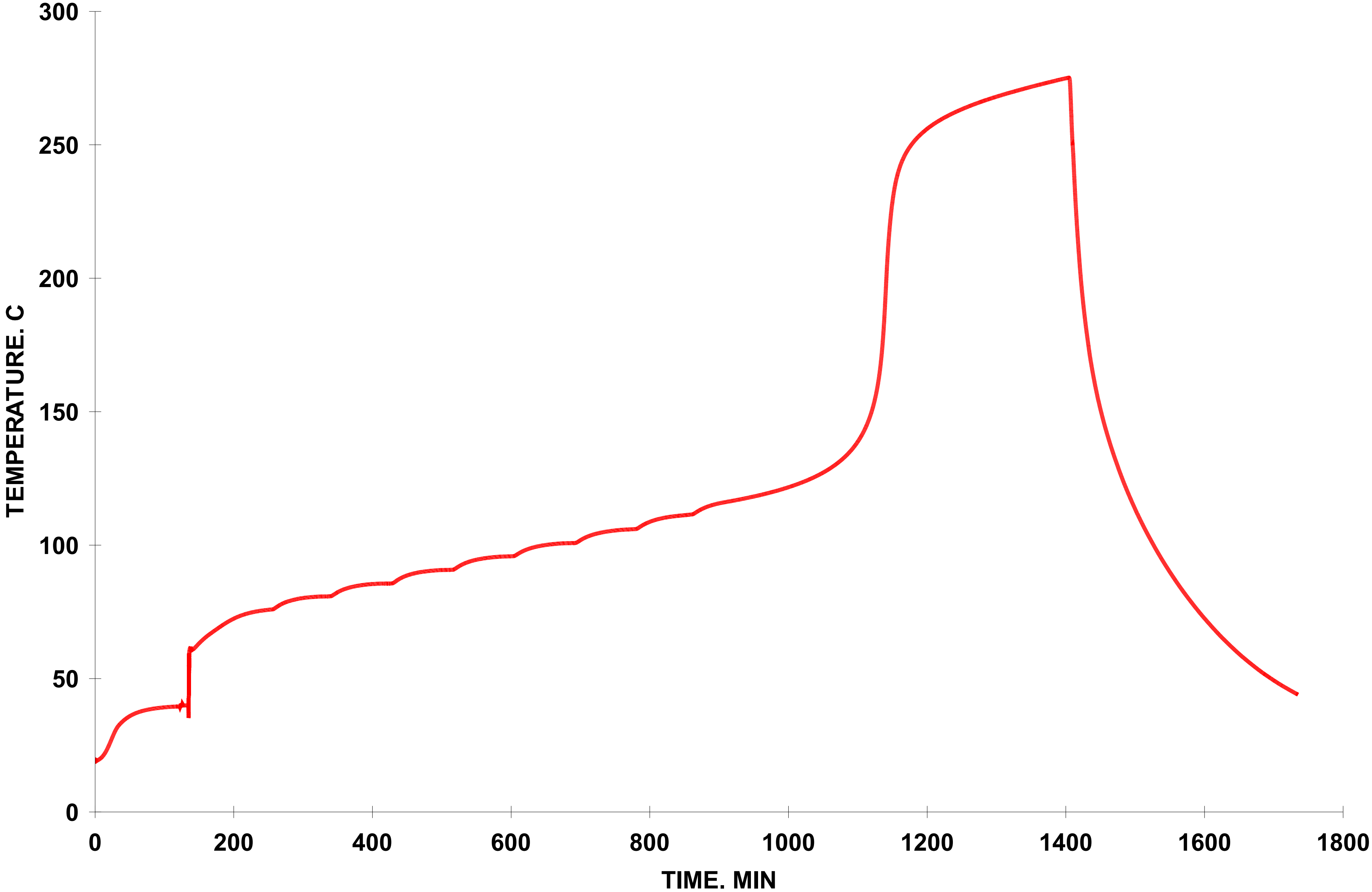
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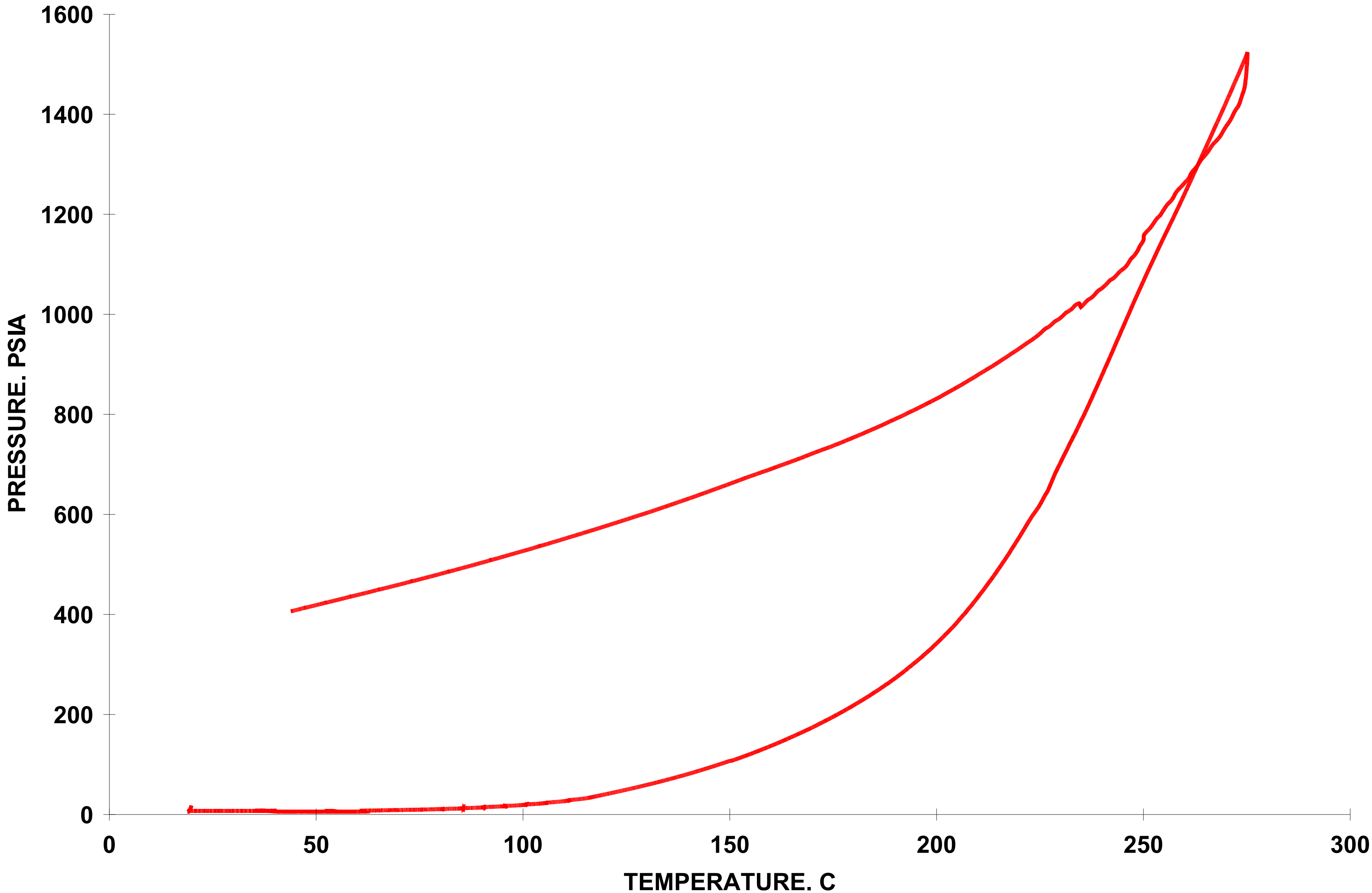

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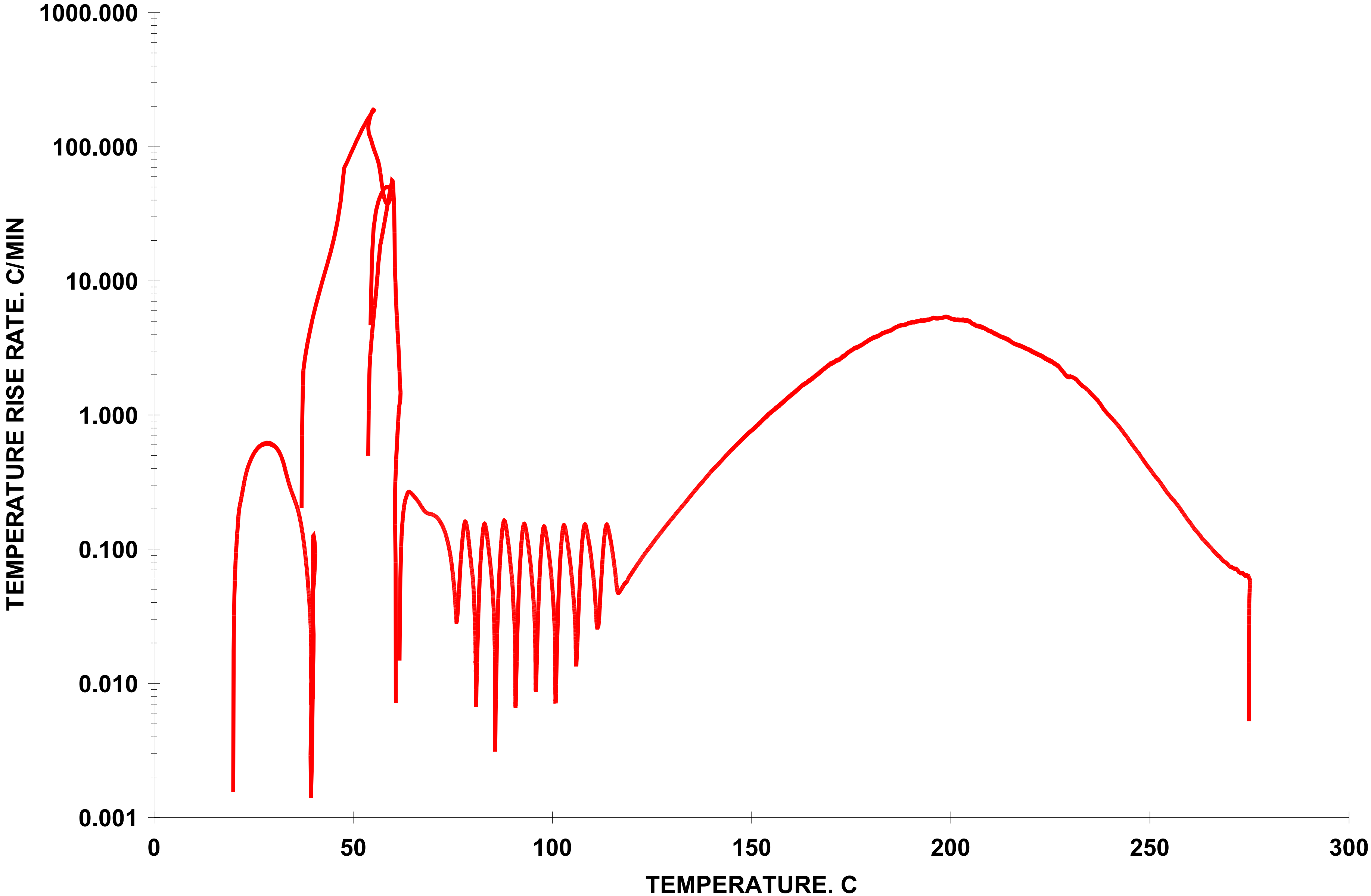

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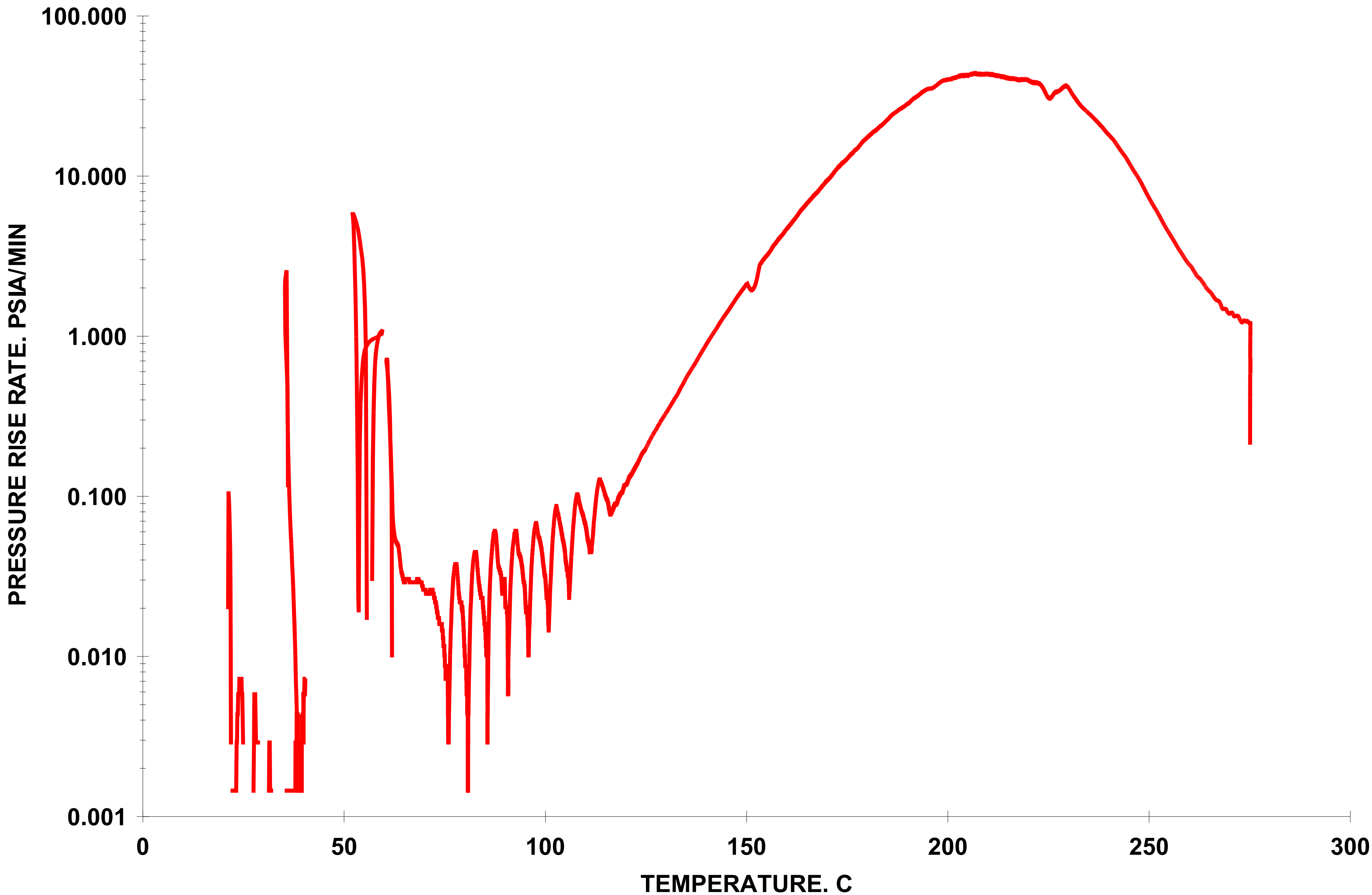

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TEMPERATURE. C

Pad Gas	AIR	
Test Cell Description	Standard Test Cell	
Test Cell Part Number	00000000	
Test Cell Material of Construction	User Specified, IRON, or STEEL	
Test Cell Mass. gms	91.48	
Test Cell Volume. ml	130.36	
Test Cell Heat Capacity. cal/g/C	0.1081545786	
Fittings Material of Construction	User Specified, Titanium, or TITAN	
Fittings Mass. gms	14.52	
Fittings Heat Capacity. cal/g/C	0.1242037143	
Foil Material of Construction	User Specified	
Foil Mass. gms	0	
Foil Heat Capacity. cal/g/C	0.1	
Stirrer Material of Construction	User Specified	
Stirrer Mass. gms	3.03	
Stirrer Heat Capacity. cal/g/C	0.1	
Time column	0	min
Time offset	0	min
Data analysis start time	0.00049	min
Data analysis end time	2157.09033	min
Temperature column	4	C
Temperature offset	0	C
dT/dt column	7	C/min
Pressure column	2	Bara
dP/dt column	8	Bara/min
Stirrer speed column. RPM	7	
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Instrument endotherm mode	-1	
Instrument heat mode	1	
Instrument wait mode	2	
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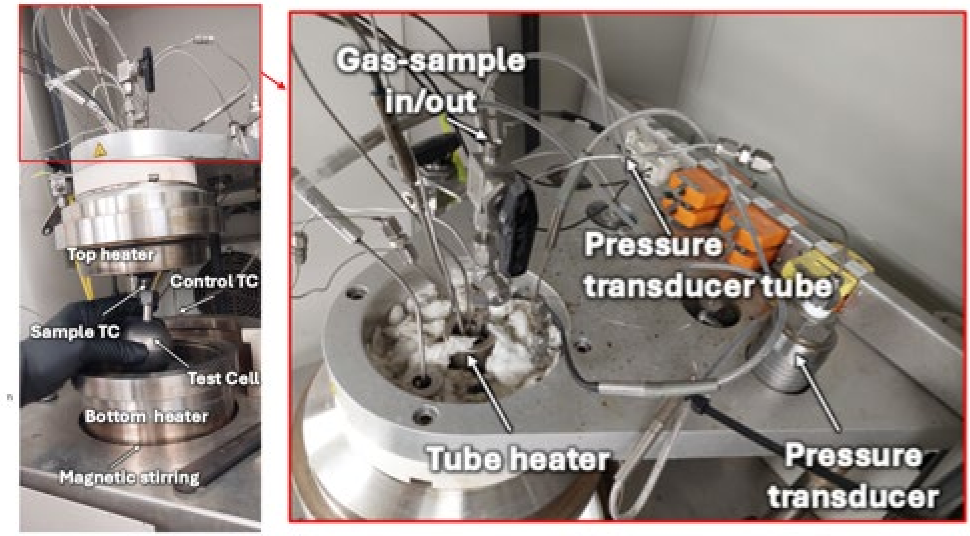
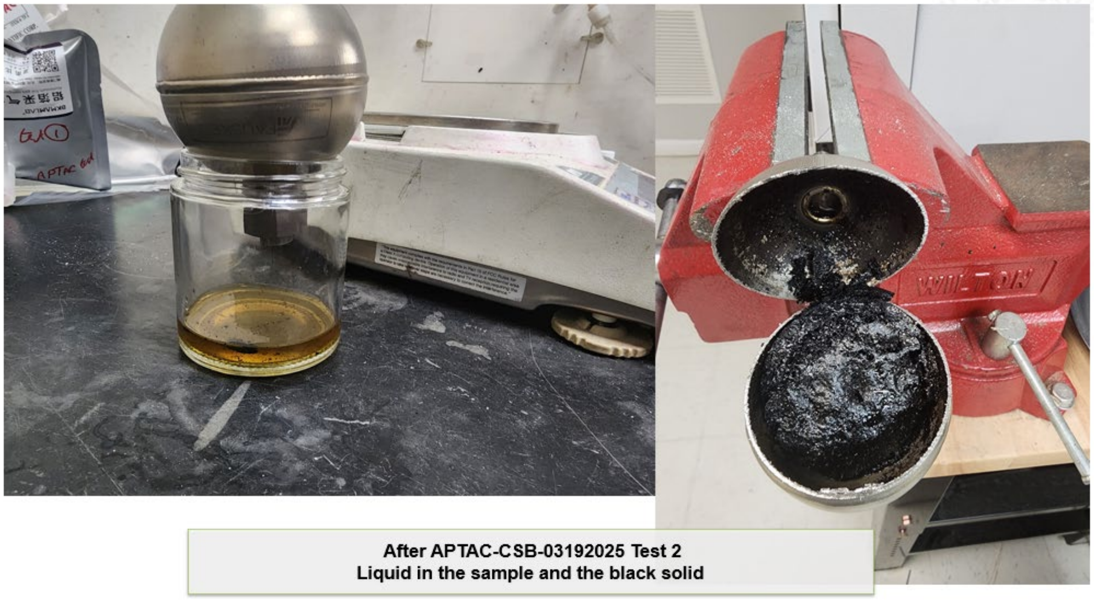
Instrument cool mode	0	
Instrument calibrate mode	-1	
Instrument manual mode	-1	
Instrument idle mode	-1	

Appendix C: Test Photos



After APTAC - CSB 03132025 Test1
Liquid in the sample and the black solid



After APTAC-CSB-03192025 Test 2
Liquid in the sample and the black solid

Accelerating Rate Calorimeter Report

Chemical Reactivity Evaluation

Invert, Phosphoric Acid, Sodium Hydroxide and Antifoam Reactions

Report to:
U.S. Chemical Safety and Hazard Investigation Board
470 L'Enfant Plaza SW
Suite 604 #23278
Washington, DC 20026

Date: September 15, 2025

This report was prepared by ioKinetic for the account of CSB. This report represents ioKinetic's best judgment in light of information made available to us. Opinions in this report are based in part upon data and information (Sample Identification) provided by CSB and / or CSB's advisors and affiliates. This report relates only to the sample as received unless otherwise noted. The reader is advised that ioKinetic has not independently verified the data or the information contained therein. This report must be read in its entirety. The reader understands that no assurances can be made that all liabilities have been identified. This report does not constitute a legal opinion. The results provided are apparatus dependent and should not be used for direct scale-up. They apply to the samples as tested and are useful as a comparison tool only.

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Report No.: ioK#: 25099 Rev. 1

AT-1922

95 Stiles Road | Salem, New Hampshire 03079
www.ioKinetic.com | P: 603.893.7009 | F: 603.386.6522

Revision History

Rev.	Date	List of Changes	Prepared by	Approved by
0	5/30/2025	Draft Final Review Copy	E. Shaaban, PhD	A. Iskandar, PhD
1	09/15/2025	Final Report	E. Shaaban, PhD	A. Iskandar, PhD

Table of Contents

List of Tables

List of Figures

Appendices

1 Study Overview

This report presents the results of Accelerating Rate Calorimeter (ARC®) testing to evaluate the chemical reactivity of pure invert and a mixture recipe. The tests' compositions were as follows:

Table 1: Samples' Compositions for ARC® Tests

Components (g) / ARC® test name (g)	ARC04252025CSB-Invert only	ARC-CSB-05162025 sugar test mixture
Invert (R0026)	4.236	[redacted]
Phosphoric Acid [redacted]	-	
Sodium Hydroxide [redacted]	-	
Water	-	
Antifoam	-	
Total	4.236	4.490

Samples preparation for the test was conducted as follows:

1. For the "ARC04252025CSB-Invert only"

In an air atmosphere, invert sugar was charged into a stainless steel ARC® test cell. A Heat-Wait-Search (HWS) program was then initiated, starting at 50 °C and increasing up to 400 °C in 5 °C increments. The test was run with an exotherm sensitivity of 0.03 °C/min and a pressure limit of 200 bar.

2. For the "ARC-CSB-05162025 sugar test mixture"

A bulk reaction mixture sample was first prepared in air at room temperature. The mixture consisted of invert, phosphoric acid [redacted], sodium hydroxide [redacted], water, and antifoam, with respective weight percentages of [redacted] To prepare the mixture, phosphoric acid was added dropwise to the invert while stirring continuously at room temperature. After 10 minutes, sodium hydroxide was also added dropwise. Water and antifoam were then added. From this mixture, 4.49 g was transferred into a stainless steel ARC® test cell, which was mounted to the instrument in air. A Heat-Wait-

Search (HWS) program was then initiated, starting at 30 °C and ramping up to 400 °C in 5 °C increments, with an exotherm sensitivity of 0.03 °C/min and a pressure limit of 2,500 psia.

The ARC® test "ARC-CSB-05162025 sugar test mixture" was based on the quantities of materials added to the cooker prior to the runaway event. These quantities are summarized in Table 2 below and referenced in the files "Cooker 6 484 Batch Sequence Day of Incident" and "Summary of Information Provided by CSB." To facilitate adiabatic measurements and feasible lab-scale testing with the instrument configuration, the multiple caustic addition steps were consolidated into a single injection at room temperature.

Table 2: Quantities of Materials Added to Cooker 6 Before the Incident.

Material	Original Recipe (Pounds)	Percent
Invert	[redacted]	[redacted]
Phosphoric Acid [redacted]		
Sodium Hydroxide [redacted]		
Water		
Antifoam		
Total	21,254.30	100.00

Information about the test setup is summarized in Table 3. Additional test details relative to samples can be found in ARC® test reports in Appendix B. The detailed ARC® test description is in Appendix A.

Table 3: ARC® Experiment Information

Sample	ARC® Test Name	Test Cell Material / Mass (g) / Volume (mL)	Sample Mass (g)	Φ without Fittings
Invert only	ARC04252025CSB-Invert only	Stainless steel / 16.5127/ 9.001	4.236	2.62
Invert, Phosphoric Acid, Sodium Hydroxide, Water, and Antifoam	ARC-CSB-05162025 sugar test mixture	Stainless steel / 17.2657/ 8.8114	4.490	2.33

2 Test Results and Discussion

The ARC® test results are summarized in Table 4. Complete data reports generated by Process Safety Office® SuperChems® are included in Appendix B.

Table 4: Summary of ARC® Test Results

Sample	Test Name	Weight Loss (%)	Observed Result	Onset T (°C)	T Rise (°C)	Adiabatic T Rise (°C)	ΔHr (cal/g)	Final P (psi)	Max dT/dt (°C/min)	Max dP/dt (psi/min)
Invert only	ARC04252025 CSB-Invert only	23.607	Exotherm Exotherm	146.33 316.10	96.97 34.83	254.23 91.31	-66.1 -23.7	433.7	1.41	12.86
Invert, Phosphoric Acid, Sodium Hydroxide, Water, and Antifoam	ARC-CSB-05162025 sugar test mixture	21.100	Exotherm Exotherm Exotherm	50.95 108.09 315.38	10.98 127.6 7.74	25.54 296.76 17.99	-8.0 -93.1 -5.64	505.4	1.94	12.57

The following observations were noted with respect to the data presented:

1. After the cooldown, the “ARC04252025 CSB-Invert only” test cell contained 433.7 psia of non-condensable gas at 21.9 °C. Upon venting the gas, a total of 1.00 g of the sample was lost. This weight loss accounts for both the vented gas and any material remaining within the pressure transfer tube.
2. After the cooldown, the “ARC-CSB-05162025 sugar test mixture” test cell contained 505.4 psia of non-condensable gas at 18.6 °C. Upon venting the gas, a total of 0.9474 g of the sample was lost. This weight loss accounts for both the vented gas and material remaining within the pressure transfer tube.

Appendix A: Detailed Test Description

The Accelerating Rate Calorimeter (ARC®) provides adiabatic pressure and temperature vs. time data for reactive systems. The ARC® can be used to obtain information about the thermal behavior of reactions and exothermic onset temperatures. The ARC® is primarily used for liquid-phase reactive systems. It is also used for the evaluation of explosives and propellants. Exotherm rates as low as 0.02°C/min can be detected. Developed by Townsend and Tou, this instrument (reference Figure 1), provides thermokinetic data that is applicable to the design and safety/performance evaluation of reactors and storage vessels. Such thermokinetic data includes:

- Adiabatic rate of self-heating
- Adiabatic time to explosion
- Rate of pressure rise
- Maximum rate of reaction
- Kinetic data such as activation energy, reaction order, and pre-exponential factor
- Heat of reaction

To conduct a test, the reaction mixture is introduced into a spherical cell whose volume is approximately 10 ml. The cell is equipped with a thermocouple mounted on the external wall. The pressure is recorded by means of a pressure transducer. The ARC® is a high thermal inertia instrument whose phi factor is greater than or equal to 1.4. Various cells can be used which have varying pressure ratings from 4,500 psi to 15,000 psi. As the pressure rating increases, the cell phi factor increases. This high phi factor requires that the temperature and pressure be adjusted. Established techniques exist that require knowledge of the heat capacity of the reaction mixture and the cell. The significant advantage that the ARC® offers over other similar techniques is exothermic onset detectability at 0.02°C/min.

In the newest ARC®, the ARC 254 (Figure 2), temperature tracking can be accomplished up to approximately 100°C/min. Operator skill ensures proper calibration. The instrument is fully automated; once operating, it needs minimal to no operator intervention.

The high phi-factor has benefits as well as deficits. It can slow a highly energetic reaction down so that tracking and measurement can be completed. For less energetic reactions there is the potential to mask some higher-temperature exotherms.

Some details on the ARC 254 include:

- Minimum detectable slope: < 0.01 K/min
- Operating test cell temperature range: room temperature to 400°C (sub-ambient optional)
- Operating test cell pressure range: 0 to 200 bar
- Pressure accuracy: 0.1% of full scale
- Sample size: 0.5 ml to 7 ml
- Tracking rate at adiabatic operation up to 100 K/min
- Test cell material options include Hastelloy- C, Titanium, Stainless Steel, Glass
- Temperature accuracy: +/-0.1°C plus thermocouple uncertainty
- Stirring, injection, and vent capability (options)
- ASTM standard: E1981

Definitions

Adiabatic Calorimeter – an instrument designed to make calorimetric measurements while maintaining a minimal heat loss or gain between the sample and its environment.

HWS – Heat, Wait, Search. The system heats the sample to a temperature, then waits to allow thermal stabilization, and finally searches if there is any adiabatic increase in the sample temperature (self-heating).

The heat of Reaction (ΔH_r) – the net calculated heat liberated during an exotherm.

Thermal Inertia (phi factor) – the ability of a system (vessel plus reactants) to store heat.

According to ASTM E1981:

Thermal inertia (Φ-factor) = $1 + \frac{m_c C_{p.c}}{m_s C_{p.s}}$

m_c = container mass
$C_{p,c}$= container heat capacity
m_s = sample mass
$C_{p,s}$= sample heat capacity

Weight loss (%)- the loss in the sample's weight after the reaction due to the release of non-condensable gases.

Total pressure change (ΔP) - the difference between the initial and final pressure after cooling down to ambient temperature.

Observed Temperature Rise – the temperature difference between the final temperature and the onset temperature of an exotherm.

Adiabatic Temperature Rise – the temperature rise which would be observed in an exothermic reaction if all of the heat liberated were used to increase the temperature of only the sample, calculated as the product of the observed adiabatic temperature rise and the thermal inertia factor.

Onset Temperature – the temperature at which the exothermic self-heating starts.

Figure 1: The Original Accelerating Rate Calorimeter (ARC®)

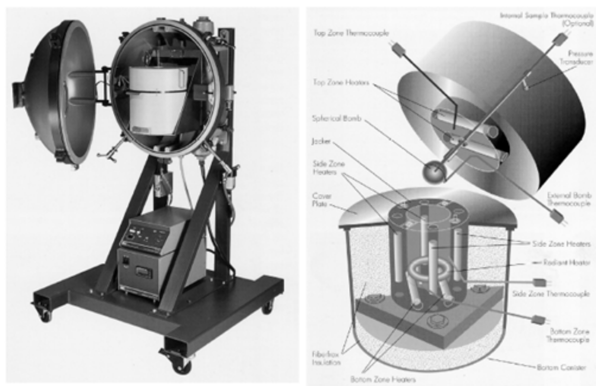

Figure 2: The Netzsch ARC® 254

Appendix B: Test Data Reports

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Today's Time and Date	04:25:55 PM, Tue Apr 29 2025
Test Date	April 25, 2025
Test Location	Salem, NH
Author	E. Shaaban
Operator	A.Iskandar
Test Description	Invert-Givaudan Test Number ARC04252025CSB-Invert only
Lab Notebook Reference	Page no.37
Comments	In an air atmosphere, the invert sugar was charged into a stainless steel ARC test cell. A Heat-Wait-Search (HWS) program was initiated, starting at 50 C and increasing up to 400 C with 5 C heat steps, a 0.03 C/min exotherm sensitivity, and a 200 bar pressure limit. The test was terminated upon reaching the pressure limit. After cooldown, the test chamber contained 433.7 psia of non-condensable gas at 29.9C. Upon venting the non-condensable gas, a total of 1.00 g of the sample was lost. This weight loss accounts for both vented gas and material remaining within the pressure transfer tube. All the remaining material was black solid
Ambient Conditions	P: 1006 mbar, T: 21.0 C, RH: 19.7%, tested under air
Sample Description	

Maximum test temperature	351.08 C
Maximum value of dT/dt	1.41 C/min
Maximum test pressure	2901.58 psia
Maximum value of dP/dt	12.86 psi/min

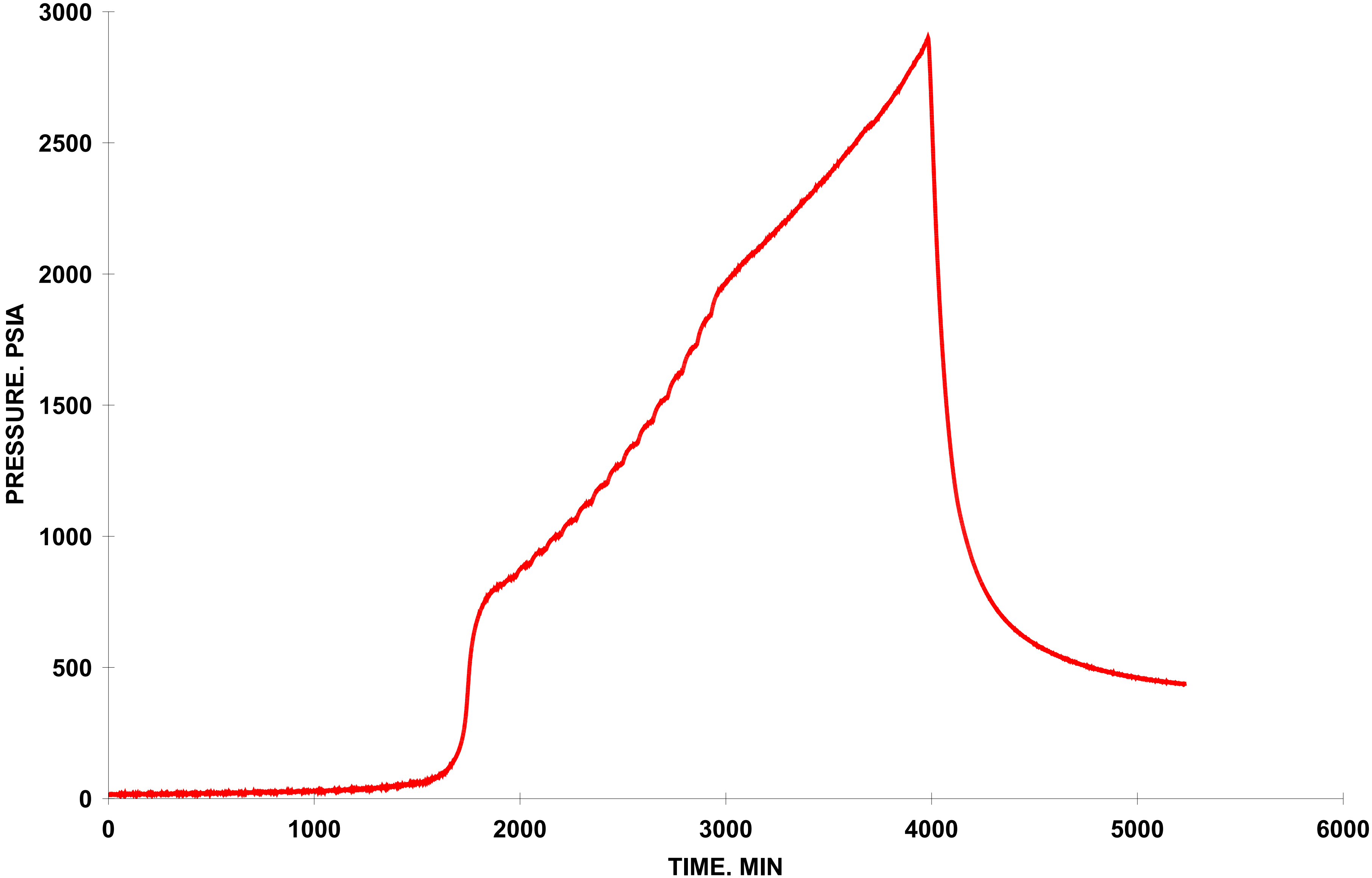
Data File Name C:\USERS\SHAABAN.E.NH\ONEDRIVE - IOMOSAIC CORP\COMPANIES\CITRINE\ARC04252025CSB-INVERT ONLY\ARC04252025CSB

Data Type ARC Instrument ID = ARC3

Chemical Component Name and/or Description	Mass g	Heat Capacity cal/g	Volume ml	Molecular Weight	Mass Fraction. %	Supplied By	Date Acquired
SUCROSE / C12H22O11 / R0026 invert	4.236	[redacted]	2.806	342.300	100.000	Givaudan	02242025
Initial	4.236		2.806				
Final after cooldown	3.236						
Lost	1.000	23.607	% Lost				

Thermal Inertia Without Fittings	2.62
Thermal Inertia With Fittings	4.18

	Exotherm 1	Exotherm 2	Total
Onset Temperature. C	146.33	316.10	
End Temperature. C	243.29	350.93	
Temperature Rise. C	96.97	34.83	
Adiabatic Temperature Rise Without Fittings. C	254.23	91.31	
Heat of Reaction Without Fittings. cal/g mix	66.08	23.73	89.81
Adiabatic Temperature Rise With Fittings. C	405.68	145.71	
Heat of Reaction With Fittings. cal/g mix	105.45	37.87	143.32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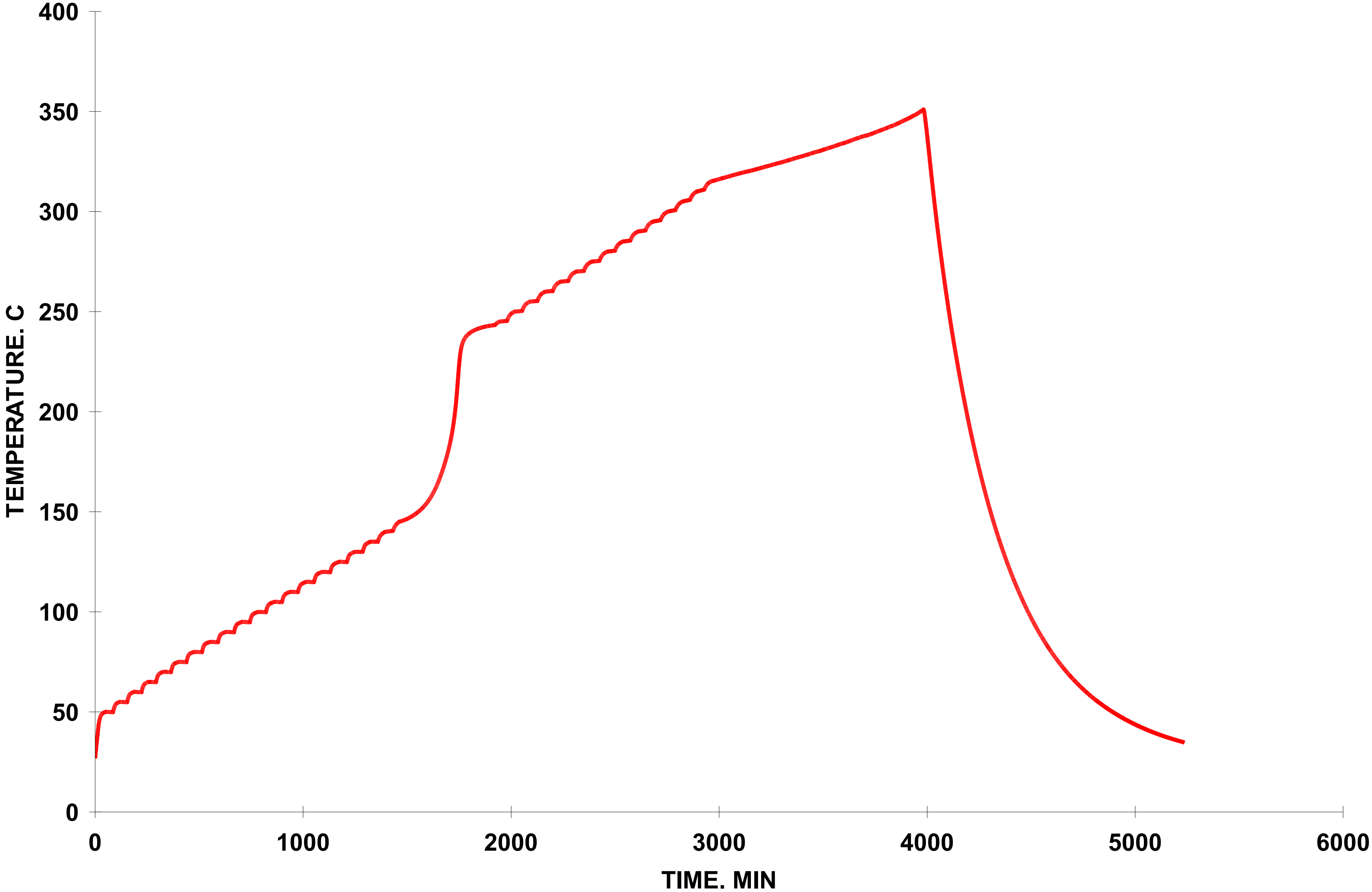
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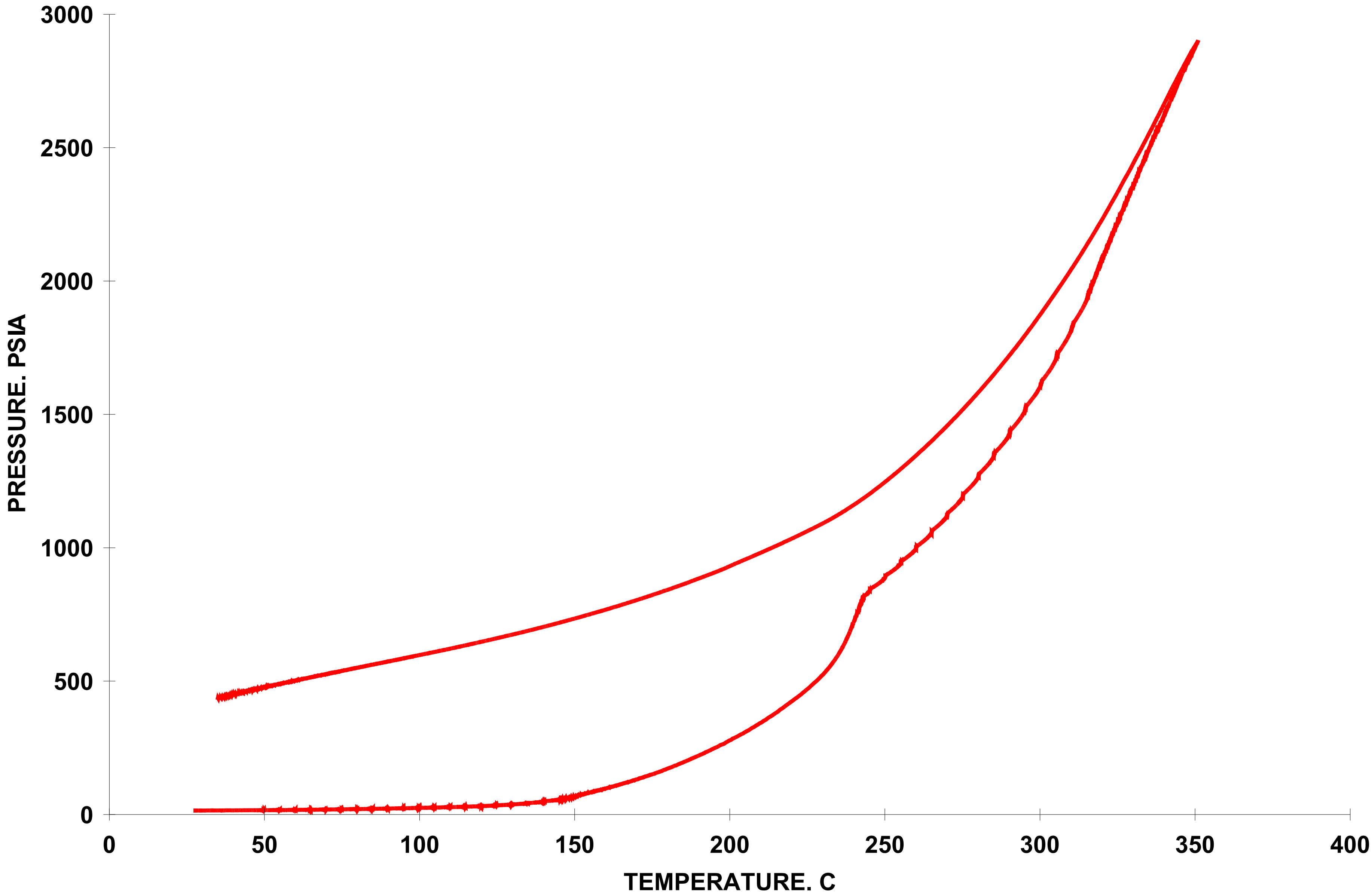
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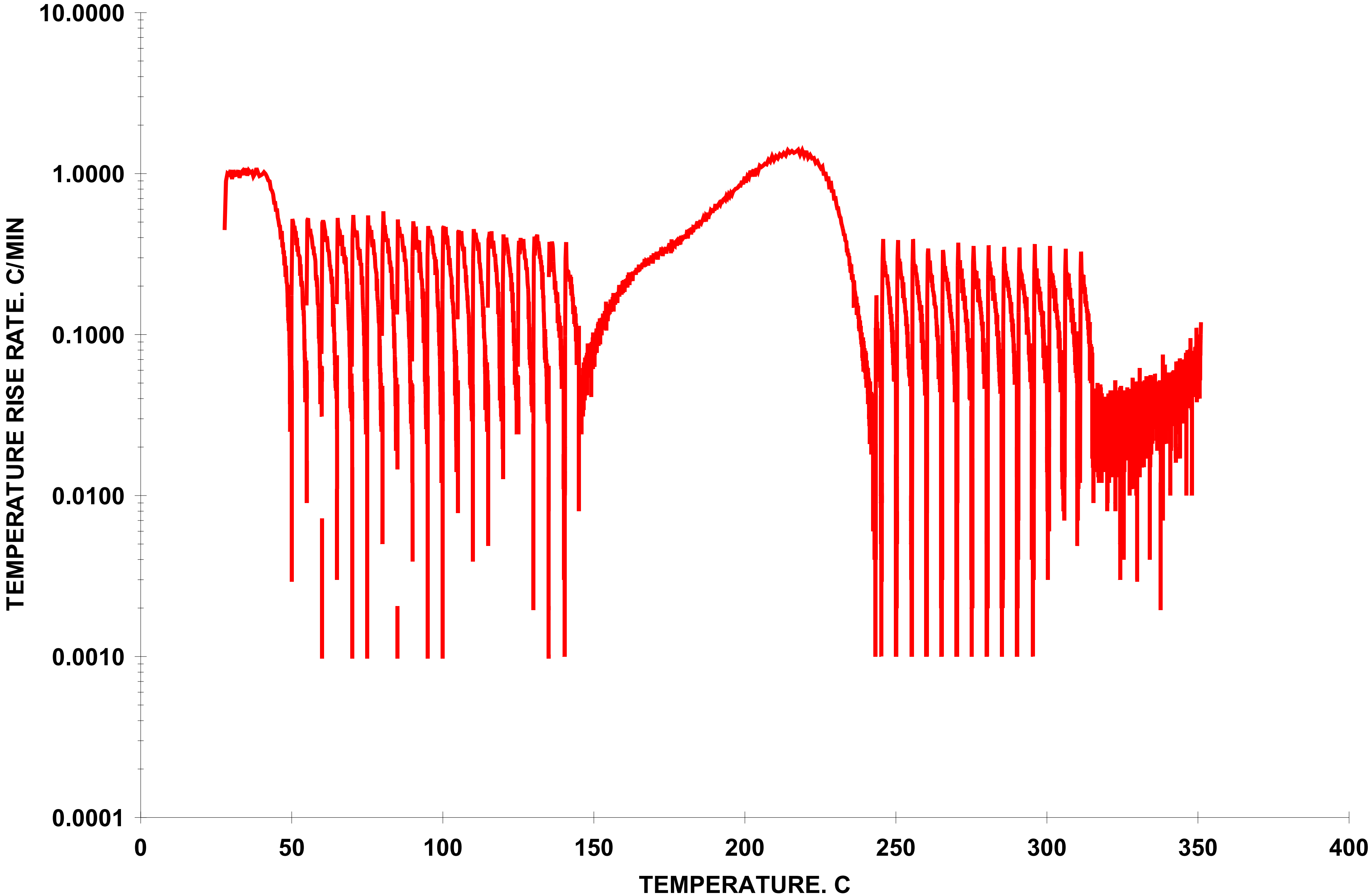

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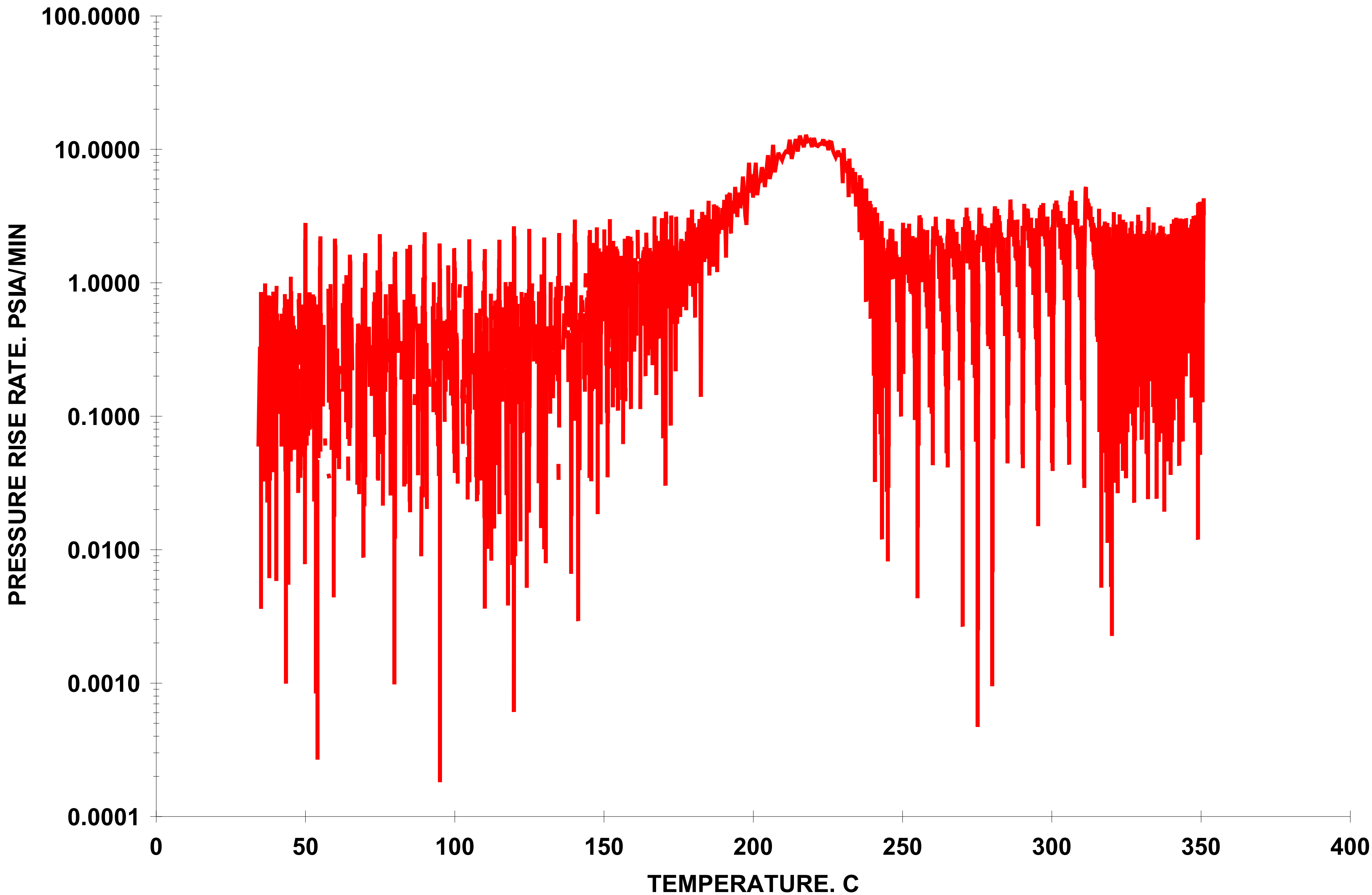

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Pad Gas	AIR	
Test Cell Description	Standard Test Cell	
Test Cell Part Number	00000000	
Test Cell Material of Construction	User Specified, IRON, or STEEL	
Test Cell Mass. gms	16.5127	
Test Cell Volume. ml	9.001	
Test Cell Heat Capacity. cal/g/C	0.1081545786	
Fittings Material of Construction	User Specified, Titanium, or TITAN	
Fittings Mass. gms	6.601	
Fittings Heat Capacity. cal/g/C	0.1242037143	
Foil Material of Construction	User Specified	
Foil Mass. gms	-1	
Foil Heat Capacity. cal/g/C	-1	
Stirrer Material of Construction	User Specified	
Stirrer Mass. gms	-1	
Stirrer Heat Capacity. cal/g/C	0.1	
Time column	0	min
Time offset	0	min
Data analysis start time	0.492	min
Data analysis end time	5228.499	min
Temperature column	1	C
Temperature offset	0	C
dT/dt column	2	C/min
Pressure column	3	bara
dP/dt column	Computed	
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Use all data points		
Instrument exotherm mode	4	
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Instrument heat mode	0	
Instrument wait mode	1	
Instrument search mode	2	
Instrument cool mode	5	
Instrument calibrate mode	-1	
Instrument manual mode	-1	
Instrument idle mode	-1	

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Today's Time and Date	03:38:27 PM, Tue May 27 2025
Test Date	May 16, 2025
Test Location	Salem, NH
Author	E. Shaaban
Operator	A.Iskandar
Test Description	Invert, Phosphoric Acid, Sodium Hydroxide, Water and Antifoam-Givaudan Test Number ARC-CSB-05162025 sugar test mixture
Lab Notebook Reference	Page no.33
Comments	A bulk reaction mixture sample was first prepared in air at room temperature. This mixture consisted of invert, phosphoric acid [redacted], sodium hydroxide [redacted], water, and antifoam, with respective weight percentages of [redacted] To prepare the mixture, phosphoric acid was added dropwise to the invert while stirring After 10 minutes, sodium hydroxide was also added dropwise. continuously at RT. Water and antifoam were then added. From this mixture, 4.49 g was transferred into a stainless steel ARC test cell, which was then mounted to the instrument in air. A Heat-Wait-Search (HWS) program was initiated, starting at 30 C and increasing up to 400 C with 5 C heat steps, a 0.03 C/min exotherm sensitivity, and a 2500 psia pressure limit. The test was terminated upon reaching the pressure limit. After cooldown, the test chamber contained 505.4 psia of non-condensable gas at 18.6 C. Upon venting the non-condensable gas, a total of 0.9474 g of the sample was lost. This weight loss accounts for both vented gas and material remaining within the pressure transfer tube.
Ambient Conditions	P: 1010 mbar, T: 20.6 C, RH: 55.1%, tested under air
Sample Description	

Maximum test temperature	339.12 C
Maximum value of dT/dt	1.94 C/min
Maximum test pressure	2493.38 psia
Maximum value of dP/dt	12.57 psi/min

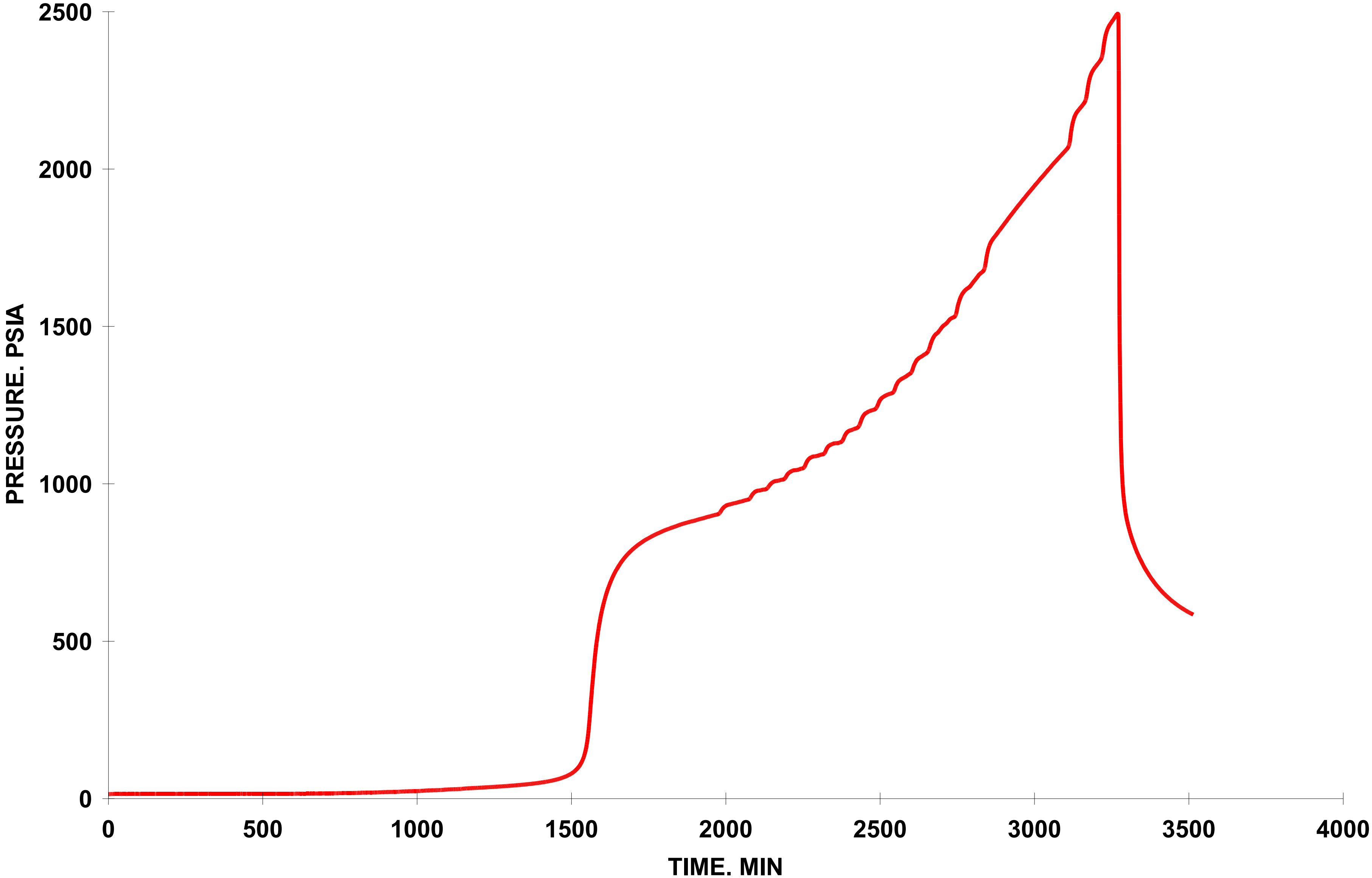
Data File Name C:\USERS\SHAABAN.E.NH\ONEDRIVE - IOMOSAIC CORP\COMPANIES\CITRINE\2 MORE ARC TESTS -COOKER 6 RECIPE-W & WO

Data Type ARC Instrument ID = ARC1

Chemical Component Name and/or Description	Mass g	Heat Capacity cal/g	Volume ml	Molecular Weight	Mass Fraction. %	Supplied By	Date Acquired
SUCROSE / C12H22O11 / R0026 invert	[redacted]	[redacted]	[redacted]	342.300	[redacted]	Givaudan	02242025
PHOSPHORIC ACID / H3O4P / Phosphoric acid [redacted]	[redacted]	[redacted]	[redacted]	97.995	[redacted]	Givaudan	02242025
SODIUM HYDROXIDE / HNaO / sodium hydroxide [redacted]	[redacted]	[redacted]	[redacted]	39.997	[redacted]	Givaudan	02242025
User Component 4 / Antifoam	[redacted]	[redacted]	[redacted]	-	[redacted]	Givaudan	02242025
WATER / H2O / Water	[redacted]	1.000	[redacted]	18.015	[redacted]	ioKinetic	-
Initial	4.490		3.103				
Final after cooldown	3.543						
Lost	0.947	21.100	% Lost				

Thermal Inertia Without Fittings	2.33
Thermal Inertia With Fittings	2.91

	Exotherm 1	Exotherm 2	Exotherm 3	Total
Onset Temperature. C	50.95	108.09	315.38	
End Temperature. C	61.93	235.69	323.12	
Temperature Rise. C	10.98	127.61	7.74	
Adiabatic Temperature Rise Without Fittings. C	25.54	296.76	17.99	
Heat of Reaction Without Fittings. cal/g mix	8.01	93.11	5.64	106.77
Adiabatic Temperature Rise With Fittings. C	31.98	371.55	22.52	
Heat of Reaction With Fittings. cal/g mix	10.03	116.57	7.07	133.67



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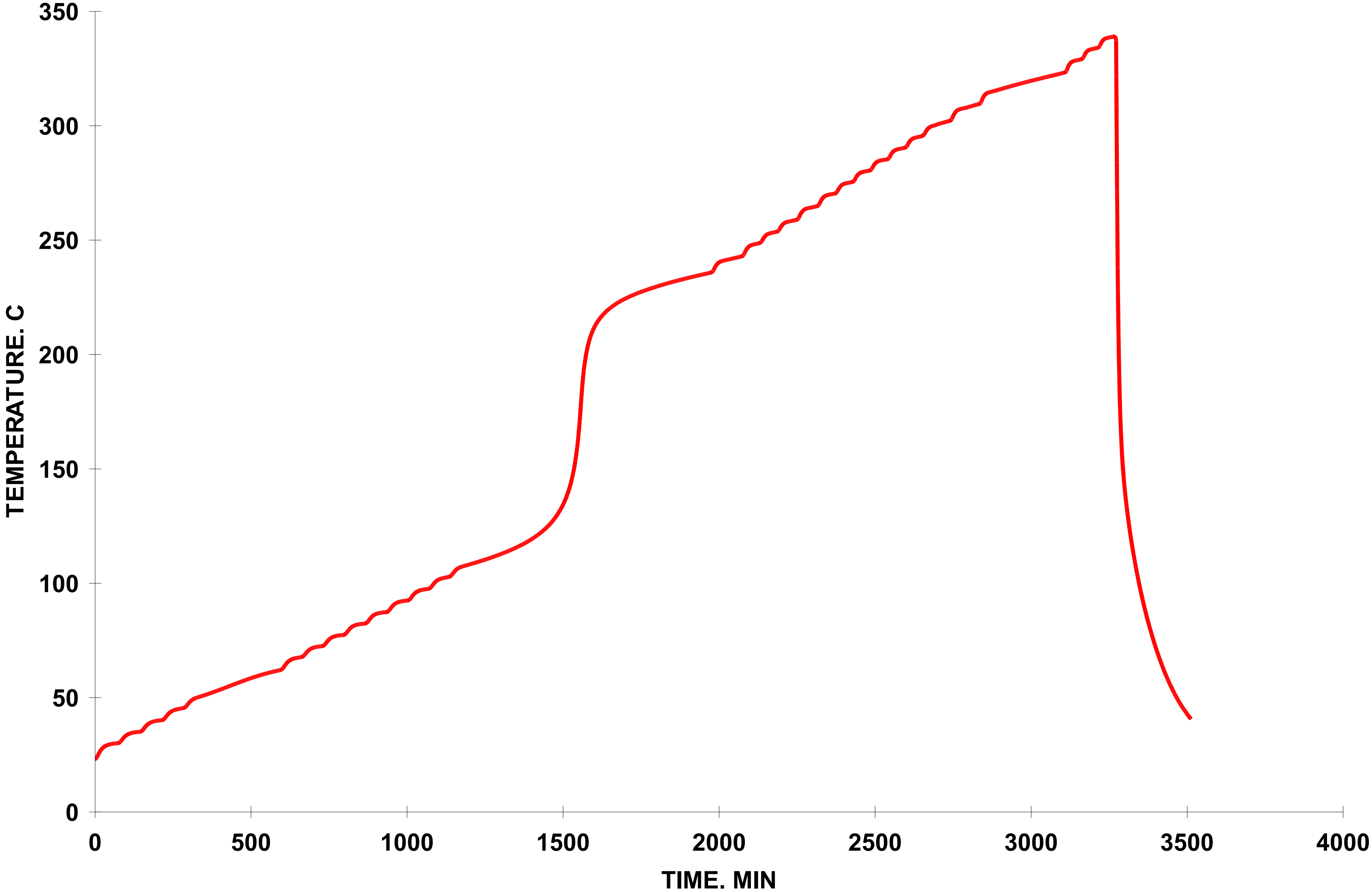
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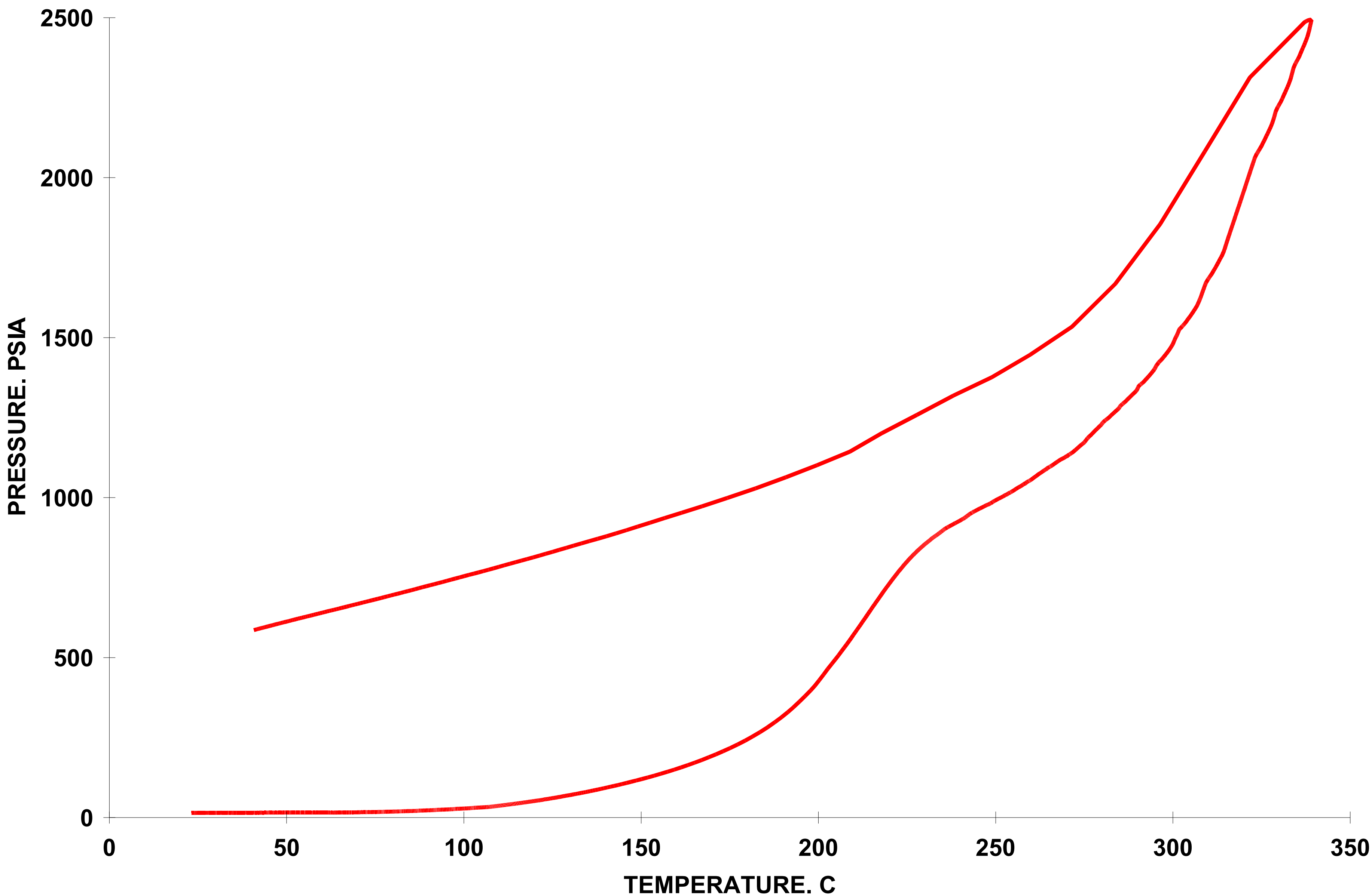
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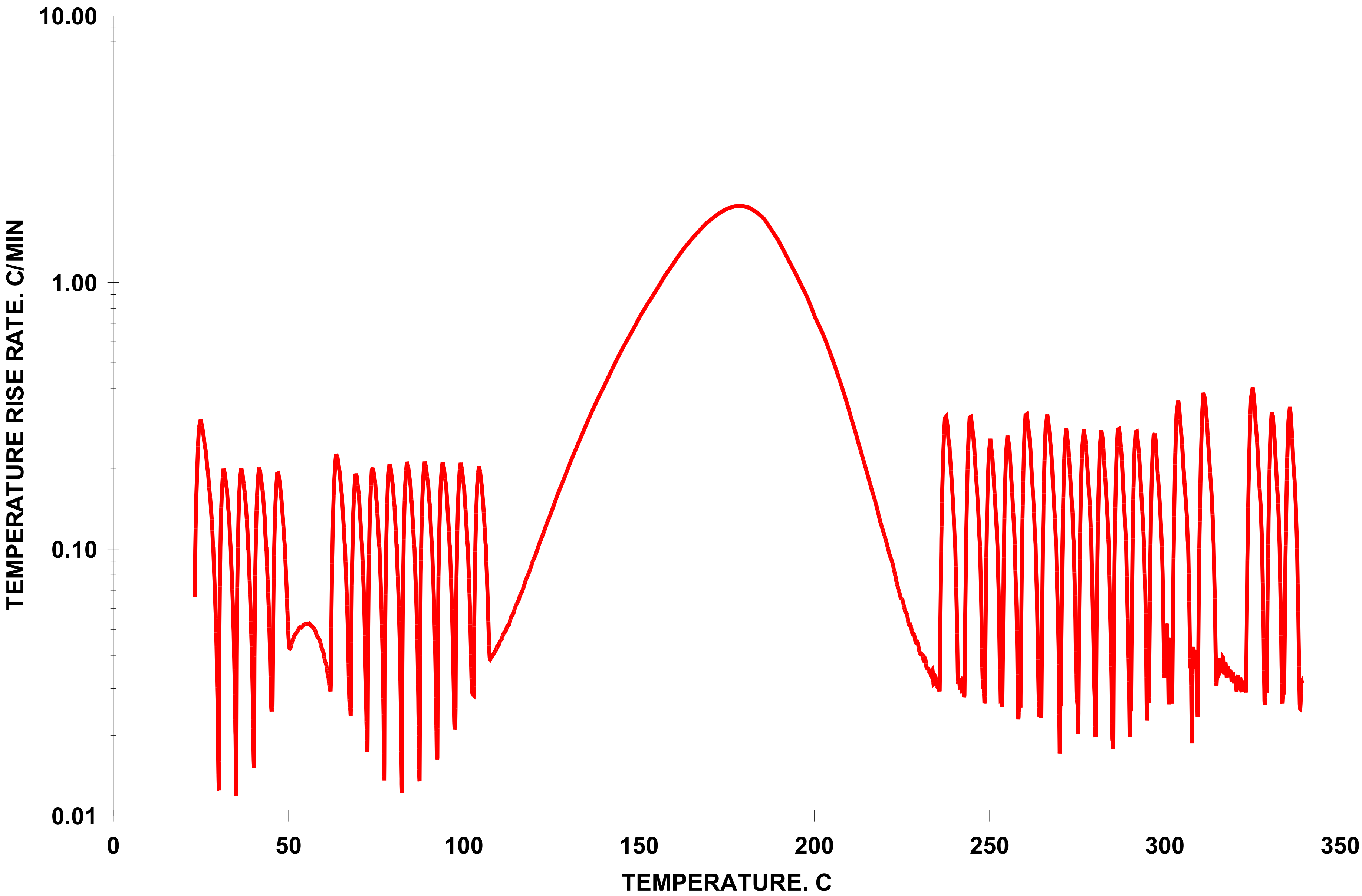
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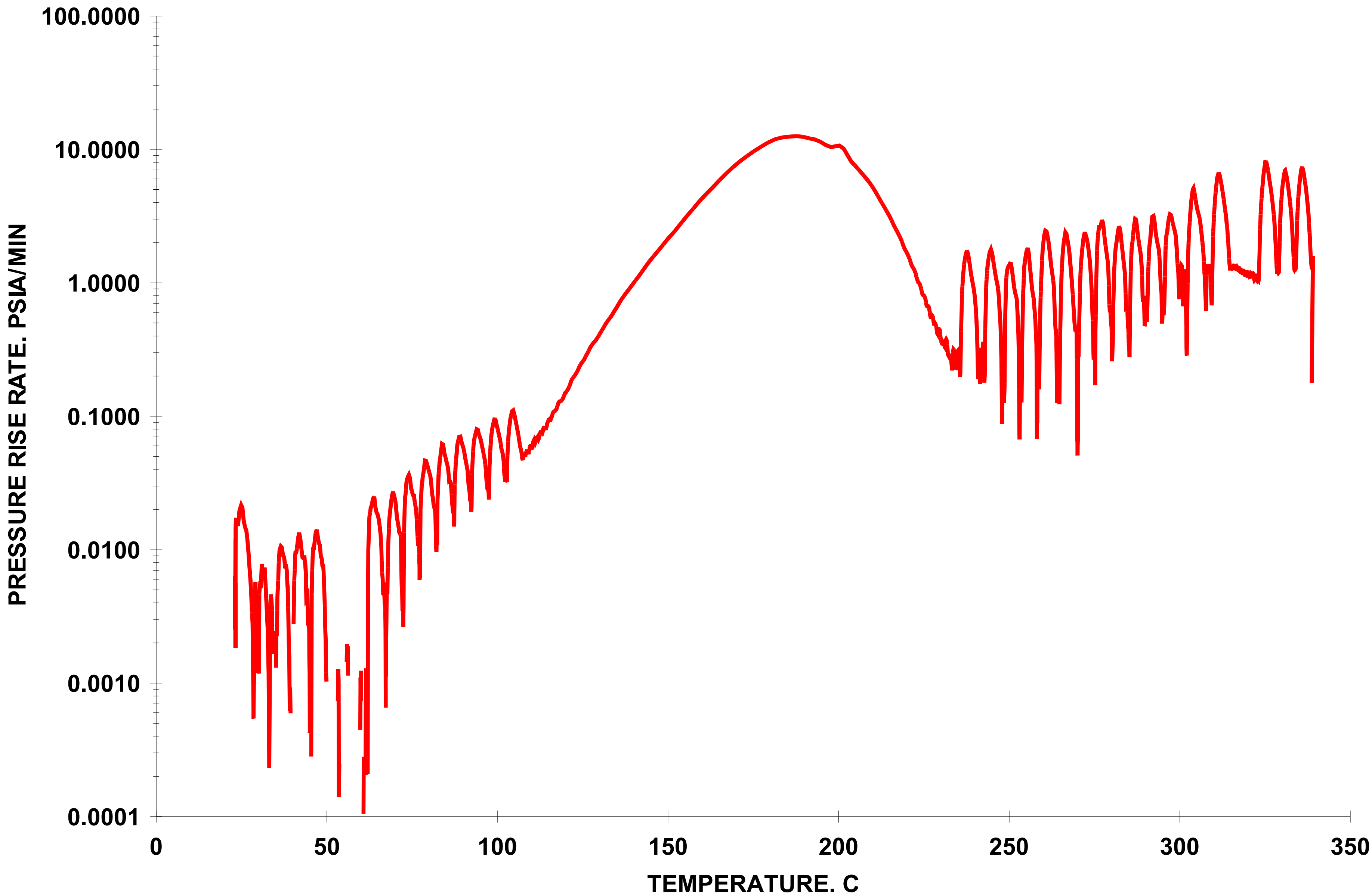
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TEMPERATURE. C

Pad Gas	AIR	
Test Cell Description	Standard Test Cell	
Test Cell Part Number	00000000	
Test Cell Material of Construction	User Specified, IRON, or STEEL	
Test Cell Mass. gms	17.2657	
Test Cell Volume. ml	8.8114	
Test Cell Heat Capacity. cal/g/C	0.1081545786	
Fittings Material of Construction	User Specified, Titanium, or TITAN	
Fittings Mass. gms	6.4738	
Fittings Heat Capacity. cal/g/C	0.1242037143	
Foil Material of Construction	User Specified	
Foil Mass. gms	0	
Foil Heat Capacity. cal/g/C	0.1	
Stirrer Material of Construction	User Specified	
Stirrer Mass. gms	0.2159	
Stirrer Heat Capacity. cal/g/C	0.1	
Time column	0	min
Time offset	0	min
Data analysis start time	0.01028	min
Data analysis end time	3508.44824	min
Temperature column	1	C
Temperature offset	0	C
dT/dt column	10	C/min
Pressure column	6	psia
dP/dt column	Computed	
Stirrer speed column. RPM	7	
Instrument mode column	14	
Use all data points		
Instrument exotherm mode	4	
Instrument endotherm mode	-1	
Instrument heat mode	1	
Instrument wait mode	2	
Instrument search mode	3	
Instrument cool mode	0	
Instrument calibrate mode	-1	
Instrument manual mode	-1	
Instrument idle mode	-1	

Accelerating Rate Calorimeter Report

Chemical Reactivity Evaluation

Invert (R0026), ARC-CSB-07102025-Invert Only

Report to:

U.S. Chemical Safety and Hazard Investigation Board

470 L'Enfant Plaza SW

Suite 604 #23278

Washington, DC 20026

Date: September 15, 2025

This report was prepared by ioKinetic for the account of CSB. This report represents ioKinetic's best judgment in light of information made available to us. Opinions in this report are based in part upon data and information (Sample Identification) provided by CSB and / or CSB's advisors and affiliates. This report relates only to the sample as received unless otherwise noted. The reader is advised that ioKinetic has not independently verified the data or the information contained therein. This report must be read in its entirety. The reader understands that no assurances can be made that all liabilities have been identified. This report does not constitute a legal opinion. The results provided are apparatus dependent and should not be used for direct scale-up. They apply to the samples as tested and are useful as a comparison tool only.

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Report No.: ioK#: 25204-01 Rev. 1

AT-1922

95 Stiles Road | Salem, New Hampshire 03079

www.ioKinetic.com | P: 603.893.7009 | F: 603.386.6522

Revision History

Rev.	Date	List of Changes	Prepared by	Approved by
0	8/5/2025	Initial Release	E. Shaaban, PhD	A. Iskandar, PhD
1	09/15/2025	Final Report	E. Shaaban, PhD	A. Iskandar, PhD

Table of Contents

List of Tables

List of Figures

Appendices

1 Study Overview

This report presents the results of Accelerating Rate Calorimeter (ARC®) testing to evaluate the chemical reactivity of a pure invert sample received from CSB. The test Composition was as follows:

Table 1: Samples' Compositions for ARC® Tests

Components (g) / ARC® test name (g)	ARC-CSB-07102025-Invert only
Invert (R0026)	4.5953
Phosphoric Acid [redacted]	-
Sodium Hydroxide [redacted]	-
Water	-
Antifoam	-
Total	4.5953

Samples preparation for the test was conducted as follows:

In an air atmosphere, the invert sugar was charged into a stainless-steel ARC® test cell. A Teflon-coated steel stirrer was used at 300 rpm. A Heat-Wait-Search (HWS) program was then initiated, starting at 50 °C and increasing up to 400 °C in 5 °C increments. The test was run with an exotherm sensitivity of 0.03 °C/min and a pressure limit of 2500 psia.

Information about the test setup is summarized in Table 2. Additional test details relative to samples can be found in ARC® test reports in Appendix B. The detailed ARC® test description is in Appendix A.

Table 2: ARC® Experiment Information

Sample	ARC® Test Name	Test Cell Material / Mass (g) / Volume (mL)	Sample Mass (g)	Φ without Fittings
Invert only	ARC-CSB-07102025-Invert only	Stainless steel / 17.1064 / 9.0304	4.5953	2.55

2 Test Results and Discussion

The ARC® test results are summarized in Table 3. Complete data reports generated by Process Safety Office® SuperChems® are included in Appendix B.

Table 3: Summary of ARC® Test Results

Sample	Test Name	Weight Loss (%)	Observed Result	Onset T (°C)	T Rise (°C)	Adiabatic T Rise (°C)	ΔHr (cal/g)	Final P (psi)	Max dT/dt (°C/min)	Max dP/dt (psi/min)
Invert only	ARC-CSB-07102025-Invert only	23.607	Exotherm	130.76	174.91	445.85	-115.9	422.8	3.55	42.39
			Exotherm	311.81	3.14	8.00	-2.08			

The following observations were made:

1. After the cooldown, the "ARC-CSB-07102025-Invert only" test cell contained 422.8 psia of non-condensable gas at 25.3 °C. Upon venting the gas, a total of 1.04 g of the sample was lost. This weight loss accounts for both the vented gas and any material remaining within the pressure transfer tube.

Appendix A: Detailed Test Description

The Accelerating Rate Calorimeter (ARC®) provides adiabatic pressure and temperature vs. time data for reactive systems. The ARC® can be used to obtain information about the thermal behavior of reactions and exothermic onset temperatures. The ARC® is primarily used for liquid-phase reactive systems. It is also used for the evaluation of explosives and propellants. Exotherm rates as low as 0.02°C/min can be detected. Developed by Townsend and Tou, this instrument (reference Figure 1), provides thermokinetic data that is applicable to the design and safety/performance evaluation of reactors and storage vessels. Such thermokinetic data includes:

- Adiabatic rate of self-heating
- Adiabatic time to explosion
- Rate of pressure rise
- Maximum rate of reaction
- Kinetic data such as activation energy, reaction order, and pre-exponential factor
- Heat of reaction

To conduct a test, the reaction mixture is introduced into a spherical cell whose volume is approximately 10 ml. The cell is equipped with a thermocouple mounted on the external wall. The pressure is recorded by means of a pressure transducer. The ARC® is a high thermal inertia instrument whose phi factor is greater than or equal to 1.4. Various cells can be used which have varying pressure ratings from 4,500 psi to 15,000 psi. As the pressure rating increases, the cell phi factor increases. This high phi factor requires that the temperature and pressure be adjusted. Established techniques exist that require knowledge of the heat capacity of the reaction mixture and the cell. The significant advantage that the ARC® offers over other similar techniques is exothermic onset detectability at 0.02°C/min.

In the newest ARC®, the ARC 254 (Figure 2), temperature tracking can be accomplished up to approximately 100°C/min. Operator skill ensures proper calibration. The instrument is fully automated; once operating, it needs minimal to no operator intervention.

The high phi-factor has benefits as well as deficits. It can slow a highly energetic reaction down so that tracking and measurement can be completed. For less energetic reactions there is the potential to mask some higher temperature exotherms.

Some details on the ARC 254 include:

- Minimum detectable slope: < 0.01 K/min
- Operating test cell temperature range: room temperature to 400°C (sub-ambient optional)
- Operating test cell pressure range: 0 to 200 bar
- Pressure accuracy: 0.1% of full scale
- Sample size: 0.5 ml to 7 ml
- Tracking rate at adiabatic operation up to 100 K/min
- Test cell material options include Hastelloy- C, Titanium, Stainless Steel, Glass
- Temperature accuracy: +/-0.1°C plus thermocouple uncertainty
- Stirring, injection, and vent capability (options)
- ASTM standard: E1981

Definitions

Adiabatic Calorimeter – an instrument designed to make calorimetric measurements while maintaining a minimal heat loss or gain between the sample and its environment.

HWS – Heat, Wait, Search. The system heats the sample to a temperature, then waits to allow thermal stabilization, and finally searches if there is any adiabatic increase in the sample temperature (self-heating).

The heat of Reaction (ΔH_r) – the net calculated heat liberated during an exotherm.

Thermal Inertia (phi factor) – the ability of a system (vessel plus reactants) to store heat.

According to ASTM E1981:

Thermal inertia (Φ-factor) = $$1 + \frac{m_c C_{p.c}}{m_s C_{p.s}}$$

m_c = container mass
$C_{p,c}$= container heat capacity
m_s = sample mass
$C_{p,s}$= sample heat capacity

Weight loss (%)- the loss in the sample's weight after the reaction due to the release of non-condensable gases.

Total pressure change (ΔP) - the difference between the initial and final pressure after cooling down to ambient temperature.

Observed Temperature Rise – the temperature difference between the final temperature and the onset temperature of an exotherm.

Adiabatic Temperature Rise – the temperature rise which would be observed in an exothermic reaction if all of the heat liberated were used to increase the temperature of only the sample, calculated as the product of the observed adiabatic temperature rise and the thermal inertia factor.

Onset Temperature – the temperature at which the exothermic self-heating starts.

Figure 1: The Original Accelerating Rate Calorimeter (ARC®)

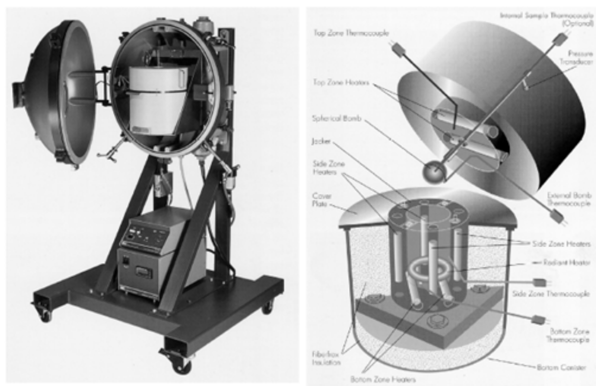

Figure 2: The Netzsch ARC® 254

Appendix B: Test Data Reports

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Today's Time and Date	08:46:28 AM, Tue Aug 05 2025
Test Date	July 10, 2025
Test Location	Salem, NH
Author	E. Shaaban
Operator	A.Iskandar
Test Description	Invert-Givaudan Test Number ARC-CSB-07102025-Invert only
Lab Notebook Reference	Page no.47
Comments	In an air atmosphere, the invert sugar was charged into a stainless steel ARC test cell. A Heat-Wait-Search (HWS) program was initiated, starting at 50 C and increasing up to 400 C with 5 C heat steps, a 0.03 C/min exotherm sensitivity, and a 200 bar pressure limit. The test was terminated upon reaching the pressure limit. After cooldown, the test chamber contained 422.8 psia of non-condensable gas at 25.3C. Upon venting the non-condensable gas, a total of 1.04 g of the sample was lost. This weight loss accounts for both vented gas and material remaining within the pressure transfer tube. All the remaining material was black solid
Ambient Conditions	P: 1005 mbar, T: 24.1 C, RH: 43.3%, tested under air
Sample Description	

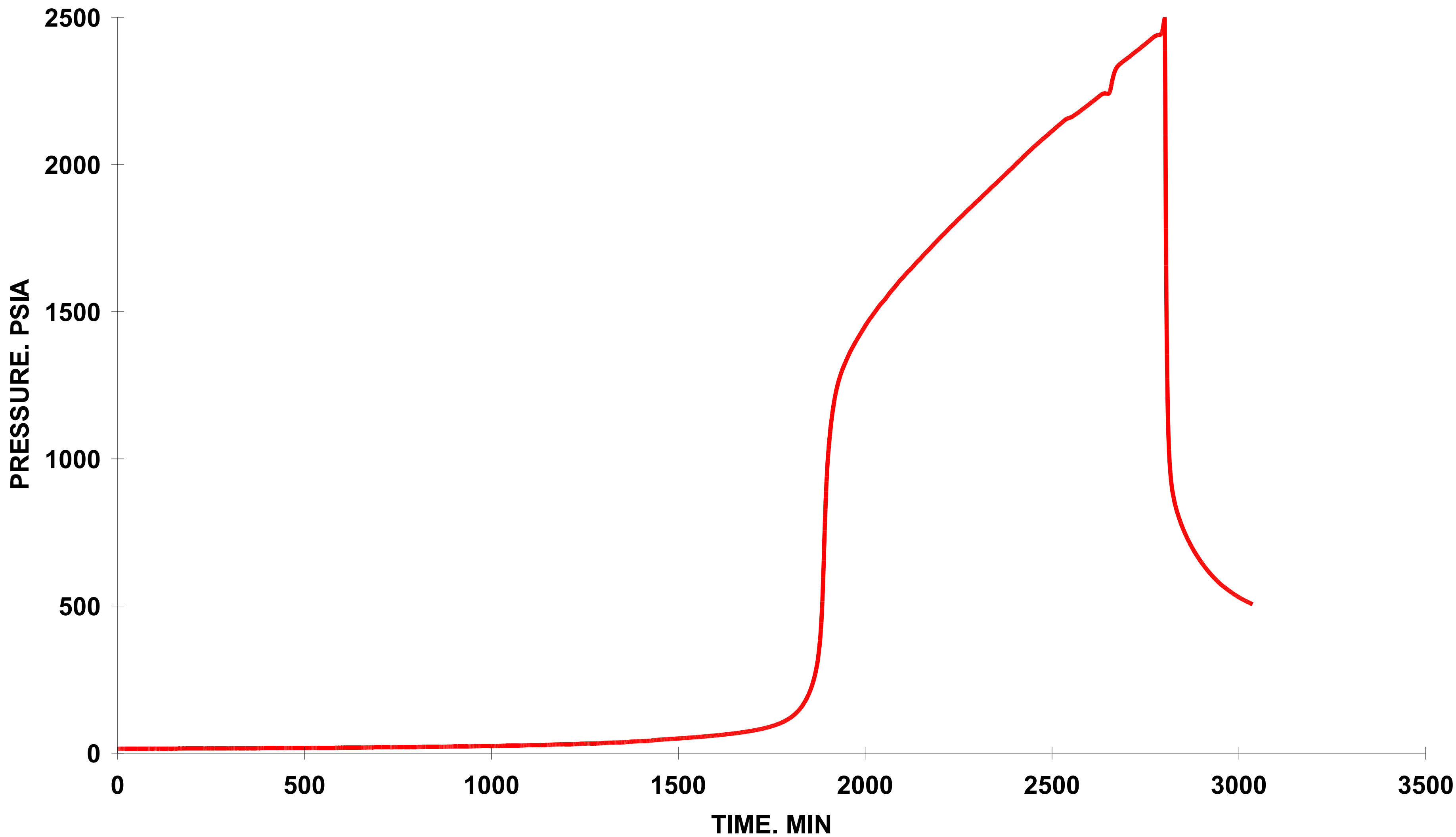
Maximum test temperature	317.07 C
Maximum value of dT/dt	3.55 C/min
Maximum test pressure	2496.49 psia
Maximum value of dP/dt	42.39 psi/min

Data File Name	C:\USERS\SHAABAN.E.NH\ONEDRIVE - IOMOSAIC CORP\COMPANIES\CITRINE\25204 CHEMICAL ANALYSIS OF BLACK SOLIDS PRODUCED FC
Data Type	ARC Instrument ID = ARC1

Chemical Component Name and/or Description	Mass g	Heat Capacity cal/g	Volume ml	Molecular Weight	Mass Fraction. %	Supplied By	Date Acquired
SUCROSE / C12H22O11 / R0026 invert	4.595	[redacted]	3.044	342.300	100.000	Givaudan	02242025
Initial	4.595		3.044				
Final after cooldown	3.554						
Lost	1.042	22.667	% Lost				

Thermal Inertia Without Fittings	2.55
Thermal Inertia With Fittings	3.25

	Exotherm 1	Exotherm 2	Total
Onset Temperature. C	130.76	311.81	
End Temperature. C	305.67	314.95	
Temperature Rise. C	174.91	3.14	
Adiabatic Temperature Rise Without Fittings. C	445.85	8.00	
Heat of Reaction Without Fittings. cal/g mix	115.89	2.08	117.97
Adiabatic Temperature Rise With Fittings. C	569.33	10.22	
Heat of Reaction With Fittings. cal/g mix	147.98	2.66	150.64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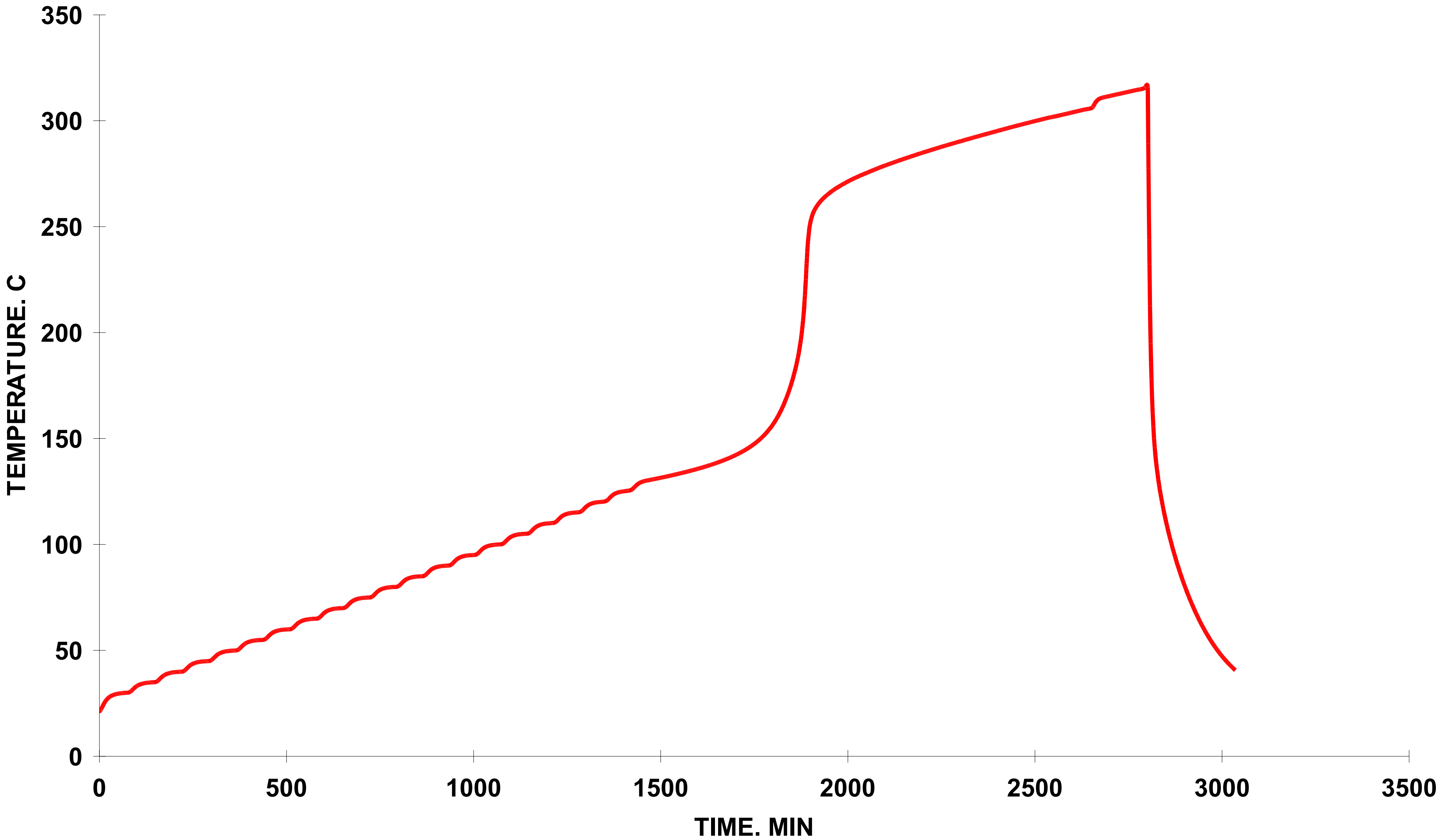
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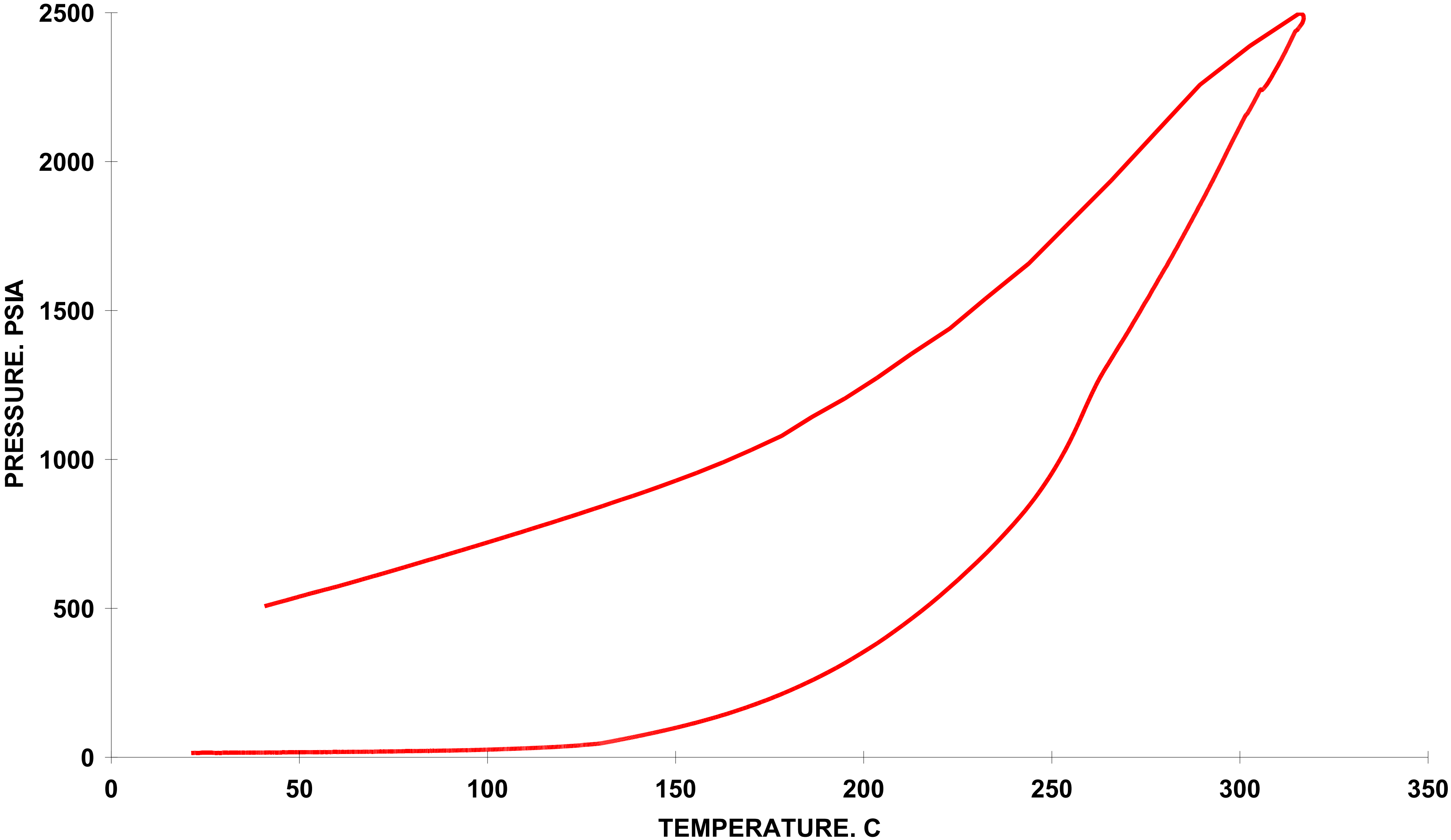
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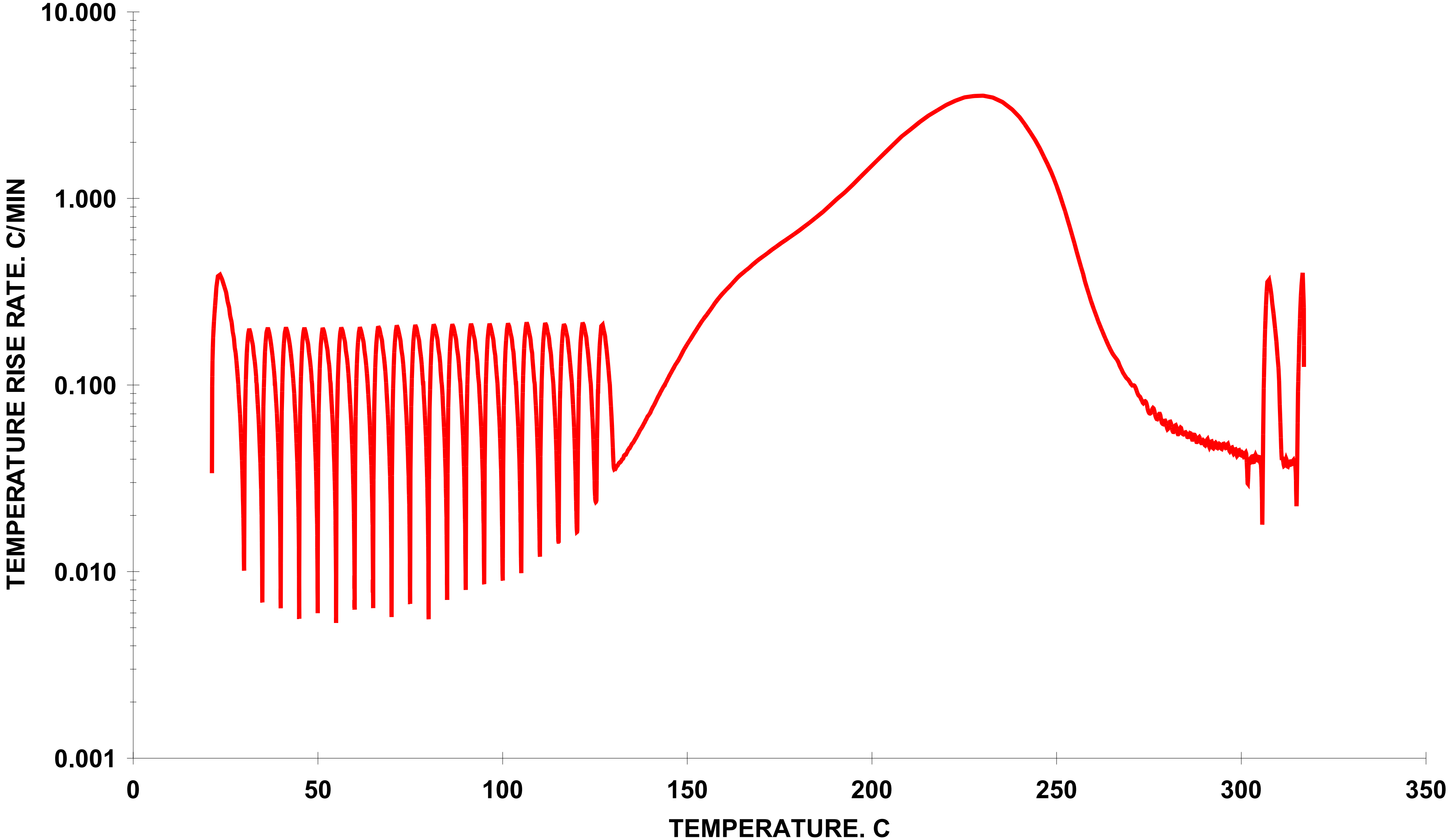
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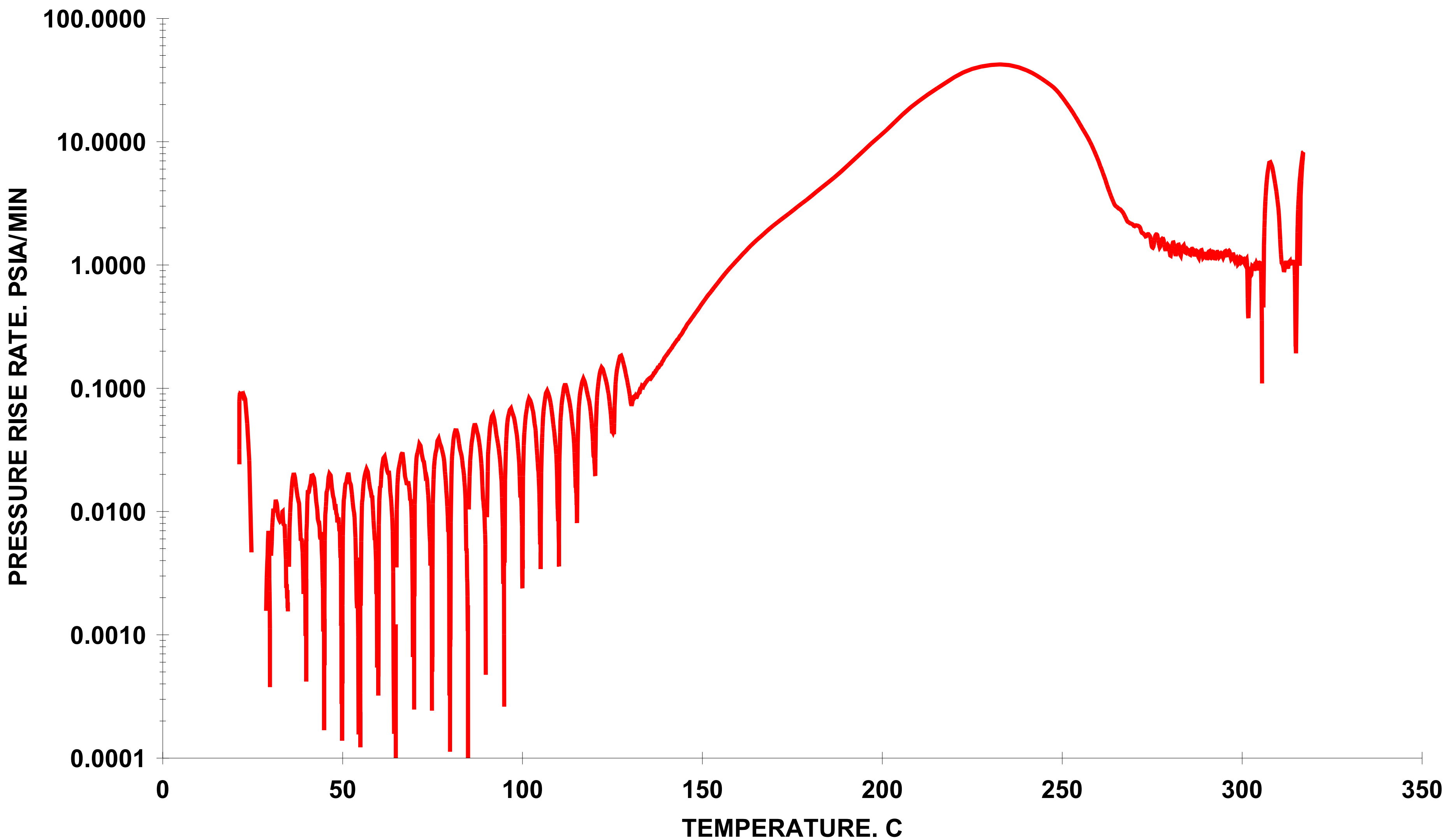
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TEMPERATURE. C

Pad Gas	AIR
Test Cell Description	Standard Test Cell
Test Cell Part Number	00000000
Test Cell Material of Construction	User Specified, IRON, or STEEL
Test Cell Mass. gms	17.1064
Test Cell Volume. ml	9.0304
Test Cell Heat Capacity. cal/g/C	0.1081545786
Fittings Material of Construction	User Specified, Titanium, or TITANIUM
Fittings Mass. gms	6.6278
Fittings Heat Capacity. cal/g/C	0.1242037143
Foil Material of Construction	User Specified
Foil Mass. gms	0
Foil Heat Capacity. cal/g/C	0.1
Stirrer Material of Construction	User Specified
Stirrer Mass. gms	0.1994
Stirrer Heat Capacity. cal/g/C	0.1
Time column	0 min
Time offset	0 min
Data analysis start time	0.01025 min
Data analysis end time	3031.51465 min
Temperature column	1 C
Temperature offset	0 C
dT/dt column	10 C/min
Pressure column	6 psia
dP/dt column	Computed
Stirrer speed column. RPM	7
Instrument mode column	14
Use all data points	
Instrument exotherm mode	4
Instrument endotherm mode	-1
Instrument heat mode	1
Instrument wait mode	2
Instrument search mode	3
Instrument cool mode	0
Instrument calibrate mode	-1
Instrument manual mode	-1
Instrument idle mode	-1

Vent Sizing Package VSP2™ Report

Chemical Reactivity Evaluation

Invert, Phosphoric Acid, Sodium Hydroxide and Antifoam Reactions

Report to:
U.S. Chemical Safety and Hazard Investigation Board
470 L'Enfant Plaza SW
Suite 604 #23278
Washington, DC 20026

Date: September 15, 2025

Report No.: ioK#: 25099 Rev. 1

AT-1922

95 Stiles Road | Salem, New Hampshire 03079
www.ioKinetic.com | P: 603.893.7009 | F: 603.386.6522

Revisions

Rev.	Date	List of Changes	Prepared by	Approved by
0	05/30/2025	Draft Final Review Copy	C. Ong	E. Shaaban, PhD
1	09/15/2025	Final Report	E. Shaaban, PhD	A. Iskandar, PhD

Table of Contents

List of Tables

Appendices

1 Study Overview

This report presents the results of a chemical reactivity study and vent sizing evaluation performed for the reaction between invert, phosphoric acid, sodium hydroxide, and antifoam.

The compositions used in the test are presented in Table 1. These materials and their quantities are based on the "Cooker 6-484 Batch Sequence – Day of Incident" and "Summary of Information Provided by CSB" documents.

Table 1: Composition Information of the VSP2-Citrine-04032025 Test 3

Components (g)	VSP2-Citrine-04032025 Test 3	
	Source	Weight (g)
Invert	Givaudan	[redacted]
Phosphoric Acid [redacted]	Givaudan	
Sodium Hydroxide [redacted]	Givaudan, item #328	
Water	ioKinetic	
Antifoam	Givaudan	
Total		110.252

Information about the test setup is summarized in Table 2. Additional test details relative to samples can be found in the VPS2 test reports in Appendix B. The detailed VSP2 test description is provided in Appendix A.

Table 2: VSP2™ Experiment Information

Test Name	Head Space	Test Cell Material / Mass(g) / Volume (ml)	Sample Mass (g)	Phi Factor Without Fittings
VSP2-Citrine-04032025 Test 3	Air	Stainless steel / 72.90 / 106.36	110.252	1.14

1.1 VSP2 ™ Sample Preparation

In an air atmosphere, invert sugar was charged into a stainless steel VSP2 test cell. A Heat-Wait-Search (HWS) program was initiated, starting at 45 °C. Once the instrument reached equilibrium at 45 °C and entered search mode, phosphoric acid was injected. Ten minutes later, sodium hydroxide solution was added. Water and antifoam were premixed, then injected, and the main valve was closed.

The test was vented when pressure reached 82.5 psig during the second exotherm, at a temperature of 134 °C.

2 Test Results and Discussions

The results of the VSP2™ tests are summarized in Table 3. Additional graphical data can be found in Appendix B.

Table 3: Test Results

Test Name	Weight Loss (%)	Observed Result	Onset T (°C)	T Rise (°C)	Adiabatic T Rise (°C)	ΔHr (cal/g)	Max dT/dt (°C/min)	Max dP/dt (psi/min)
VSP2-Citrine-04032025 Test 3	1.295	Exotherm Exotherm	45.24 118.58	17.61 14.88	19.99 16.89	-10.58 - 8.94	17.43	41.75

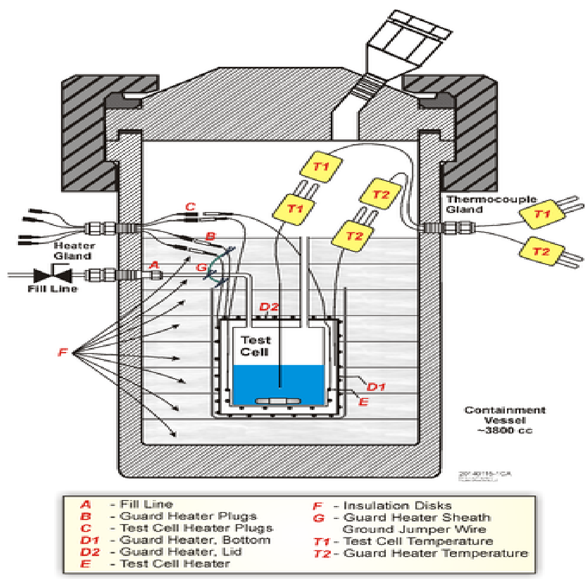
The following observations were noted with respect to the data presented:

1. The test was vented when the Pressure reached 82.5 psig during the 2nd exotherm, the temperature was 134°C. A black-brown liquid sample vented through a 1/8 tube, amounting to 35.91g was collected in a glass vessel.
2. After the cell cooled down to room temperature, the remaining sample in the cell was 72.914g of black-brown liquid.
3. Upon venting the non-condensable gas, a total of 1.43 g of the sample was lost. This weight loss accounts for both vented gas and material remaining within the pressure transfer tube.

Appendix A: Test Description

The Vent Sizing Package 2™ (VSP2™) is a low thermal inertia adiabatic calorimeter used for process hazard characterization that utilizes state-of-the-art DIERS technology to obtain critical upset process design data. It is the commercial version of the original DIERS bench scale apparatus developed by Fauske & Associates, LLC's (FAI).

Figure A1: VSP2™ illustration



Its versatile design allows the VSP2™ to simulate upset (abnormal) conditions which might lead to a runaway chemical reaction (e.g. loss of cooling, loss of stirring, mischarge of reagents, mass-loaded upset, batch contamination, fire exposure heating, etc). Resulting temperature and pressure rise rates are directly scalable since it is a low thermal inertia (phi-factor) apparatus. FAI not only utilizes the VSP2™ in our fully equipped hazards laboratory but we also manufacture and sell the calorimeter for use by our clients.

Benefit

The VSP2™ utilizes established DIERS technology to identify and quantify process safety hazards so they can be prevented or accommodated by process design.

Test data includes adiabatic rates of temperature and pressure change which, due to the low thermal inertia, can be directly applied to process scale to determine relief vent sizes, quench tank designs and other relief system design parameters related to process safety management. Adiabatic data obtained with the VSP2™ can be used to characterize reactive chemical and consequences that could occur due to process upset conditions.

Optimizing Temperature Measurement

To get the best temperature readings from VSP2™ tests, it is important to remember to ground the sheath of each element of the guard heater to the test cell fill line as shown in Figure 1. Both the sheath of the lid and side elements of the guard heater should be jumpered using alligator clips to the test cell fill line. This eliminates electrical interference from the heaters with the test cell thermocouple. In addition (as per the VSP2™ Manual), the containment vessel should be grounded to the VSP2™ control box chassis. Finally, the shields of the thermocouple cables where they plug in to the thermocouple gland should also be grounded to the outside of the containment vessel. These measures help assure noise free temperature measurements. If the FAI Super Magnetic stirrer is being used, the thermocouple cables should be oriented radially away from the containment vessel and kept above the Super Magnetic Stirrer. This avoids interference from the strong magnetic field of the stirrer.

Features

The versatile configurations offered by the VSP2™ design directly simulates process conditions including:

- Loss of cooling or agitation
- Accumulation or mischarge of reactants
- Contamination of batch
- Thermally initiated decomposition
- Resident incubation time
- In-situ liquid/gas dosing or sampling

Applications

Use of the VSP2™ can help users obtain complete chemical system data such as:

- Low thermal inertia testing allows data to be directly applied to process scale Temperature and pressure rise rates applicable to relief system design "Based on DIERS two-phase flow technology, recognized by OSHA as an example of "good engineering practice"
- Many testing configurations
    - Solids, liquids or two-phase mixtures
    - Closed or open (vented) tests
    - Scaled blowdown simulation
    - Test cells are available in 304 & 316 SS, Hastelloy C, Titanium, and glass
- Accurate adiabatic data
    - Onset temperature
    - Total adiabatic temperature rise (ΔTad)
    - Heat of reaction or mixing room temperature to 400C.
    - Vapor pressure data: 0 to 3000psia
- Time to maximum rate (tmr)
    - Self-accelerating decomposition temperature (SADT)
- Relief vent sizing
- Quench tank design
- Effluent handling
- Critical temperature
- Effect of two-phase flow

Onset temperature: The temperature at which the heat that is released by a reaction can no longer be completely removed from the reaction vessel, and consequently, results in a detectable temperature increase.

Measure T rise: The measured temperature rise of self-heating reaction under adiabatic conditions without consideration of the PHI-factor

Adiabatic T rise: is the observed temperature rise of a self-heating reaction under adiabatic conditions in consideration of the PHI-factor

PHI-factor: The ratio of mass and specific heat capacity of a sample or sample mixture compared to that of the vessel or sample container. The closer the PHI-factor is to 1, the lower the influence of the container and the more representative the result is of the sample itself.

Heat of Reaction: The energy that is released or absorbed when chemicals are transformed in a chemical reaction

DP: The change in pressure in the test cell between the start of the test and the end of the test. Primarily useful for determining the presence of non-condensable gases in the test cell at the end of the run.

Appendix B: Test Results

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Today's Time and Date	10:57:43 AM, Fri Apr 04 2025
Test Date	April 03, 2025
Test Location	Salem, NH
Author	A.Iskandar and E.Shaaban
Operator	A.Iskandar
Test Description	PRV at 82.5 psig for Invert, Phosphoric Acid, and Sodium Hydroxide Test Number VSP2-Citrine-04032025 Test 3
Lab Notebook Reference	Page no.6x
Comments	In an air atmosphere, the invert sugar was charged into a stainless steel VSP2 test cell. A Heat-Wait-Search (HWS) program was initiated, starting at 45 C Once the instrument reached equilibrium at 45 C and during the search mode, phosphoric acid was injected. Ten minutes after the phosphoric acid addition, the sodium hydroxide solution was introduced. Water + Antifoam amounts were mixed then injected, and the main valve was closed. The test was vented when the Pressure reached 82.5 PSIG during the 2nd exotherm, the temperature was 134 A black-brown liquid sample vented through a 1/8 tube and collected in a glass vessel was 35.91g After the cell cooled down to RT, the remaining sample in the cell was 72.914 g black-brown liquid. Upon venting the non-condensable gas, a total of 1.43 g of the sample was lost. This weight loss accounts for both vented gas and material remaining within the pressure transfer tube.
Ambient Conditions	P: 1007 mbar, T: 21.3C, RH: 17.8%, tested under air
Sample Description	

Maximum test temperature	134.95 C
Maximum value of dT/dt	17.43 C/min
Maximum test pressure	96.33 psia
Maximum value of dP/dt	41.75 psi/min

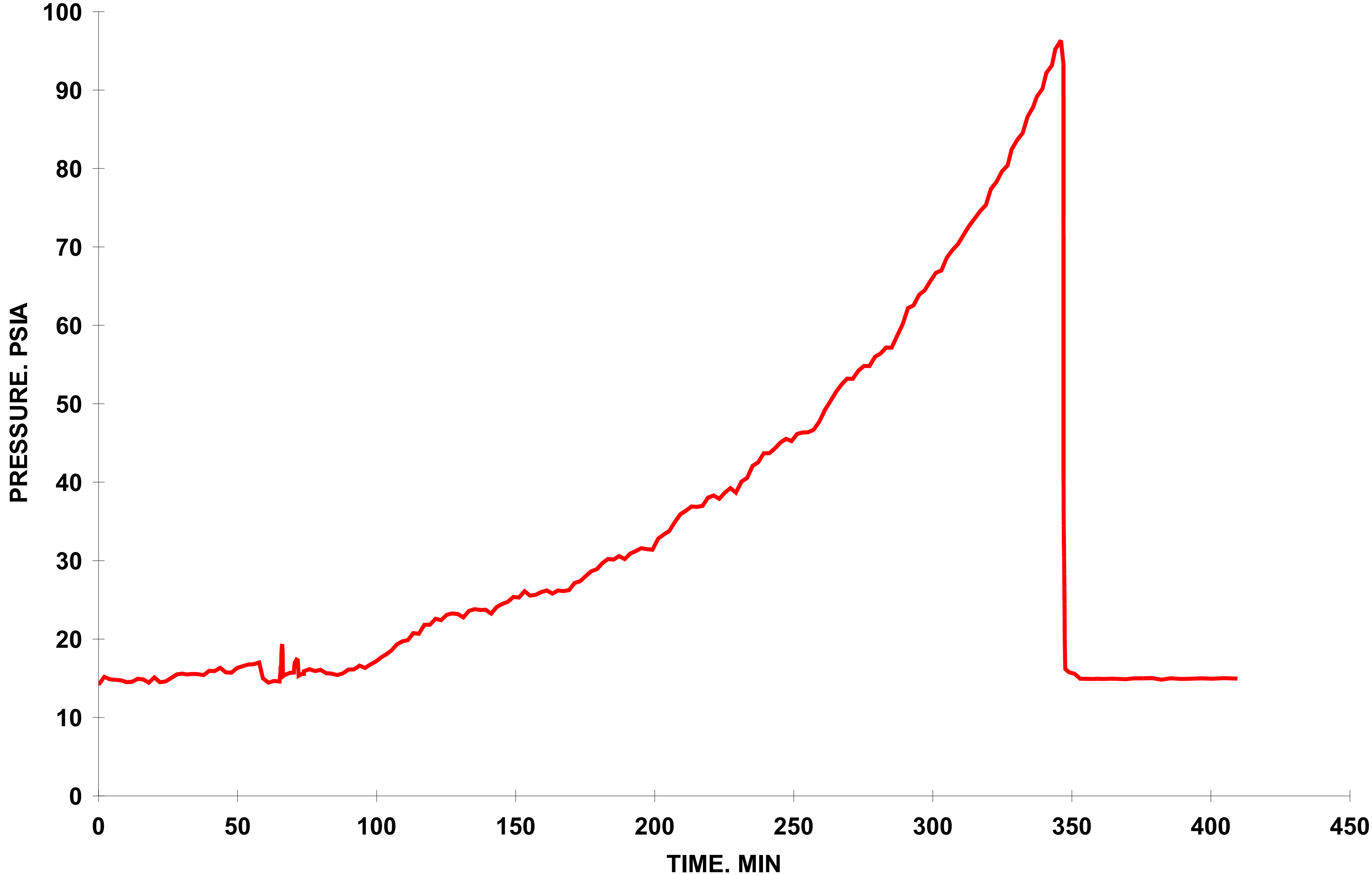
Data File Name C:\USERS\SHAABAN.E.NH\ONEDRIVE - IOMOSAIC CORP\COMPANIES\CITRINE\TEST 3 VSP2\VSP2-CITRINE-04032025 TEST 3

Data Type VSP Instrument ID = VSP2

Chemical Component Name and/or Description	Mass g	Heat Capacity cal/g	Volume ml	Molecular Weight	Mass Fraction. %	Supplied By	Date Acquired
SUCROSE / C12H22O11 / R0026 invert	[redacted]	[redacted]	[redacted]	342.300	[redacted]	Givaudan	02242025
PHOSPHORIC ACID / H3O4P / Phosphoric acid [redacted]	[redacted]	[redacted]	[redacted]	97.995	[redacted]	Givaudan	02242025
SODIUM HYDROXIDE / HNaO / sodium hydroxide [redacted]	[redacted]	[redacted]	[redacted]	39.997	[redacted]	Givaudan	02242025
User Component 4 / Antifoam	[redacted]	[redacted]	[redacted]	0.000	[redacted]	Givaudan	02242025
WATER / H2O / Water	[redacted]	1.000	[redacted]	18.015	[redacted]	ioKinetic	-
Initial	110.252		79.346				
Final after cooldown	108.824						
Lost	1.428	1.295	% Lost				

Thermal Inertia Without Fittings	1.14
Thermal Inertia With Fittings	1.14

	Exotherm 1	Exotherm 2	Total
Onset Temperature. C	45.24	118.58	
End Temperature. C	62.85	133.46	
Temperature Rise. C	17.61	14.88	
Adiabatic Temperature Rise Without Fittings. C	19.99	16.89	
Heat of Reaction Without Fittings. cal/g mix	10.58	8.94	19.51
Adiabatic Temperature Rise With Fittings. C	19.99	16.89	
Heat of Reaction With Fittings. cal/g mix	10.58	8.94	19.51



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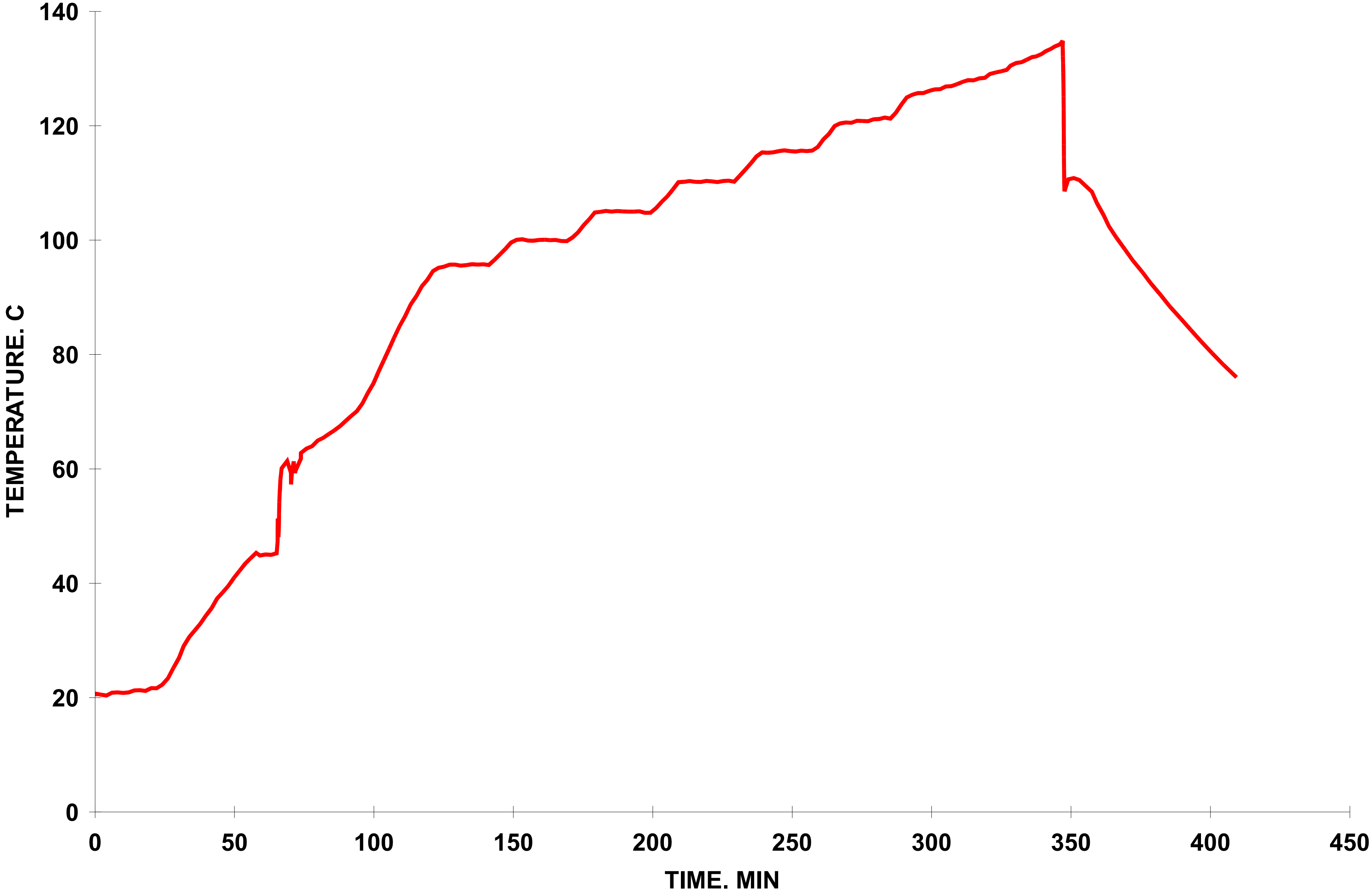

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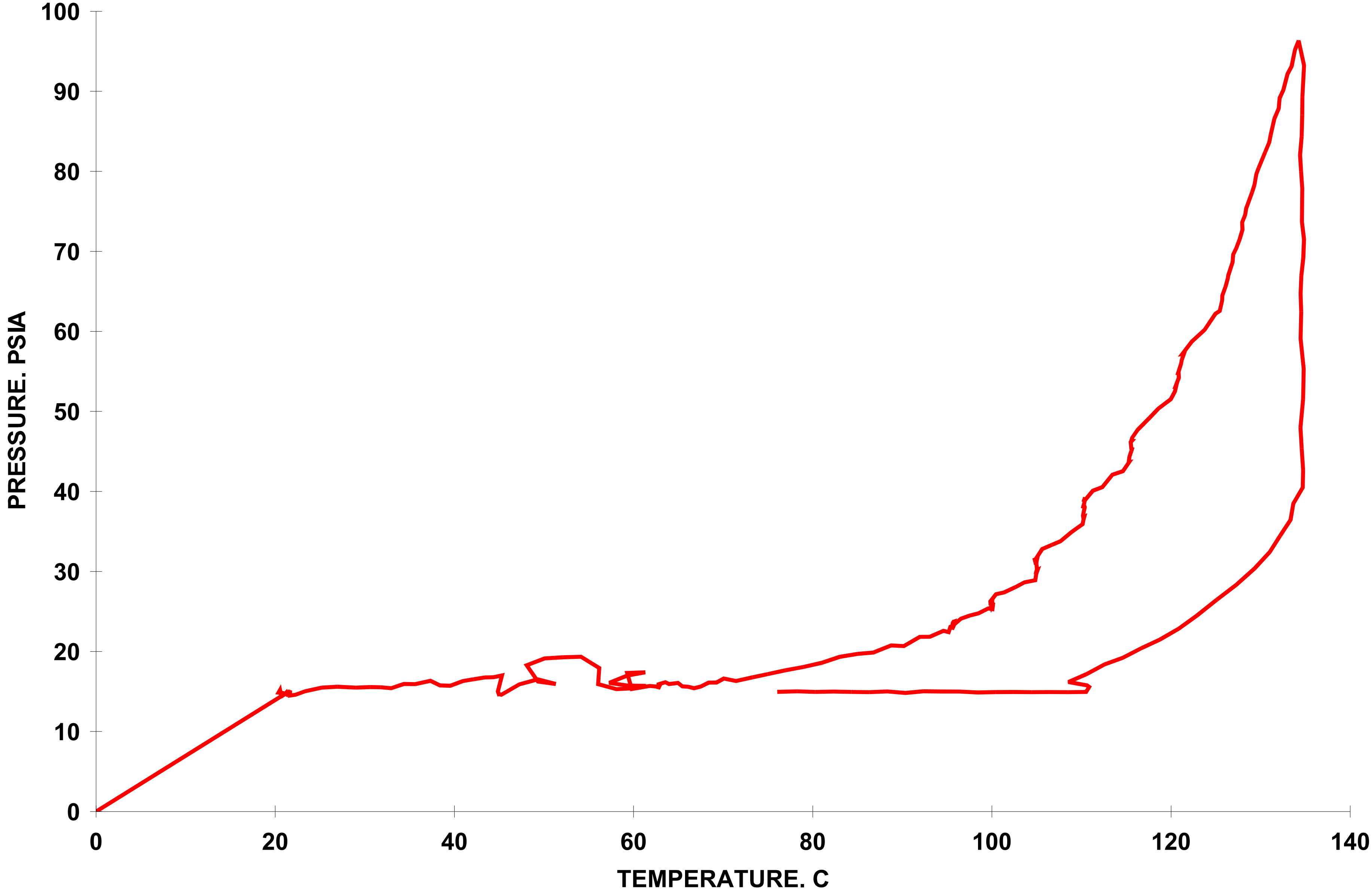

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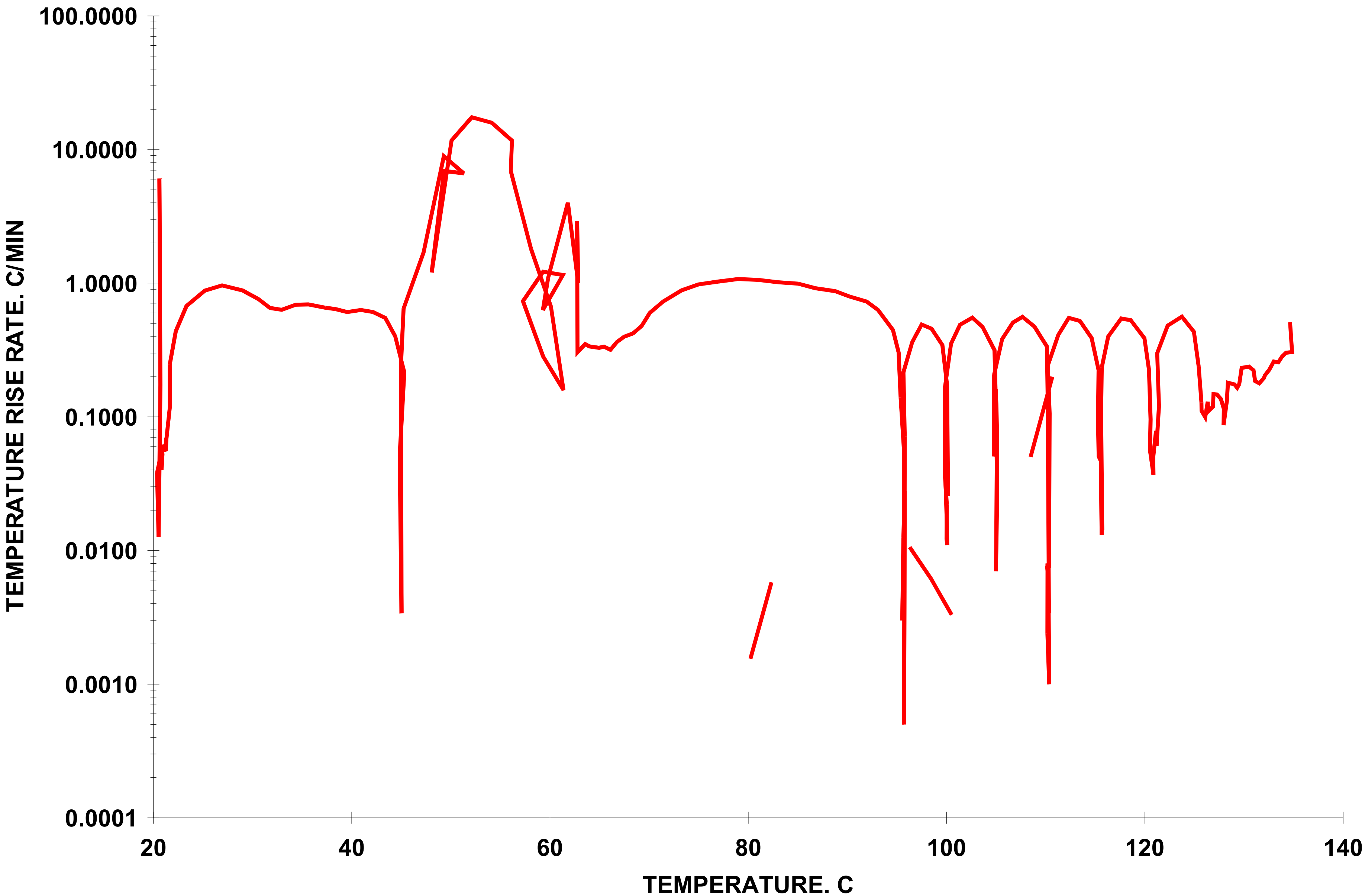

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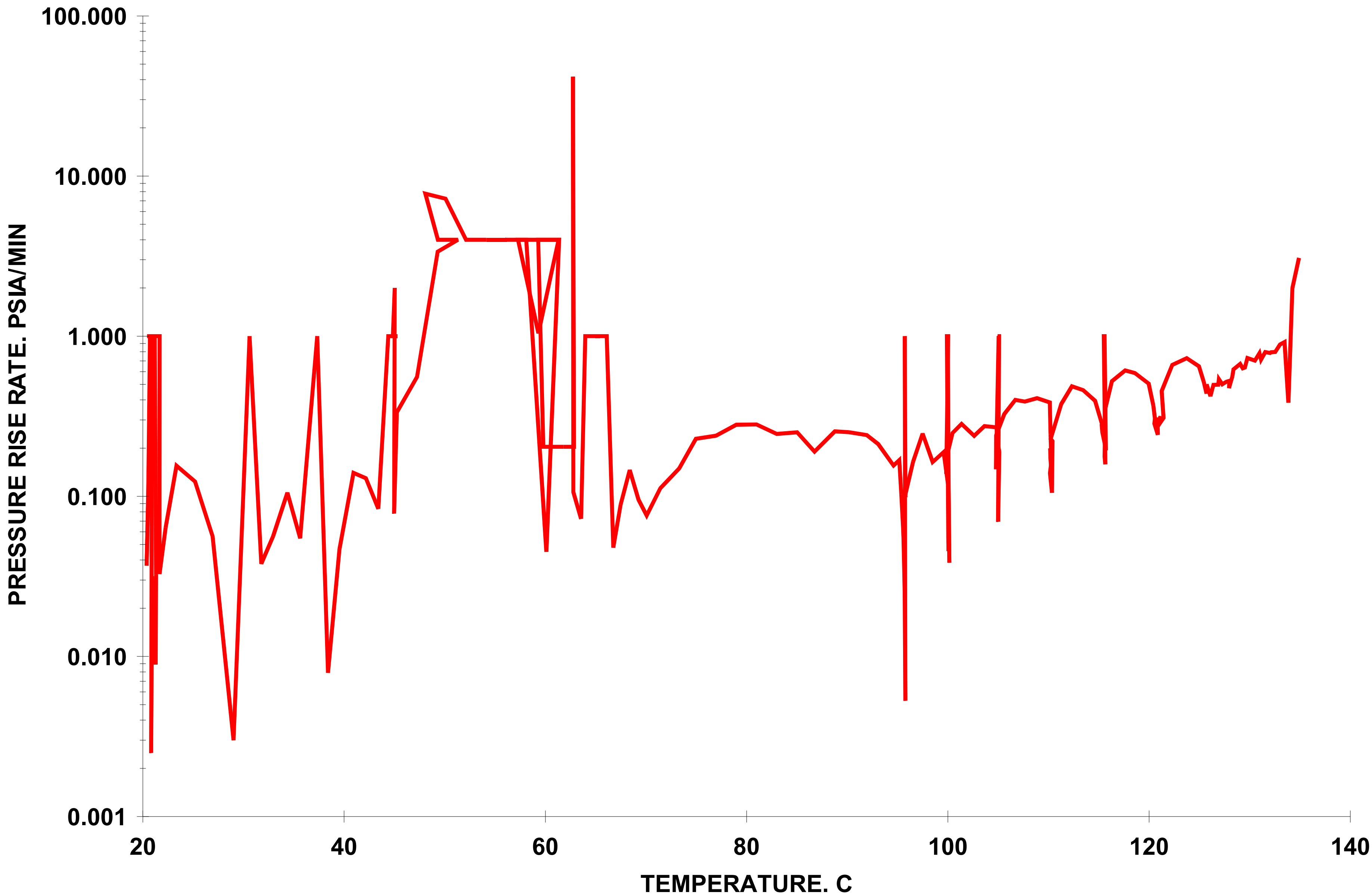
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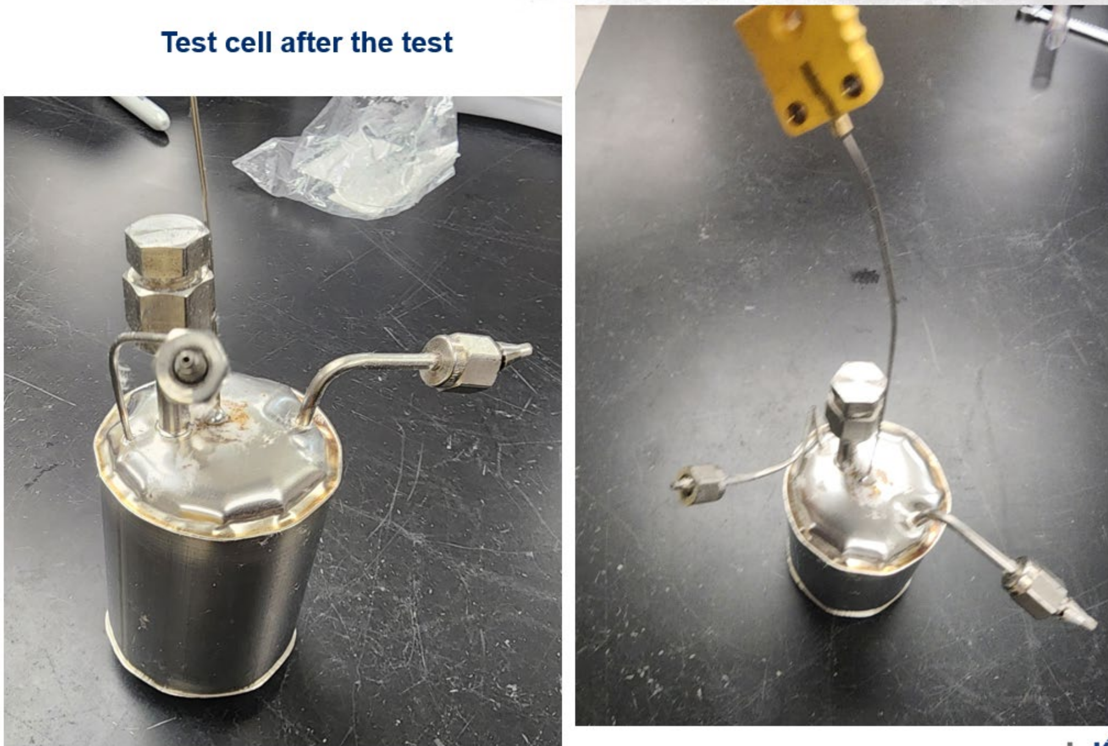
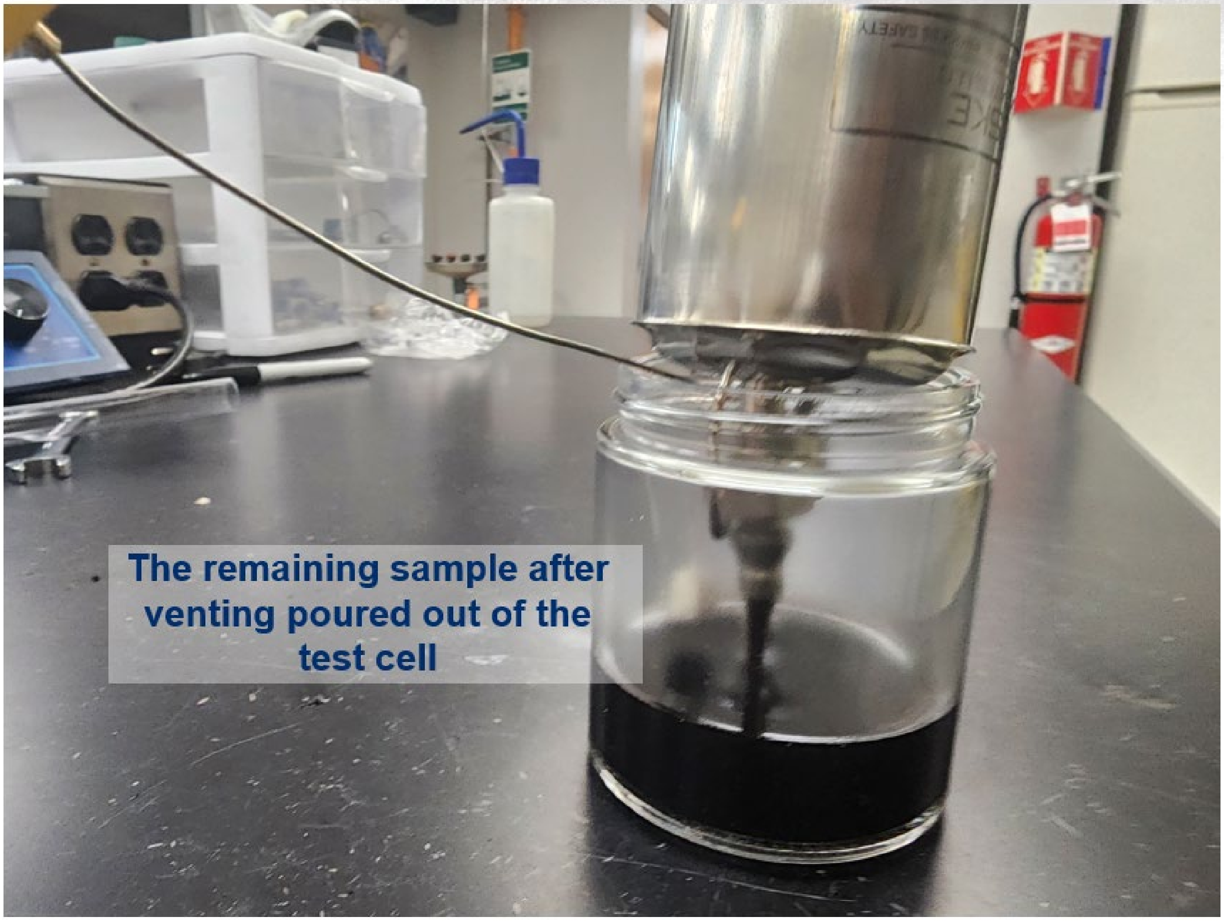
TEMPERATURE. C

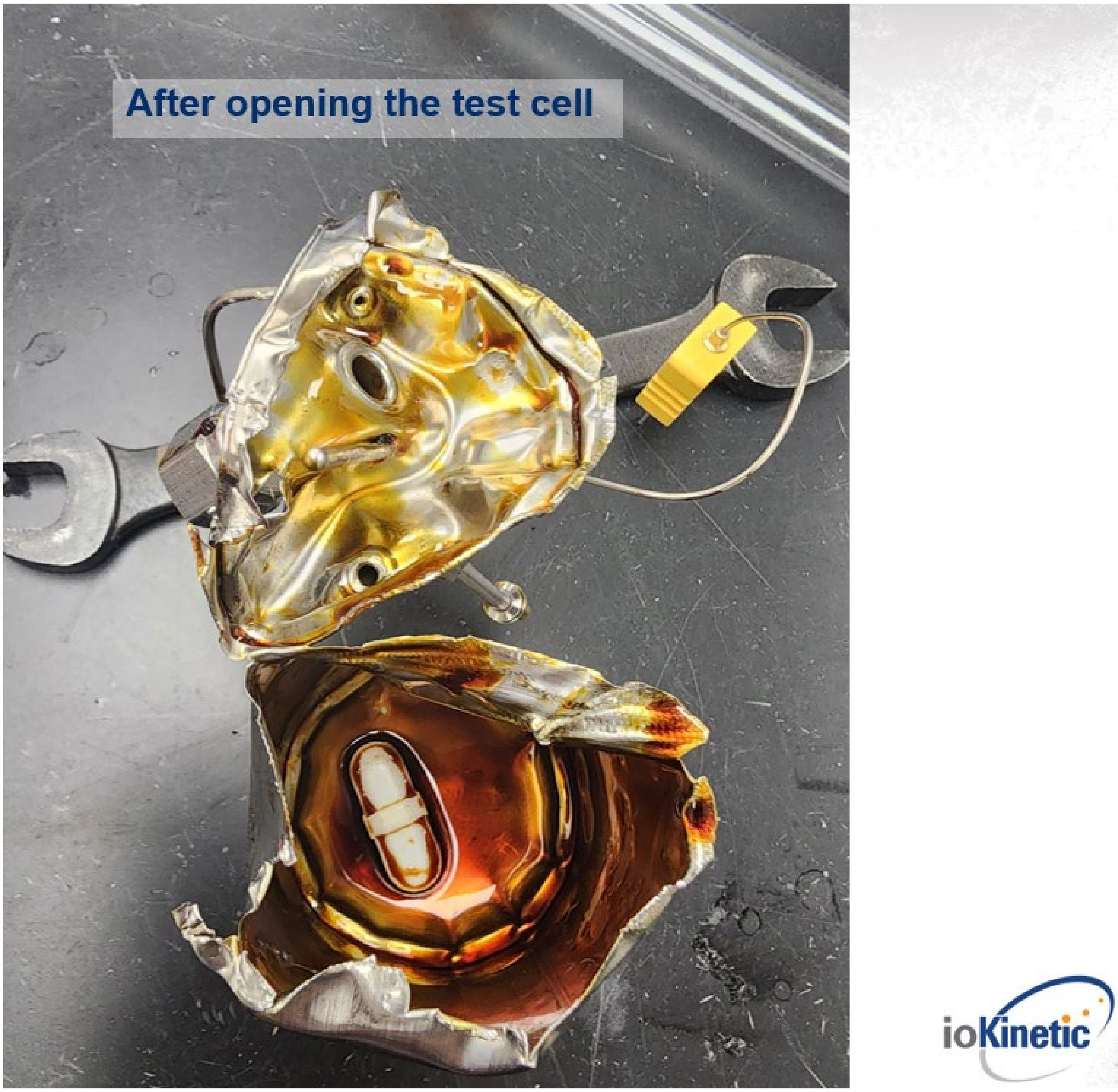
Pad Gas	AIR	
Test Cell Description	Standard Test Cell with the stirre	
Test Cell Part Number	00000000	
Test Cell Material of Construction	User Specified, IRON, or STEEL	
Test Cell Mass. gms	72.9	
Test Cell Volume. ml	106.36	
Test Cell Heat Capacity. cal/g/C	0.1081545786	
Fittings Material of Construction	User Specified	
Fittings Mass. gms	0	
Fittings Heat Capacity. cal/g/C	0.1	
Foil Material of Construction	User Specified	
Foil Mass. gms	0	
Foil Heat Capacity. cal/g/C	0.1	
Stirrer Material of Construction	User Specified	
Stirrer Mass. gms	0	
Stirrer Heat Capacity. cal/g/C	0.1	
Time column	1	min
Time offset	0	min
Data analysis start time	0	min
Data analysis end time	408.80835	min
Temperature column	2	C
Temperature offset	0	C
dT/dt column	13	C/min
Pressure column	4	psia
dP/dt column	14	psia/min
Instrument mode column	15	
Use all data points		
Instrument exotherm mode	4	
Instrument endotherm mode	-1	
Instrument heat mode	1	
Instrument wait mode	2	
Instrument search mode	3	
Instrument cool mode	0	
Instrument calibrate mode	-1	
Instrument manual mode	-1	
Instrument idle mode	-1	

Appendix C: Test Photos

Test cell after the test




The remaining sample after venting poured out of the test cell


After opening the test cell

Gas Analysis Reports

The following reports detail the Gas Chromatography-Mass Spectrometry (GC-MS) tests conducted to identify the composition of the gases generated during the APTAC and ARC tests.

APTAC™ Head Space Gas Analysis using GC-MS Report

Chemical Reactivity Evaluation

APTAC™ - CSB 03132025 Test 1 and APTAC-CSB-03192025 Test 2

Report to:

U.S. Chemical Safety and Hazard Investigation Board

470 L'Enfant Plaza SW

Suite 604 #23278

Washington, DC 20026

Date: September 15, 2025

Report No.: ioK#: 25099 Rev.1

AT-1922

95 Stiles Road | Salem, New Hampshire 03079

www.ioKinetic.com | P: 603.893.7009 | F: 603.386.6522

Revisions

Rev.	Date	List of Changes	Prepared by	Approved by
0	5/30/2025	Draft Final Review Copy	E. Shaaban, PhD	A.Iskandar, PhD
1	09/15/2025	Final Report	E. Shaaban, PhD	A. Iskandar, PhD

Table of Contents

List of Tables

List of Figures

Appendices

1 Study Overview

This report presents the results of gas analysis for the headspace after the following Automatic Pressure-Tracking Adiabatic Calorimeter (APTAC™) tests: 'APTAC-CSB03132025 Test 1' and 'APTAC-CSB03192025 Test 2'.

After the APTAC had cooled down, gaseous samples were collected in Tedlar bags and injected into the GC-MS using a gas-tight syringe.

The analysis was performed using a GC-MS system (Agilent 6890N coupled with 5973 MS) equipped with a PLOT column (Agilent J&W PoraBOND Q for volatile solvents and hydrocarbons, 25 m × 0.25 mm × 3 µm, –100 °C to 300/320 °C). Helium was used as the carrier gas.

The oven temperature program started at 40 °C (held for 10 minutes), increased at 10 or 20 °C/min to 250 °C, and was then held at the final temperature for 5 minutes.

The injector was operated in splitless mode at 200 °C.

Nitrogen and carbon monoxide co-eluted and were detected in the same peak in the GC-MS. Both N_2 and CO produce signals at m/z = 28, making them indistinguishable in the same peak.

A detailed test description is provided in Appendix A. For further information regarding the APTAC test, see the APTAC test reports.

2 Test Results

The GC-MS results for the headspace of 'APTAC-CSB03132025 Test 1' are summarized in Table 1 and Figure 1.

The GC-MS results for the headspace of 'APTAC-CSB03192025 Test 2' are summarized in Table 2 and Figure 2.

For the detailed MS signal of each peak, please see Appendix B.

Table 1: GC-MS Test Results for the Headspace of 'APTAC-CSB03132025 Test 1'

Peak #	Retention time (min)	Area % of total	Compound
1	1.93	22%	Nitrogen and carbon monoxide*
2	2.216	70.9%	Carbon dioxide
3	13.70	6.6%	Hexane

Table 2: GC-MS Test Results for the Headspace of 'APTAC-CSB03192025 Test 2'

Peak #	Retention time (min)	Area % of total	Compound
1	2.02	15.4%	Nitrogen and carbon monoxide*
2	2.36	84.6%	Carbon dioxide

** Nitrogen and carbon monoxide co-eluted and were detected in the same peak in the GC-MS due to their similar physical properties. Nitrogen and carbon monoxide produce signals at m/z = 28, making them indistinguishable under standard GC-MS conditions.*

Figure 1: GC-MS Main Peaks Versus Retention Time for the Headspace of 'APTAC-CSB03132025 Test 1'

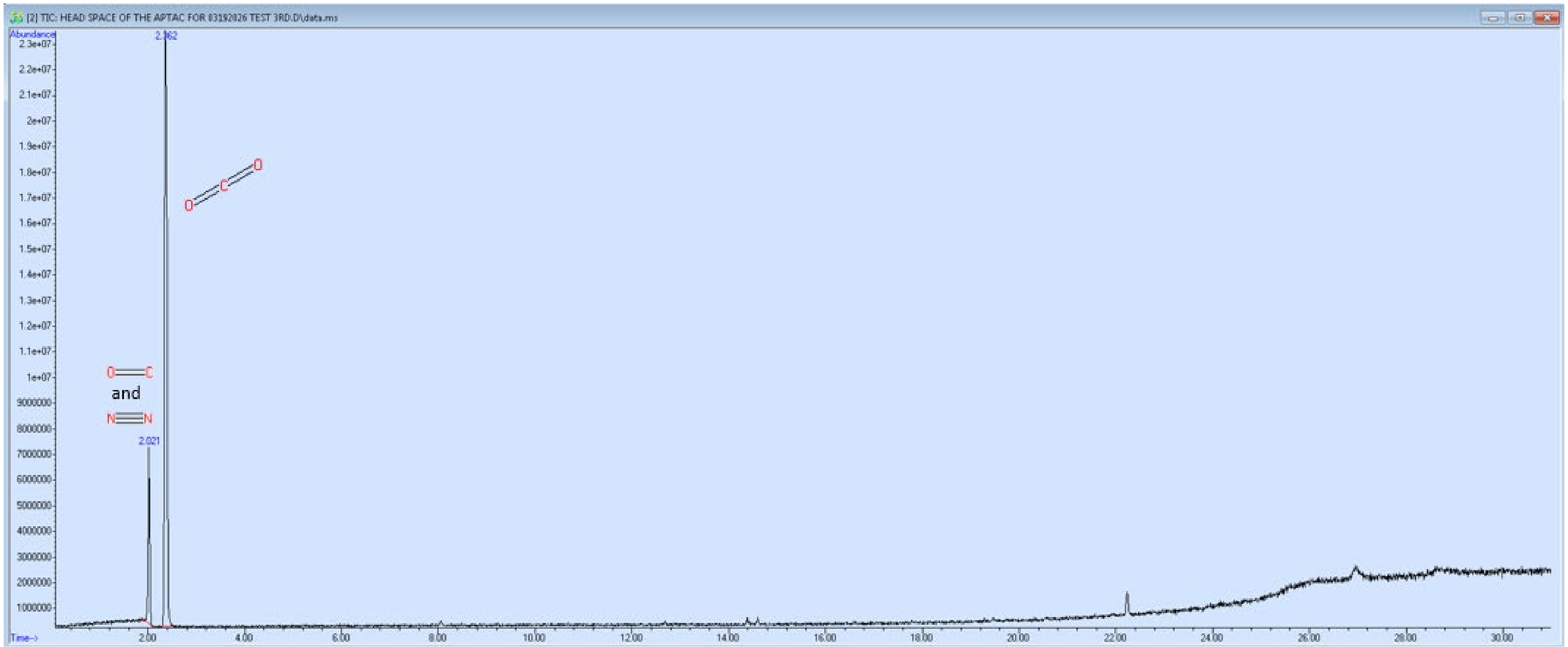
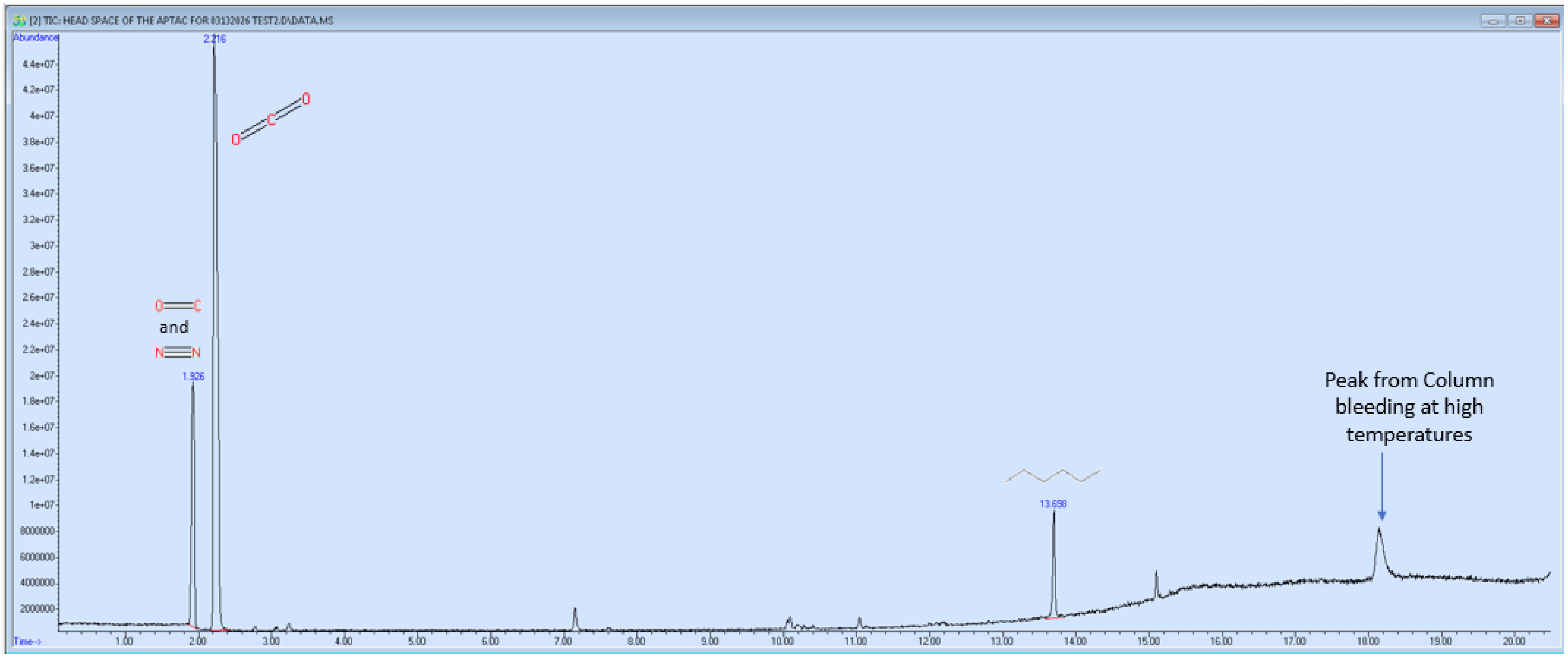


Figure 2: GC-MS Main Peaks Versus Retention Time for the Headspace of 'APTAC-CSB03192025 Test 2'



Appendix A: Test Description

GC-MS

Gas Chromatography Mass Spectrometry (GC-MS) is a technique that combines the separation capacity of gas chromatography with the sensitivity and selective capacity of the mass detector. This combination allows analyzing and quantifying trace compounds in complex mixtures with a high degree of effectiveness. This technique is indicated for the separation of volatile and semi-volatile organic compounds. GC-MS can be used to study liquid, gaseous or solid samples. The use of GC-MS is restricted to the separation of compounds of formula weight lower than 1000 or molecular weight lower than 1000 kg/kgmol and a maximum working temperature of about 400ºC.

To conduct a test, The sample is first introduced into the Gas Chromatograph (GC) manually with a syringe or by an autosampler and it enters the carrier gas (typically hydrogen, helium or nitrogen) via the GC inlet. If the sample is in the liquid form, it is vaporized and transferred to the analytical column The sample components, the “analytes”, are separated by their differences in splitting between the mobile phase and the liquid stationary phase (held within the column), or for more volatile gases their adsorption by a solid stationary phase. The analytes are then propelled by an inert carrier gas. As components of the mixture are separated, each compound elutes from the column at a different time based on its boiling point and polarity. Once the components leave the GC column, they are ionized and fragmented by the mass spectrometer using electron ionization. These ionized molecules are separated based on their different mass-to-charge (m/z) ratios by the mass analyzer. The separated ions then reach the ion detector where the signal is recorded to produce a chromatogram and a mass spectrum for each data point. A complex sample produces multiple peaks in the gas chromatogram. Each peak generates a unique mass spectrum, which is used for compound identification through libraries of mass spectra.

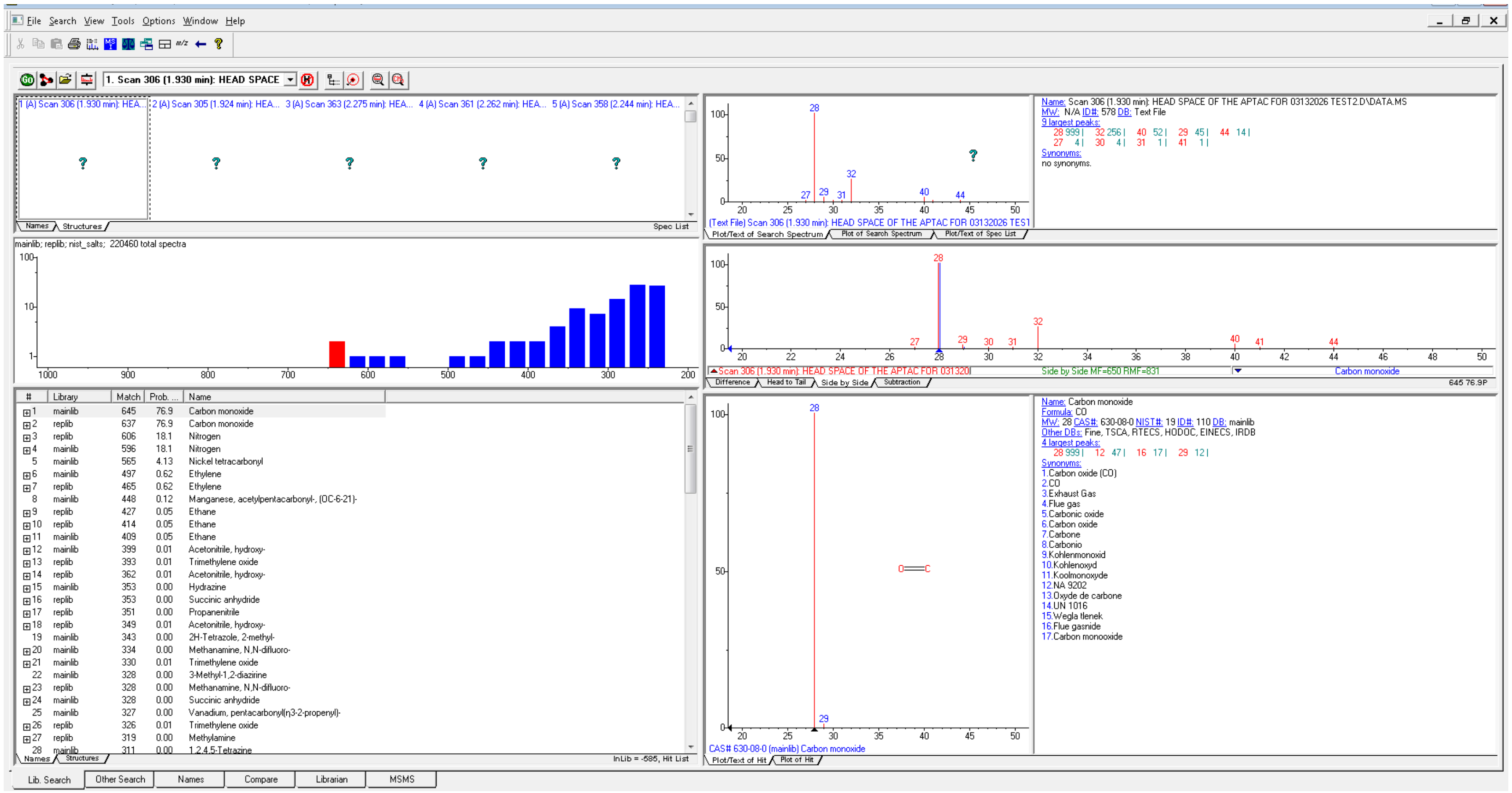
Some details on the Agilent MS5973N GC 6890 with Autosampler include:

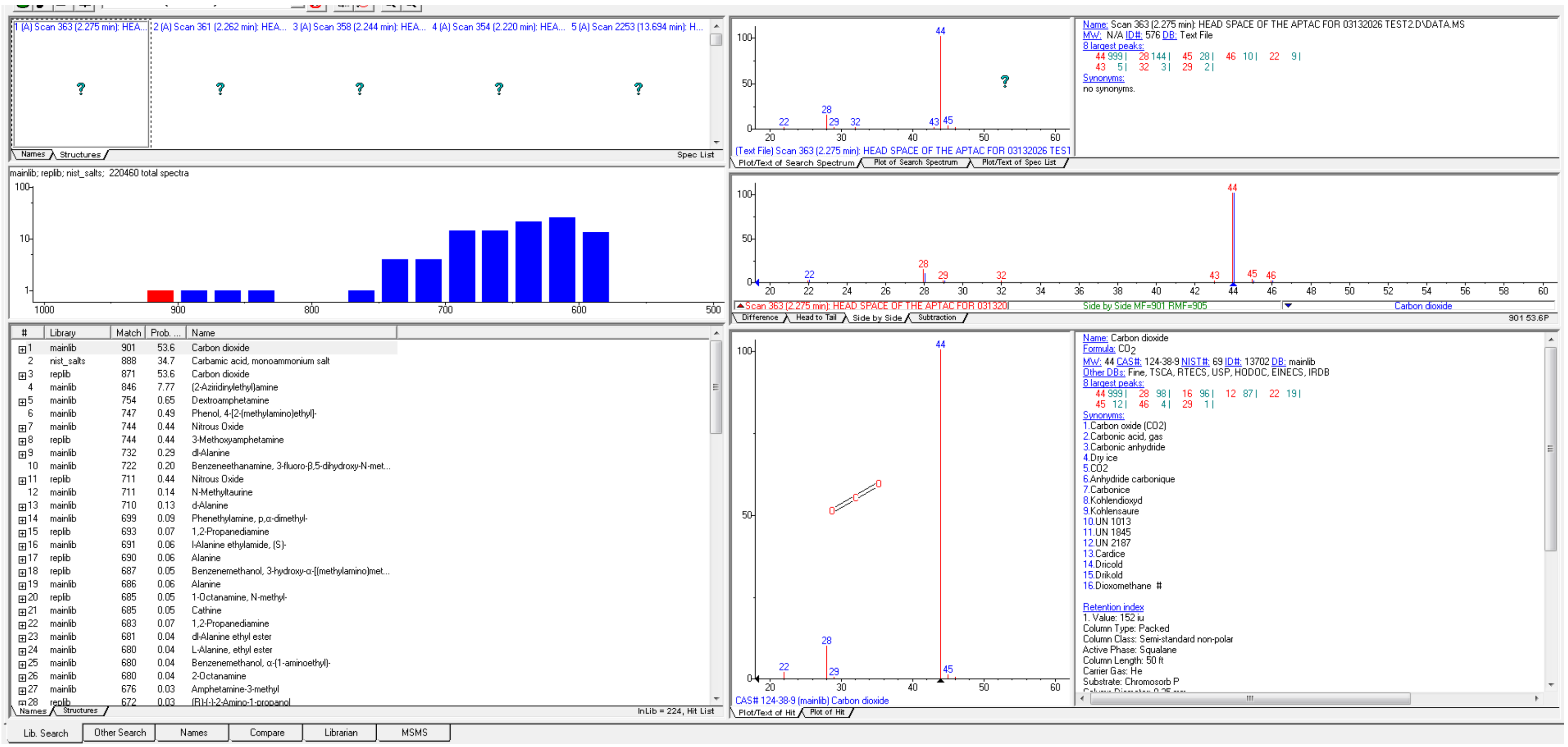
- Scan rates up to 5,200 amu/sec with 0.1 amu scan step size, with eight sampling rates.
- Total ADC (analog/digital converter) dynamic range is 10^6.
- Mass axis stability is +0.15 amu over 12 hours
- Up to 50 group of masses with 30 masses per group
- Any value between 10-9,999 msecs per mass, selectable by the user
- Filament Voltage is user-selectable over the range 5-240 eV. Dual Filament for EI; single filament for CI.

- Filament emission current is user-selectable over the range 0-315 uA in all modes of operation.
- Temperature of the independently heated ion source can be controlled up to 250°C for EI and up to 300°C for CI.
- Temperature of the independently heated quadrupole can be controlled up to 200°C
- Temperature of the interface can be controlled up to 350°C

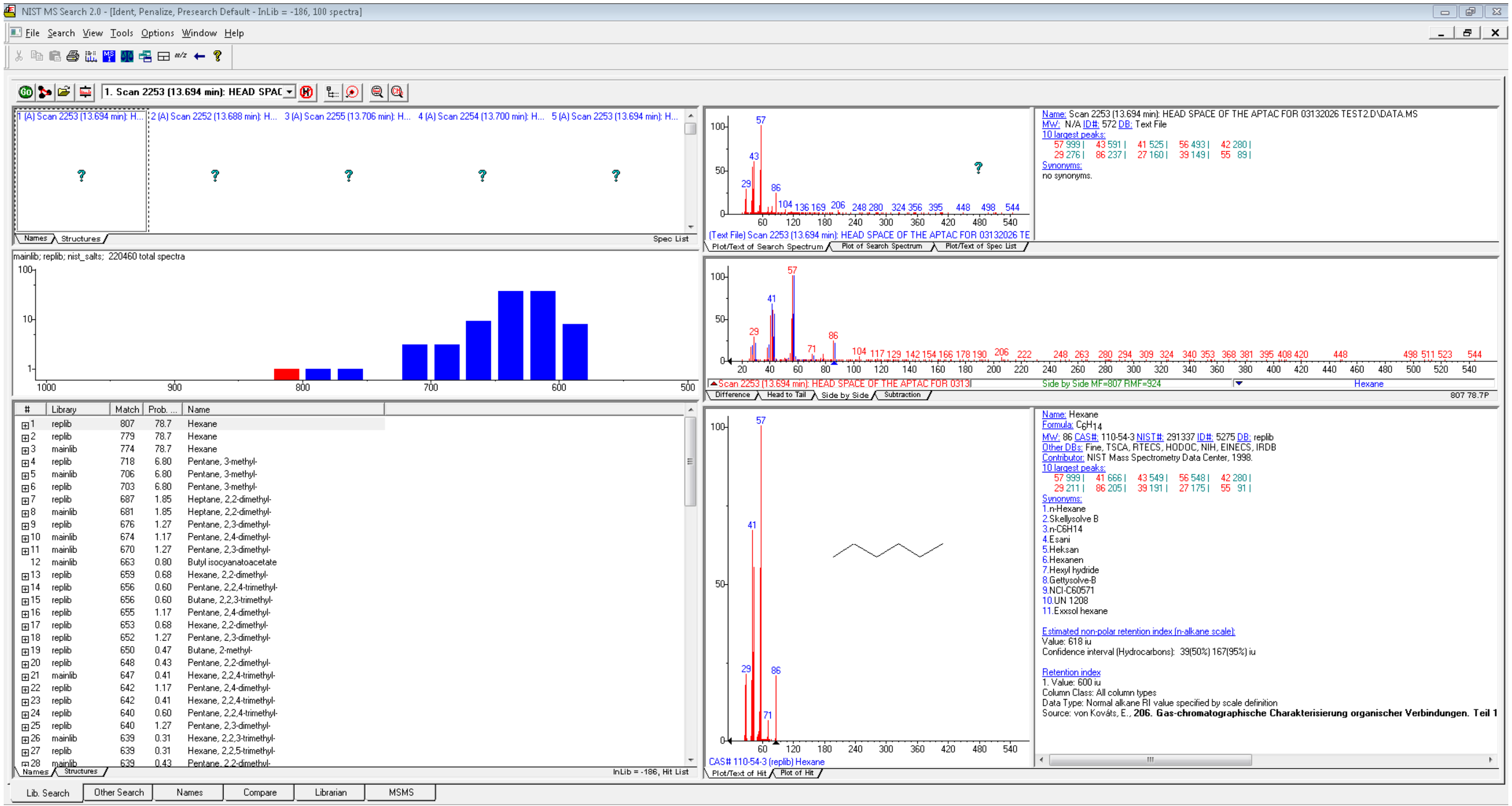
Appendix B: Detailed Peak Analysis of GC-MS Data

Figure: The MS detailed peak analysis for the gases in the headspace of 'APTAC-CSB03132025 Test 1'



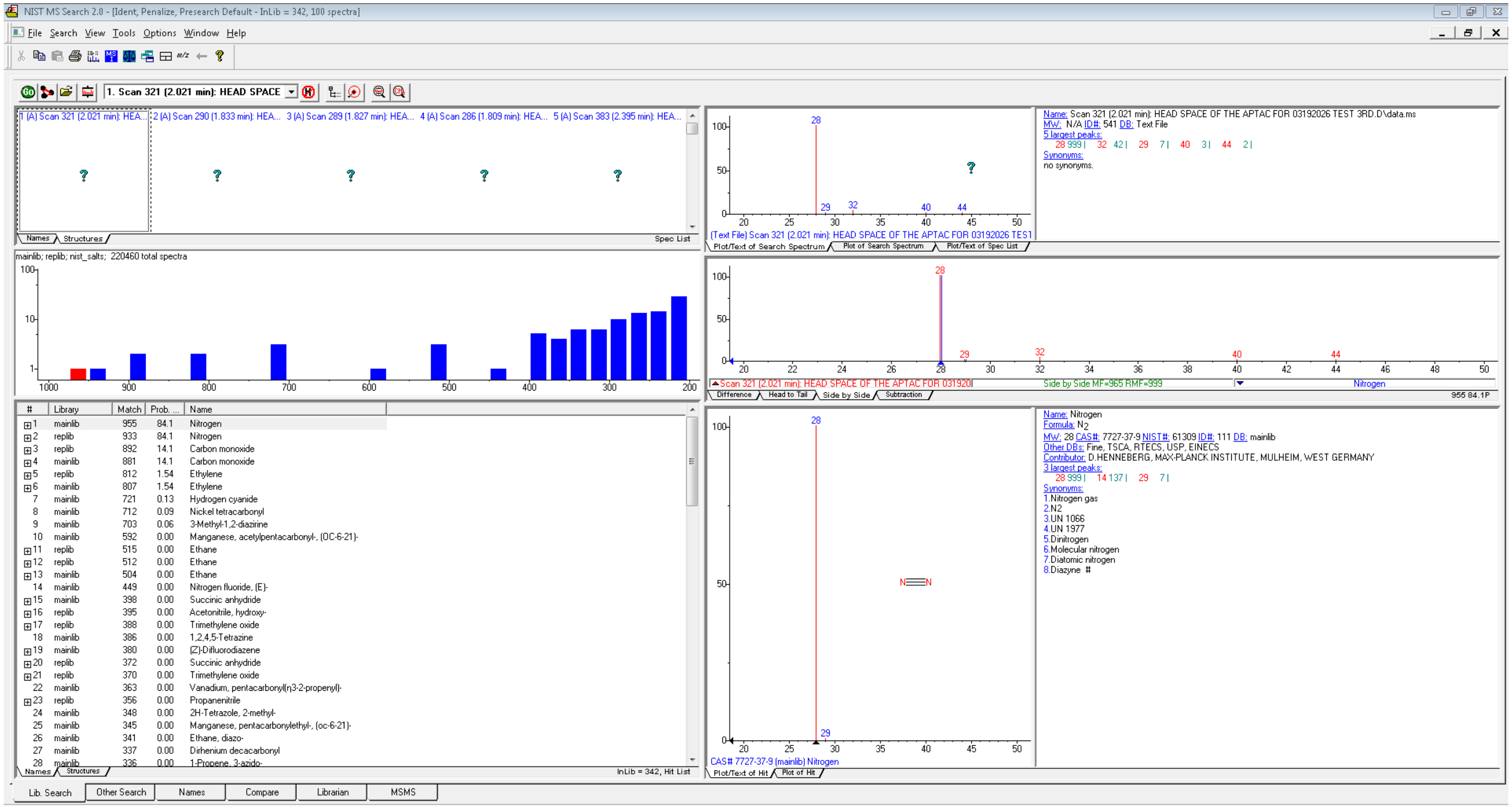


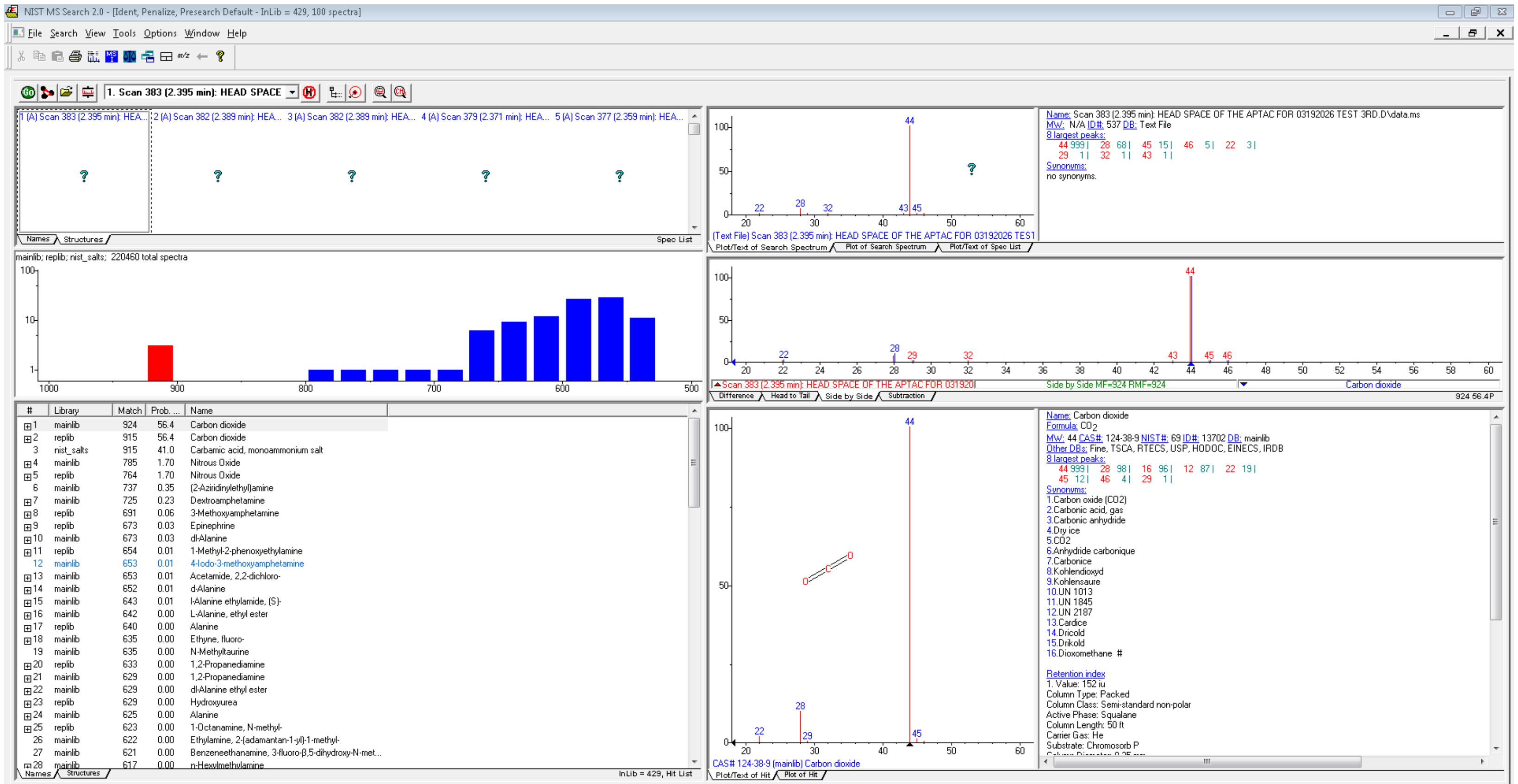
1 (A) Scan 363 (2.275 min): HEA... 2 (A) Scan 361 (2.262 min): HEA... 3 (A) Scan 358 (2.244 min): HEA... 4 (A) Scan 354 (2.220 min): HEA... 5 (A) Scan 2253 (13.694 min): H...
mainlib; replib; nist_salts; 220460 total spectra
(Text File) Scan 363 (2.275 min): HEAD SPACE OF THE APTAC FOR 03132026 TEST
Name: Scan 363 (2.275 min): HEAD SPACE OF THE APTAC FOR 03132026 TEST2.D\DATA.MS
MW: N/A ID#: 576 DB: Text File
8 largest peaks:
44 999 | 28 144 | 45 28 | 46 10 | 22 9 |
43 5 | 32 3 | 29 2 |
Synonyms:
no synonyms.
Scan 363 (2.275 min): HEAD SPACE OF THE APTAC FOR 031320
Side by Side MF=901 RMF=905
Carbon dioxide
1 mainlib 901 53.6 Carbon dioxide
2 nist_salts 888 34.7 Carbamic acid, monoammonium salt
3 replib 871 53.6 Carbon dioxide
4 mainlib 846 7.77 (2-Aziridinylethyl)amine
5 mainlib 754 0.65 Dextroamphetamine
6 mainlib 747 0.49 Phenol, 4-[2-(methylamino)ethyl]-
7 mainlib 744 0.44 Nitrous Oxide
8 replib 744 0.44 3-Methoxyamphetamine
9 mainlib 732 0.29 dl-Alanine
10 mainlib 722 0.20 Benzeneethanamine, 3-fluoro-β,5-dihydroxy-N-met...
11 replib 711 0.44 Nitrous Oxide
12 mainlib 711 0.14 N-Methyltaurine
13 mainlib 710 0.13 d-Alanine
14 mainlib 699 0.09 Phenethylamine, p,α-dimethyl-
15 replib 693 0.07 1,2-Propanediamine
16 mainlib 691 0.06 l-Alanine ethylamide, (S)-
17 replib 690 0.06 Alanine
18 replib 687 0.05 Benzenemethanol, 3-hydroxy-α-[(methylamino)met...
19 mainlib 686 0.06 Alanine
20 replib 685 0.05 1-Octanamine, N-methyl-
21 mainlib 685 0.05 Cathine
22 mainlib 683 0.07 1,2-Propanediamine
23 mainlib 681 0.04 dl-Alanine ethyl ester
24 mainlib 680 0.04 L-Alanine, ethyl ester
25 mainlib 680 0.04 Benzenemethanol, α-(1-aminoethyl)-
26 mainlib 680 0.04 2-Octanamine
27 mainlib 676 0.03 Amphetamine-3-methyl
28 replib 672 0.03 (R)-(-)-2-Amino-1-propanol
InLib = 224, Hit List
CAS# 124-38-9 (mainlib) Carbon dioxide
Name: Carbon dioxide
Formula: CO2
MW: 44 CAS#: 124-38-9 NIST#: 69 ID#: 13702 DB: mainlib
Other DBs: Fine, TSCA, RTECS, USP, HODOC, EINECS, IRDB
8 largest peaks:
44 999 | 28 98 | 16 96 | 12 87 | 22 19 |
45 12 | 46 4 | 29 1 |
Synonyms:
1.Carbon oxide (CO2)
2.Carbonic acid, gas
3.Carbonic anhydride
4.Dry ice
5.CO2
6.Anhydride carbonique
7.Carbonice
8.Kohlendioxyd
9.Kohlensaure
10.UN 1013
11.UN 1845
12.UN 2187
13.Cardice
14.Dricold
15.Drikold
16.Dioxomethane #
Retention index
1. Value: 152 iu
Column Type: Packed
Column Class: Semi-standard non-polar
Active Phase: Squalane
Column Length: 50 ft
Carrier Gas: He
Substrate: Chromosorb P
Lib. Search
Other Search
Names
Compare
Librarian
MSMS



NIST MS Search 2.0 - [Ident, Penalize, Presearch Default - InLib = -186, 100 spectra]
File Search View Tools Options Window Help
1. Scan 2253 (13.694 min): HEAD SPAC
1 (A) Scan 2253 (13.694 min): H...
2 (A) Scan 2252 (13.688 min): H...
3 (A) Scan 2255 (13.706 min): H...
4 (A) Scan 2254 (13.700 min): H...
5 (A) Scan 2253 (13.694 min): H...
Names Structures Spec List
mainlib; replib; nist_salts; 220460 total spectra
(Text File) Scan 2253 (13.694 min): HEAD SPACE OF THE APTAC FOR 03132026 TE
Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List
Name: Scan 2253 (13.694 min): HEAD SPACE OF THE APTAC FOR 03132026 TEST2.D\DATA.MS
MW: N/A ID#: 572 DB: Text File
10 largest peaks:
57 999 | 43 591 | 41 525 | 56 493 | 42 280 |
29 276 | 86 237 | 27 160 | 39 149 | 55 89 |
Synonyms:
no synonyms.
Scan 2253 (13.694 min): HEAD SPACE OF THE APTAC FOR 0313
Side by Side MF=807 RMF=924
Hexane
Difference Head to Tail Side by Side Subtraction
807 78.7P
Library Match Prob. Name
1 replib 807 78.7 Hexane
2 replib 779 78.7 Hexane
3 mainlib 774 78.7 Hexane
4 replib 718 6.80 Pentane, 3-methyl-
5 mainlib 706 6.80 Pentane, 3-methyl-
6 replib 703 6.80 Pentane, 3-methyl-
7 replib 687 1.85 Heptane, 2,2-dimethyl-
8 mainlib 681 1.85 Heptane, 2,2-dimethyl-
9 replib 676 1.27 Pentane, 2,3-dimethyl-
10 mainlib 674 1.17 Pentane, 2,4-dimethyl-
11 mainlib 670 1.27 Pentane, 2,3-dimethyl-
12 mainlib 663 0.80 Butyl isocyanatoacetate
13 replib 659 0.68 Hexane, 2,2-dimethyl-
14 replib 656 0.60 Pentane, 2,2,4-trimethyl-
15 replib 656 0.60 Butane, 2,2,3-trimethyl-
16 replib 655 1.17 Pentane, 2,4-dimethyl-
17 replib 653 0.68 Hexane, 2,2-dimethyl-
18 replib 652 1.27 Pentane, 2,3-dimethyl-
19 replib 650 0.47 Butane, 2-methyl-
20 replib 648 0.43 Pentane, 2,2-dimethyl-
21 mainlib 647 0.41 Hexane, 2,2,4-trimethyl-
22 replib 642 1.17 Pentane, 2,4-dimethyl-
23 replib 642 0.41 Hexane, 2,2,4-trimethyl-
24 replib 640 0.60 Pentane, 2,2,4-trimethyl-
25 replib 640 1.27 Pentane, 2,3-dimethyl-
26 mainlib 639 0.31 Hexane, 2,2,3-trimethyl-
27 replib 639 0.31 Hexane, 2,2,5-trimethyl-
28 mainlib 639 0.43 Pentane, 2,2-dimethyl-
InLib = -186, Hit List
CAS# 110-54-3 (replib) Hexane
Plot/Text of Hit Plot of Hit
Name: Hexane
Formula: C6H14
MW: 86 CAS#: 110-54-3 NIST#: 291337 ID#: 5275 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1998.
10 largest peaks:
57 999 | 41 666 | 43 549 | 56 548 | 42 280 |
29 211 | 86 205 | 39 191 | 27 175 | 55 91 |
Synonyms:
1.n-Hexane
2.Skellysolve B
3.n-C6H14
4.Esani
5.Heksan
6.Hexanen
7.Hexyl hydride
8.Gettysolve-B
9.NCI-C60571
10.UN 1208
11.Exxsol hexane
Estimated non-polar retention index (n-alkane scale):
Value: 618 iu
Confidence interval (Hydrocarbons): 39(50%) 167(95%) iu
Retention index
1. Value: 600 iu
Column Class: All column types
Data Type: Normal alkane RI value specified by scale definition
Source: von Kováts, E., 206. Gas-chromatographische Charakterisierung organischer Verbindungen. Teil 1
Lib. Search Other Search Names Compare Librarian MSMS

Figure: The MS Detailed Peak Analysis for the Gases in the Headspace of 'APTAC-CSB03192025 Test 2'




NIST MS Search 2.0 - [Ident, Penalize, Presearch Default - InLib = 429, 100 spectra]
File Search View Tools Options Window Help
1. Scan 383 (2.395 min): HEAD SPACE
1 (A) Scan 383 (2.395 min): HEA... 2 (A) Scan 382 (2.389 min): HEA... 3 (A) Scan 382 (2.389 min): HEA... 4 (A) Scan 379 (2.371 min): HEA... 5 (A) Scan 377 (2.359 min): HEA...
mainlib; replib; nist_salts; 220460 total spectra
Library Match Prob. Name
1 mainlib 924 56.4 Carbon dioxide
2 replib 915 56.4 Carbon dioxide
3 nist_salts 915 41.0 Carbamic acid, monoammonium salt
4 mainlib 785 1.70 Nitrous Oxide
5 replib 764 1.70 Nitrous Oxide
6 mainlib 737 0.35 (2-Aziridinylethyl)amine
7 mainlib 725 0.23 Dextroamphetamine
8 replib 691 0.06 3-Methoxyamphetamine
9 replib 673 0.03 Epinephrine
10 mainlib 673 0.03 dl-Alanine
11 replib 654 0.01 1-Methyl-2-phenoxyethylamine
12 mainlib 653 0.01 4-Iodo-3-methoxyamphetamine
13 mainlib 653 0.01 Acetamide, 2,2-dichloro-
14 mainlib 652 0.01 d-Alanine
15 mainlib 643 0.01 l-Alanine ethylamide, (S)-
16 mainlib 642 0.00 L-Alanine, ethyl ester
17 replib 640 0.00 Alanine
18 mainlib 635 0.00 Ethyne, fluoro-
19 mainlib 635 0.00 N-Methyltaurine
20 replib 633 0.00 1,2-Propanediamine
21 mainlib 629 0.00 1,2-Propanediamine
22 mainlib 629 0.00 dl-Alanine ethyl ester
23 replib 629 0.00 Hydroxyurea
24 mainlib 625 0.00 Alanine
25 replib 623 0.00 1-Octanamine, N-methyl-
26 mainlib 622 0.00 Ethylamine, 2-(adamantan-1-yl)-1-methyl-
27 mainlib 621 0.00 Benzeneethanamine, 3-fluoro-β,5-dihydroxy-N-met...
28 mainlib 617 0.00 n-Hexylmethylamine
InLib = 429, Hit List
Name: Scan 383 (2.395 min): HEAD SPACE OF THE APTAC FOR 03192026 TEST 3RD.D\data.ms
MW: N/A ID#: 537 DB: Text File
8 largest peaks:
44 999 | 28 68 | 45 15 | 46 5 | 22 3 |
29 1 | 32 1 | 43 1 |
Synonyms:
no synonyms.
(Text File) Scan 383 (2.395 min): HEAD SPACE OF THE APTAC FOR 03192026 TEST
Scan 383 (2.395 min): HEAD SPACE OF THE APTAC FOR 031920
Side by Side MF=924 RMF=924
Carbon dioxide
CAS# 124-38-9 (mainlib) Carbon dioxide
Name: Carbon dioxide
Formula: CO2
MW: 44 CAS#: 124-38-9 NIST#: 69 ID#: 13702 DB: mainlib
Other DBs: Fine, TSCA, RTECS, USP, HODOC, EINECS, IRDB
8 largest peaks:
44 999 | 28 98 | 16 96 | 12 87 | 22 19 |
45 12 | 46 4 | 29 1 |
Synonyms:
1.Carbon oxide (CO2)
2.Carbonic acid, gas
3.Carbonic anhydride
4.Dry ice
5.CO2
6.Anhydride carbonique
7.Carbonice
8.Kohlendioxyd
9.Kohlensaure
10.UN 1013
11.UN 1845
12.UN 2187
13.Cardice
14.Dricold
15.Drikold
16.Dioxomethane #
Retention index
1. Value: 152 iu
Column Type: Packed
Column Class: Semi-standard non-polar
Active Phase: Squalane
Column Length: 50 ft
Carrier Gas: He
Substrate: Chromosorb P

Gas Chromatography-Mass Spectrometry Report

For The Head Space of ARC - 07102025 Pure Invert Sugar Test

Report to:
U.S. Chemical Safety and Hazard Investigation Board
470 L'Enfant Plaza SW
Suite 604 #23278
Washington, DC 20026

Date: September 15, 2025

Report No.: ioK#: 25204-01 Rev. 1

AT-1922

95 Stiles Road | Salem, New Hampshire 03079
www.ioKinetic.com | P: 603.893.7009 | F: 603.386.6522

Revisions

Rev.	Date	List of Changes	Prepared by	Approved by
0	8/5/2025	Initial Release	E. Shaaban, PhD	A. Iskandar, PhD
1	09/15/2025	Final Report	E. Shaaban, PhD	A. Iskandar, PhD

Table of Contents

List of Tables

List of Figures

Appendices

1 Study Overview

This report presents the results of gas analysis for the headspace after the following accelerated rate calorimetry (ARC®) test:

1. ARC - 07102025 Pure Invert Sugar

After the ARC® had cooled down, gaseous samples were collected in Tedlar bags and injected into the GC-MS using a gas-tight syringe.

The analysis was performed using a GC-MS system (Agilent 6890N coupled with 5973 MS) equipped with a PLOT column (Agilent J&W PoraBOND Q for volatile solvents and hydrocarbons, 25 m × 0.25 mm × 3 µm, –100 °C to 300/320 °C). Helium was used as the carrier gas.

The oven temperature program started at 40 °C (held for 10 minutes), increased at 10 or 20 °C/min to 250 °C, and was then held at the final temperature for 5 minutes.

The injector was operated in splitless mode at 200 °C.

Nitrogen and carbon monoxide co-eluted and were detected in the same peak in the GC-MS. Both N_2 and CO produce signals at m/z = 28, making them indistinguishable in the same peak.

A detailed test description is provided in Appendix A. For further information regarding the ARC® test, see the ARC® test reports.

2 Test Results

The GC-MS results for the headspace of ‘ARC - 07102025 Pure Invert Sugar' are summarized in Table 1 and Figure 1.

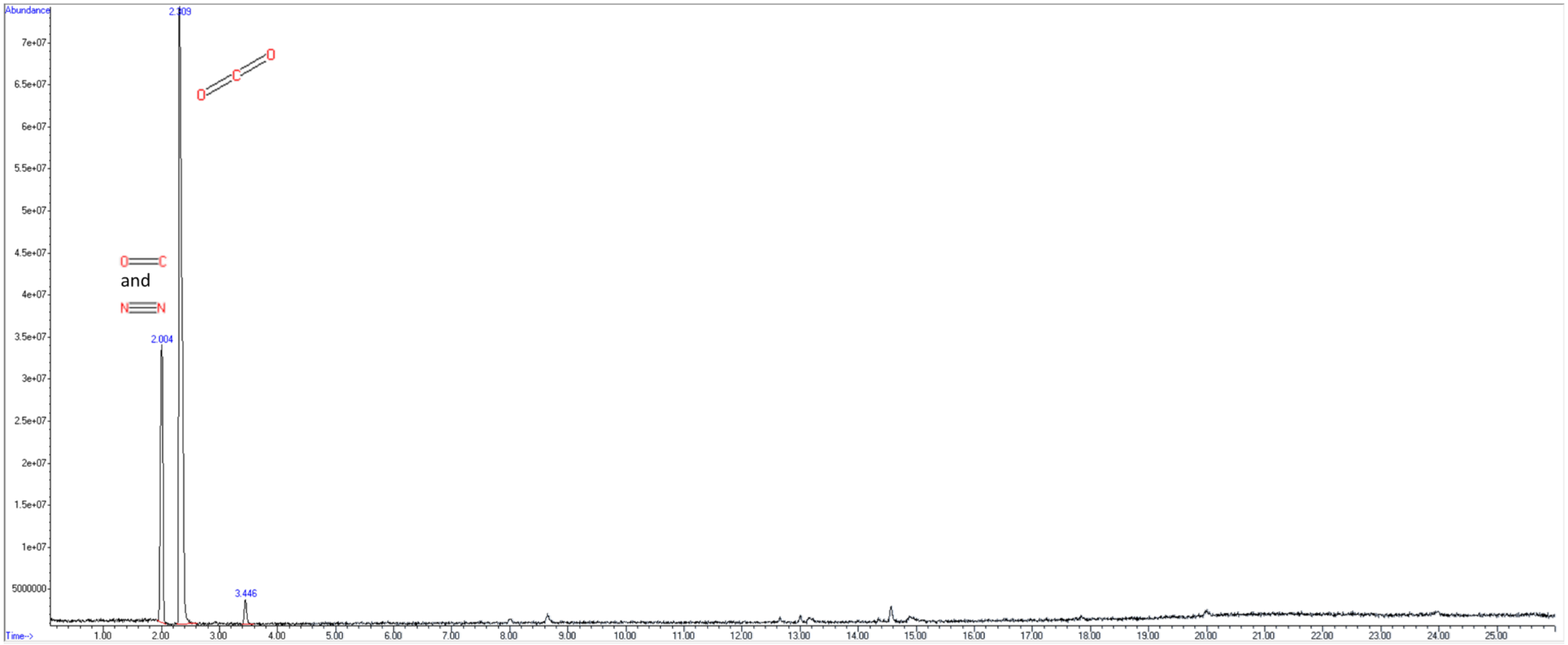
For the detailed MS signal of each peak, please see Appendix B.

Table 1: GC-MS Test Results for the Headspace of 'ARC - 07102025 Pure Invert Sugar'

Peak #	Retention time (min)	Area % of total	Compound
1	2.00	26.66%	Nitrogen and carbon monoxide*
2	2.216	70.98%	Carbon dioxide
3	13.70	2.36%	Ethane

** Nitrogen and carbon monoxide co-eluted and were detected in the same peak in the GC-MS due to their similar physical properties. Nitrogen and carbon monoxide produce signals at m/z = 28, making them indistinguishable under standard GC-MS conditions.*

Figure 1: GC-MS Main Peaks Versus Retention Time for the Headspace of ' ARC - 07102025 Pure Invert Sugar '



Source: Agilent MS5973N GC 6890 with Autosampler

Appendix A: Test Description

GC-MS

Gas Chromatography Mass Spectrometry (GC-MS) is a technique that combines the separation capacity of gas chromatography with the sensitivity and selective capacity of the mass detector. This combination allows analyzing and quantifying trace compounds in complex mixtures with a high degree of effectiveness. This technique is indicated for the separation of volatile and semi-volatile organic compounds. GC-MS can be used to study liquid, gaseous or solid samples. The use of GC-MS is restricted to the separation of compounds of formula weight lower than 1000 or molecular weight lower than 1000 kg/kgmol and a maximum working temperature of about 400ºC.

To conduct a test, The sample is first introduced into the Gas Chromatograph (GC) manually with a syringe or by an autosampler and it enters the carrier gas (typically hydrogen, helium or nitrogen) via the GC inlet. If the sample is in the liquid form, it is vaporized and transferred to the analytical column The sample components, the “analytes”, are separated by their differences in splitting between the mobile phase and the liquid stationary phase (held within the column), or for more volatile gases their adsorption by a solid stationary phase. The analytes are then propelled by an inert carrier gas. As components of the mixture are separated, each compound elutes from the column at a different time based on its boiling point and polarity. Once the components leave the GC column, they are ionized and fragmented by the mass spectrometer using electron ionization. These ionized molecules are separated based on their different mass-to-charge (m/z) ratios by the mass analyzer. The separated ions then reach the ion detector where the signal is recorded to produce a chromatogram and a mass spectrum for each data point. A complex sample produces multiple peaks in the gas chromatogram. Each peak generates a unique mass spectrum, which is used for compound identification through libraries of mass spectra.

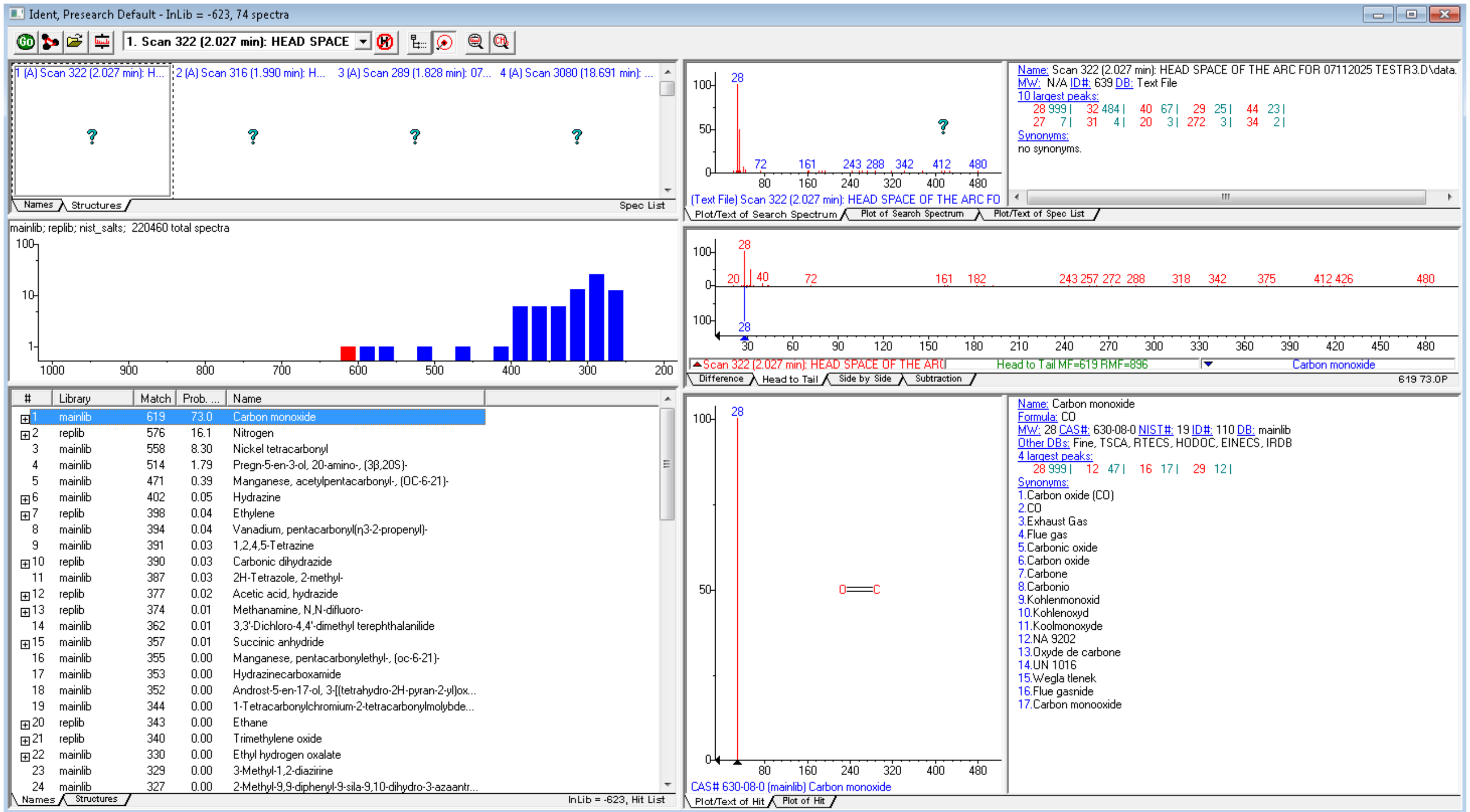
Some details on the Agilent MS5973N GC 6890 with Autosampler include:

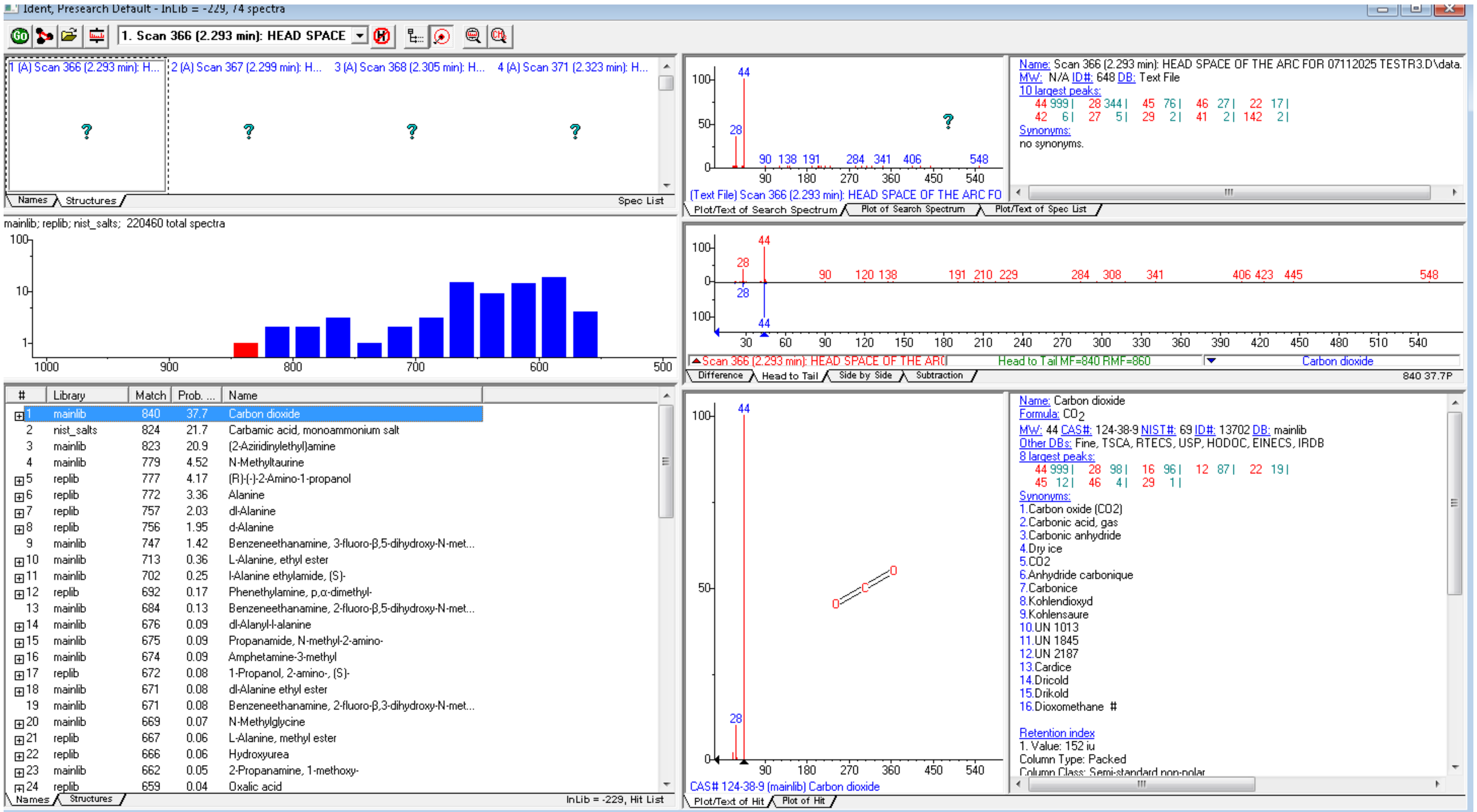
- Scan rates up to 5,200 amu/sec with 0.1 amu scan step size, with eight sampling rates.
- Total ADC (analog/digital converter) dynamic range is 10^6.
- Mass axis stability is +0.15 amu over 12 hours
- Up to 50 group of masses with 30 masses per group
- Any value between 10-9,999 msecs per mass, selectable by the user
- Filament Voltage is user-selectable over the range 5-240 eV. Dual Filament for EI; single filament for CI.

- Filament emission current is user-selectable over the range 0-315 uA in all modes of operation.
- Temperature of the independently heated ion source can be controlled up to 250°C for EI and up to 300°C for CI.
- Temperature of the independently heated quadrupole can be controlled up to 200°C
- Temperature of the interface can be controlled up to 350°C

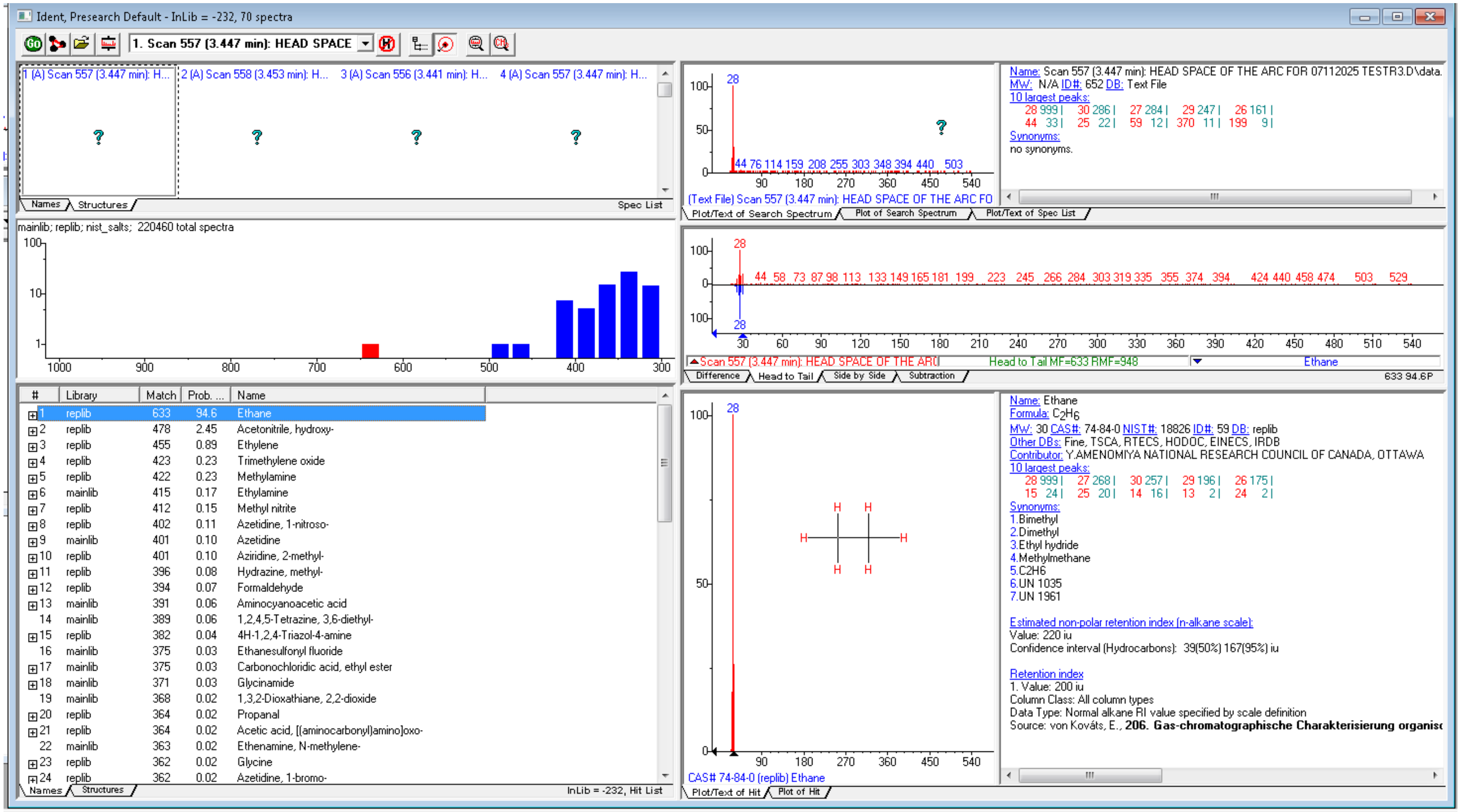
Appendix B: Detailed Peak Analysis of GC-MS Data.

The MS detailed peak analysis for the gases in the headspace of ARC - 07102025 Pure Invert Sugar test





Proprietary Information Use or disclosure of data contained on this sheet is subject to the restriction on the title page of this document.



Proprietary Information Use or disclosure of data contained on this sheet is subject to the restriction on the title page of this document.

SOLIDS ANALYSIS REPORTS

The following reports analyze the composition of black residue recovered by the CSB from the Reactor 6 (Cooker 6) vessel, as well as the composition of the black residue generated in the test cell during the APTAC test. The test results indicate that the black residue recovered from Reactor 6 (Cooker 6) was the byproduct of the decomposition reaction of the Product 484 ingredients.

Gas Chromatography Mass Spectrometry Report

For Washout Liquids from 10.1 Sample Remnants Inside Cooker 6, and Solids from APTAC-CSB-03192025 Test 2.

Report to:
U.S. Chemical Safety and Hazard Investigation Board
470 L'Enfant Plaza SW
Suite 604 #23278
Washington, DC 20026

Date: September 15, 2025

Notice:

This report was prepared by ioKinetic for the account of CSB. This report represents ioKinetic's best judgment in light of information made available to us. Opinions in this report are based in part upon data and information (Sample Identification) provided by CSB and / or CSB's advisors and affiliates. This report relates only to the sample as received unless otherwise noted. The reader is advised that ioKinetic has not independently verified the data or the information contained therein. This report must be read in its entirety. The reader understands that no assurances can be made that all liabilities have been identified. This report does not constitute a legal opinion. The results provided are apparatus dependent and should not be used for direct scale-up. They apply to the samples as tested and are useful as a comparison tool only.

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Report No.: ioK#: 25204-01 Rev.2

AT-1922

Revisions

Rev.	Date	List of Changes	Prepared by	Approved by
0	8/5/2025	Initial Release	E. Shaaban, PhD	A. Iskandar, PhD
1	08/07/2025	Include full sample name as 10.1 Sample Remnants Inside Cooker 6	E. Shaaban, PhD	A. Iskandar, PhD
2	09/15/2025	Final Report	E. Shaaban, PhD	A. Iskandar, PhD

Table of Contents

List of Tables

Appendices

1 Study Overview

This report presents the results of gas analysis using Gas Chromatography-Mass Spectrometry (GC-MS) for the washout liquids from:

1. 10.1 Sample Remnants Inside Cooker 6,
2. Solids from APTAC-CSB-03192025 Test 2.

For sample preparation, methanol, dimethyl chloride, and acetonitrile were screened as extraction solvents. Methanol was the only solvent capable of fully dissolving the caramel color, so it was used for liquid phase extraction from all solid samples. Each solid sample was combined with methanol at a solvent-to-sample mass ratio of 5:1 to ensure efficient extraction. After thorough mixing, the resulting washout liquid was filtered to remove particulates. An aliquot of the filtered extract was injected into the GC-MS system for analysis.

The analysis was performed using a GC-MS system (Agilent 6890N coupled with 5973 MS) equipped with a low-polarity fused silica column (Agilent J&W HP-5ms Ultra Inert, 30 m × 0.25 mm × 0.25 μm). Helium was used as the carrier gas.

The oven temperature program began at 40 °C with a 10-minute hold, then ramped at 10 °C per minute to a final temperature of 300 °C, with no additional final hold time. The maximum oven temperature was set at 320 °C, and the total run time was 36 minutes, allowing for complete elution of analytes. The front inlet was operated in split mode at 280 °C with a split ratio of 300:1, running helium as the carrier gas at a constant flow rate of 1.2 mL/min. Injections were performed manually with a 10 μL syringe.

A detailed test description is provided in Appendix A.

2 Test Results and Discussions

The GC-MS results for the washout liquids produced from the 10.1 Sample Remnants Inside Cooker 6 showed no volatile organics, see Figure 1.

The GC-MS results for the washout liquid produced from APTAC-CSB-03192025 Test 2 solids are summarized in Table 1 and Figure 2.

For the detailed MS signal of each peak, please see Appendix B:.

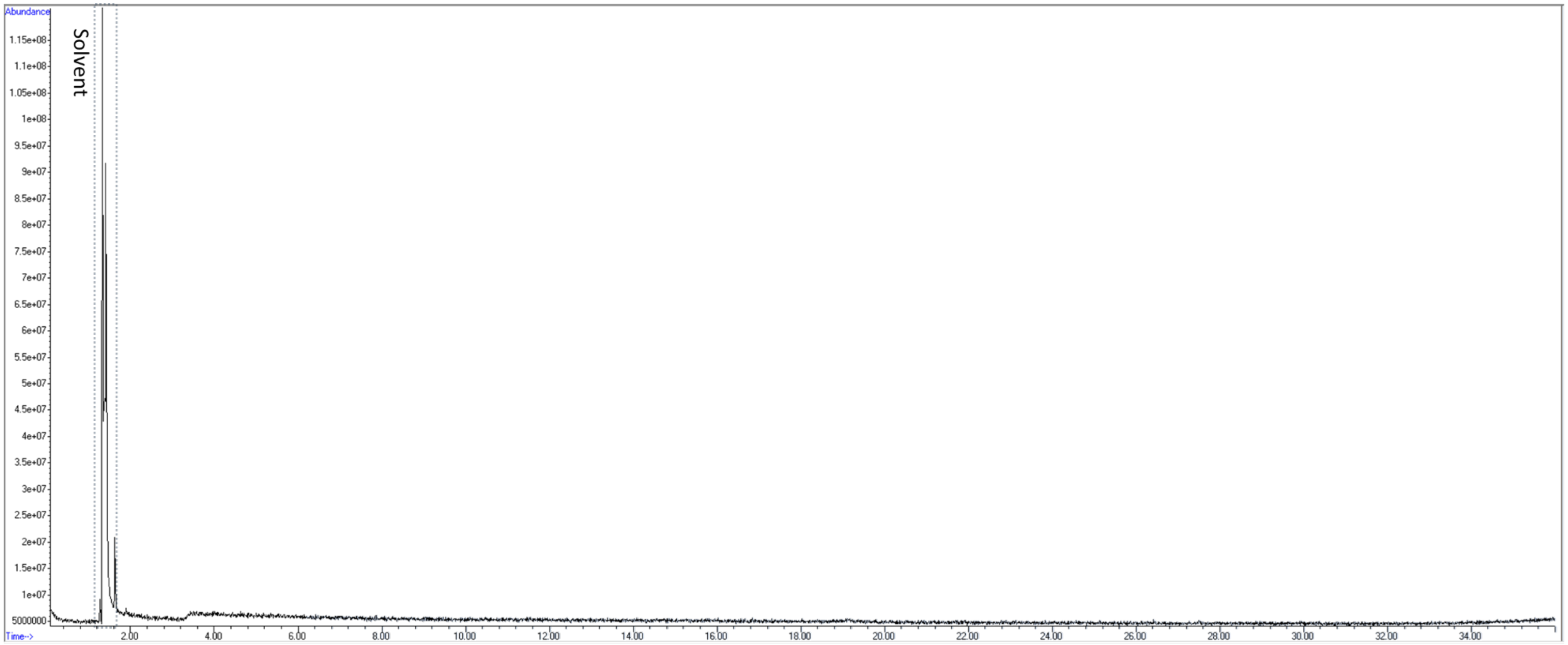
Table 1: GC-MS Test Results of Washout Liquids Produced from APTAC-CSB-03192025 Test 2 Solids.

Peak #	Retention time (min)	% of total	Compound	Match
1	2.121	76.204%	Acetic acid Ammonium acetate Propanedioic acid Acetic acid, anhydride with formic acid Hydrazine, ethyl-	884 830 703 674 673
2	14.507	5.452%	2-Hydroxy-gamma-butyrolactone Trimethylene oxide Propylene Carbonate 1,3-Propanediol Butanedial	676 651 614 609 596
3	2.046	13.906%	2-Pyrrolidinone, 1-ethenyl- Pyrazol-4-amine, 1,5-dimethyl- 2(1H)-Pyrimidinone, 4-amino- N-Methylmaleimide 4-Amino-6-hydroxypyrimidine	892 693 645 639 635
4	2.519	4.438%	[S]-[+]-2',3'-Dideoxyribonolactone 5-Hydroxymethyldihydrofuran-2-one [1-Methoxy-pentyl)-cyclopropane 5-0xotetrahydrofuran-2-carboxylic acid, ethyl ester 5-0xotetrahydrofuran-2-carboxylic acid	738 732 730 693 686

The following observation was made:

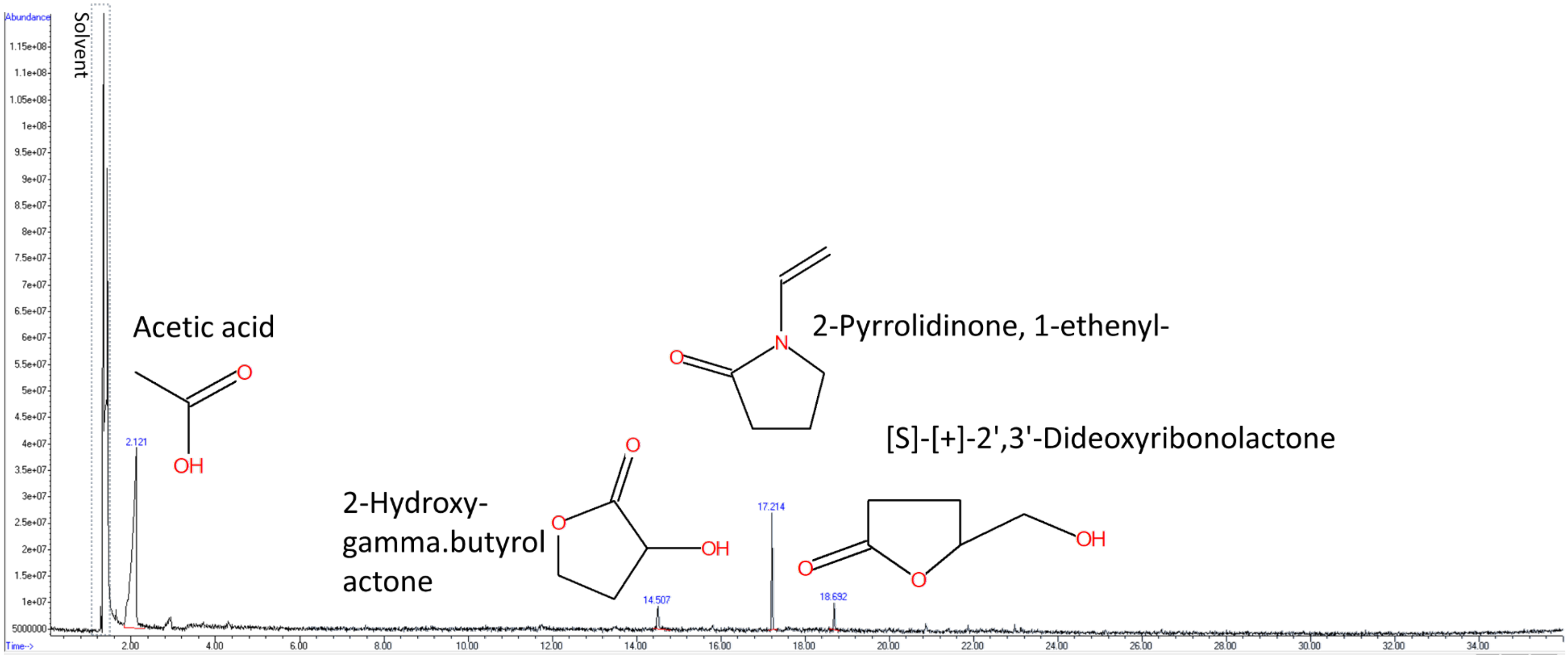
1. Despite the caramel color observed after filtering the methanol solutions of the two samples (see Appendix C), the washout liquid from APTAC-CSB-03192025 Test 2 Solids showed only a limited amount of volatile organics. No volatile organics were detected in the washout from the 10.1 Sample Remnants Inside Cooker 6. These results suggest that both the Remnants Inside Cooker 6 and the APTAC-CSB-03192025 Test 2 Solids primarily contain higher molecular weight compounds, including the brown-colored polymers responsible for the caramel hue—caramelan, caramelen, and caramelin.

Figure 1: GC-MS Peaks Versus Retention Time of the Washout Liquids Produced from 10.1 Sample Remnants Inside Cooker 6.



Source: Agilent MS5973N GC 6890 with Autosampler

Figure 2: GC-MS Peaks Versus Retention Time of the Washout Liquids Produced from APTAC-CSB-03192025 Test 2 Solids



Source: Agilent MS5973N GC 6890 with Autosampler

Appendix A: Test Description

GC-MS

Gas Chromatography Mass Spectrometry (GC-MS) is a technique that combines the separation capacity of gas chromatography with the sensitivity and selective capacity of the mass detector. This combination allows analyzing and quantifying trace compounds in complex mixtures with a high degree of effectiveness. This technique is indicated for the separation of volatile and semi-volatile organic compounds. GC-MS can be used to study liquid, gaseous or solid samples. The use of GC-MS is restricted to the separation of compounds of formula weight lower than 1000 or molecular weight lower than 1000 kg/kgmol and a maximum working temperature of about 400ºC.

To conduct a test, The sample is first introduced into the Gas Chromatograph (GC) by an autosampler and it enters the carrier gas (typically hydrogen, helium or nitrogen) via the GC inlet. If the sample is in the liquid form, it is vaporized and transferred to the analytical column The sample components, the “analytes”, are separated by their differences in splitting between the mobile phase and the liquid stationary phase (held within the column), or for more volatile gases their adsorption by a solid stationary phase. The analytes are then propelled by an inert carrier gas. As components of the mixture are separated, each compound elutes from the column at a different time based on its boiling point and polarity. Once the components leave the GC column, they are ionized and fragmented by the mass spectrometer using electron ionization. These ionized molecules are separated based on their different mass-to-charge (m/z) ratios by the mass analyzer. The separated ions then reach the ion detector where the signal is recorded to produce a chromatogram and a mass spectrum for each data point. A complex sample produces multiple peaks in the gas chromatogram. Each peak generates a unique mass spectrum, which is used for compound identification through libraries of mass spectra.

Some details on the Agilent MS5973N GC 6890 with Autosampler include:

- Scan rates up to 5,200 amu/sec with 0.1 amu scan step size, with eight sampling rates.
- Total ADC (analog/digital converter) dynamic range is 10^6.
- Mass axis stability is +0.15 amu over 12 hours
- Up to 50 group of masses with 30 masses per group
- Any value between 10-9,999 msecs per mass, selectable by the user
- Filament Voltage is user-selectable over the range 5-240 eV. Dual Filament for EI; single filament for CI.

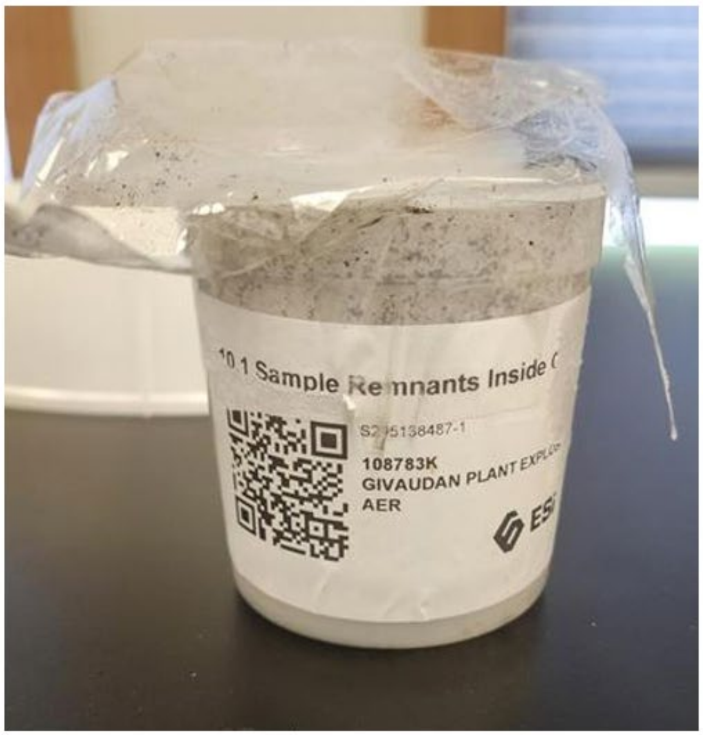
- Filament emission current is user-selectable over the range 0-315 uA in all modes of operation.
- Temperature of the independently heated ion source can be controlled up to 250°C for EI and up to 300°C for CI.
- Temperature of the independently heated quadrupole can be controlled up to 200°C
- Temperature of the interface can be controlled up to 350°C

Appendix B: Test Data Reports

Figure 3: Detailed MS Signal of Each Peak for APTAC-CSB-03192025 Test 2 Solids Test.

Source: Agilent MS5973N GC 6890 with Autosampler

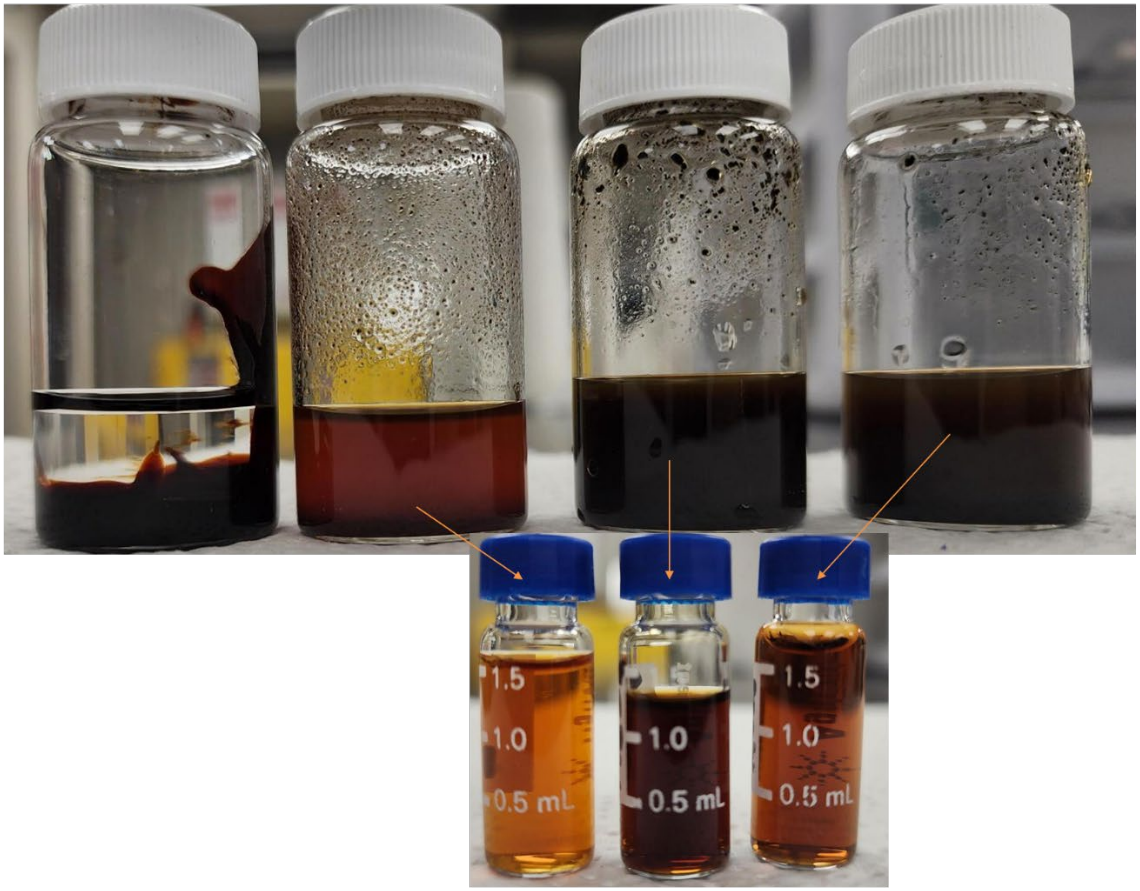
Appendix C: Sample Photos



10.1 Sample Remnants Inside Cooker 6

Solids from APTAC-CSB-03192025 Test 2

Caramel Color DMC and ACN | Caramel Color Methanol | Remnants inside cooker 6 + Methanol | Remnants from APTAC + Methanol



Thermogravimetric Analysis-Fourier Transform Infrared Report

10.1 Sample Remnants Inside Cooker 6, and Solids from APTAC-CSB-03192025 Test 2

Report to:
U.S. Chemical Safety and Hazard Investigation Board
470 L'Enfant Plaza SW
Suite 604 #23278
Washington, DC 20026

Date: September 15, 2025

This report was prepared by ioKinetic for the account of CSB. This report represents ioKinetic's best judgment in light of information made available to us. Opinions in this report are based in part upon data and information (Sample Identification) provided by CSB and / or CSB's advisors and affiliates. This report relates only to the sample as received unless otherwise noted. The reader is advised that ioKinetic has not independently verified the data or the information contained therein. This report must be read in its entirety. The reader understands that no assurances can be made that all liabilities have been identified. This report does not constitute a legal opinion. The results provided are apparatus dependent and should not be used for direct scale-up. They apply to the samples as tested and are useful as a comparison tool only.

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Report No.: ioK#: 25204-01 Rev.2

AT-1922

95 Stiles Road | Salem, New Hampshire 03079
www.ioKinetic.com | P: 603.893.7009 | F: 603.386.6522

Revisions

Rev.	Date	List of Changes	Prepared by	Approved by
0	08/04/2025	First Release	E. Shaaban, PhD	A. Iskandar, PhD
1	08/07/2025	Include full sample name as 10.1 Sample Remnants Inside Cooker 6	E. Shaaban, PhD	A. Iskandar, PhD
2	09/15/2025	Final Report	E. Shaaban, PhD	A. Iskandar, PhD

Table of Contents

List of Tables

Appendices

1 Study Overview

This report presents the results of a Thermogravimetric Analyzer-Fourier Transform Infrared (TGA-FTIR) Report on the following samples:

1. 10.1 Sample Remnants Inside Cooker 6
2. Solids from APTAC-CSB-03192025 Test 2

Each of the samples was heated from 30 to 1000°C at 10 °C per minute under nitrogen. A heated transfer line (150°C) was used to connect the TGA evolved gases to the two-meter heated gas cell of the FTIR instrument. FTIR data were collected with a DTGS detector every two minutes in the range of 4000–1000 cm^{-1} (a CaF_2 window was used) with a 32 cm^{-1} scanning rate and a resolution of 4 cm^{-1}.

The TGA tests were conducted according to ASTM E2550, Standard Test Method for Thermal Stability by Thermogravimetry. A detailed test description is provided in Appendix A. The testing is ISO/IEC 17025-accredited by ANAB.

Test setup details for each TGA run are summarized in the table below.

Table 1: TGA Sample Information

TGA Test #	Test Name	Sample mass (mg)	Gas Flowed	Heating Rate (°C/min)	Crucible Material
1	TGA 07092025CSB 10.1 Sample Remnants Inside Cooker 6	28.2	Nitrogen	10	Alumina
2	TGA 07162025CSB APTAC Solids 03192025 Test	15	Nitrogen	10	Alumina

2 Test Results and Discussions

The results of the sample TGA analysis are summarized in Table 2. Graphical results are presented in Appendix B.

Table 2: Summary of TGA-FTIR Test Results

Sample	Temperature range for mass loss (°C)	Mass Change (%)	Outgassed Species
10.1 Sample Remnants Inside Cooker 6	30 - 174	-26.81	H_2O
	174 - 400	-19.10	CO, CO_2, H_2O
	400 -742		CO, CO_2, $C_xH_yO_z$, H_2O
	742-1000	-13.20	CO, ↑↑CO_2^*, H_2O
Solids from APTAC-CSB-03192025 Test 2	30 - 174	-24.76	H_2O
	174 - 300	-27.89	H_2O
	300- 400		CO_2, H_2O
	400 -742		CO, CO_2, $C_xH_yO_z$, H_2O
	742-1000	-17.02	CO, ↑↑CO_2^*, H_2O

* Saturation of IR detector Signal was observed for CO_2 gas.

The following observations were made:

1. Based on the observed mass loss profile in the TGA curves and the evolved gases detected via FTIR, the TGA curves were generally divided into three distinct regions:
    a. Dehydration 30 - 174°C: Initial mass loss attributed to the removal of water.
    b. Decomposition 174-742 °C: mass reduction associated with thermal decomposition due to the release of gaseous products such as CO, CO_2, H_2O, and volatile organic compounds ($C_xH_yO_z$).
    c. Full carbonization (>700°C): Final stage involving further mass loss corresponding to the complete carbonization of the material, with CO and CO_2 released.
2. The 10.1 Sample Remnants Inside Cooker 6 and Solids from APTAC-CSB-03192025 Test 2 have similar TGA curves and evolved Gas. In the case of 10.1 Sample Remnants Inside Cooker 6, the mass loss due to decomposition started at slightly earlier temperatures (around 200°C) when compared to Solids from APTAC-CSB-03192025 Test 2.
3. The FTIR data were also analyzed by tracking the intensity of the four evolved gases—H_2O, CO, CO_2, and $C_xH_yO_z$ —as a function of temperature, from the TGA thermal profile, see Appendix B.

Appendix A: Test Description

TGA-FTIR, a system that combines a Thermogravimetric Analyzer (TGA) with Fourier-Transform-Infrared (FT-IR) spectroscopy, is the most commonly used type of Evolved Gas Analysis (EGA) system.

TGA measures the amount and rate of change in the mass of a sample as a function of temperature and time in a controlled atmosphere. Changes in mass (loss or gain) are often associated with loss of volatiles, decomposition, and oxidation.

FTIR is a vital tool in gas analysis, offering precise identification of gases based on their unique infrared spectra. It enables real-time monitoring and detection of even trace amounts of gases, making it suitable for dynamic studies. FTIR is non-destructive and versatile, applicable across various industries such as environmental monitoring, chemical processing, and combustion analysis. Its sensitivity and accuracy make it indispensable for detailed gas composition analysis.

In a TGA-FTIR test setup, a small sample is placed in the TGA furnace and heated under a controlled atmosphere, usually nitrogen or air. As the temperature increases, the instrument measures any change in the sample's weight due to decomposition, oxidation, or loss of volatiles. The gases released during heating are carried by the purge gas through a heated transfer line to the FTIR detector. The FTIR analyzes the gas composition in real-time by detecting the unique infrared absorption of different compounds, such as CO_2, H_2O, or other organics. This combined system helps identify the temperature at which gases evolve and what those gases are, which is useful for thermal stability studies, decomposition behavior, and safety evaluations.

The measurements from the TGA instrument (TG 209 F3 Tarsus Thermogravimetric Analyzer manufactured by Netzsch™ Group of Selb, Germany) provide quantitative information about chemical changes that involve weight loss.

The TGA instrument is used primarily to determine the thermal and / or oxidative stabilities of materials as well as their compositional properties. TGA measurements provide valuable information that can be used for selecting materials, identifying reactivity, quantifying composition and / or impurity levels, moisture, and volatile contents.

Table 3: TGA Results Summary

Results	Description	Unit
T_o	Onset temperature of mass change	°C
T_p	Peak temperature	°C
ΔM	Change in mass	%

Approximately 10 mg of the reaction mixture is introduced into an open cylindrical cell. The cell is placed into the instrument. Sample mass vs. time and temperature is recorded continuously. The most frequently operates in a scanning mode, ranging from 1-20 °C/min. Operator skill ensures proper calibration. The instrument is fully automated; once operating, it needs minimal to no operator intervention. Various atmospheres can be imposed during test.

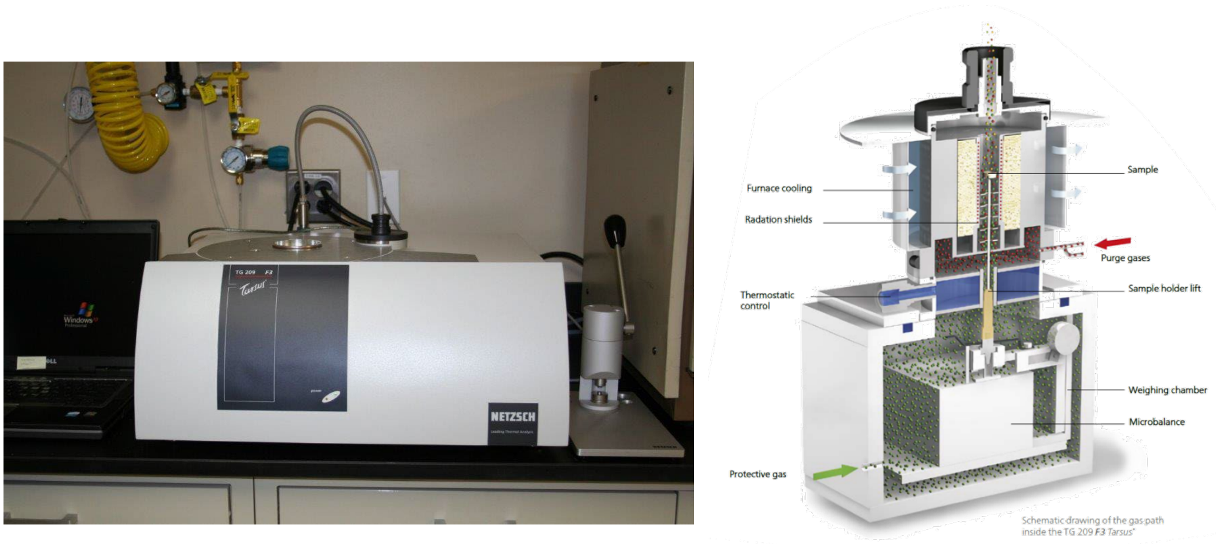
Some details on the TG 209 F3 Tarsus include:

- Operating test cell temperature range: room temperature to 900°C
- Temperature Accuracy: +/-0.1°C
- Operating test cell pressure: Atmospheric pressure
- Sample size: 5-10 mg standard
- Test cell material options include alumina, stainless steel.

Applicable Standard

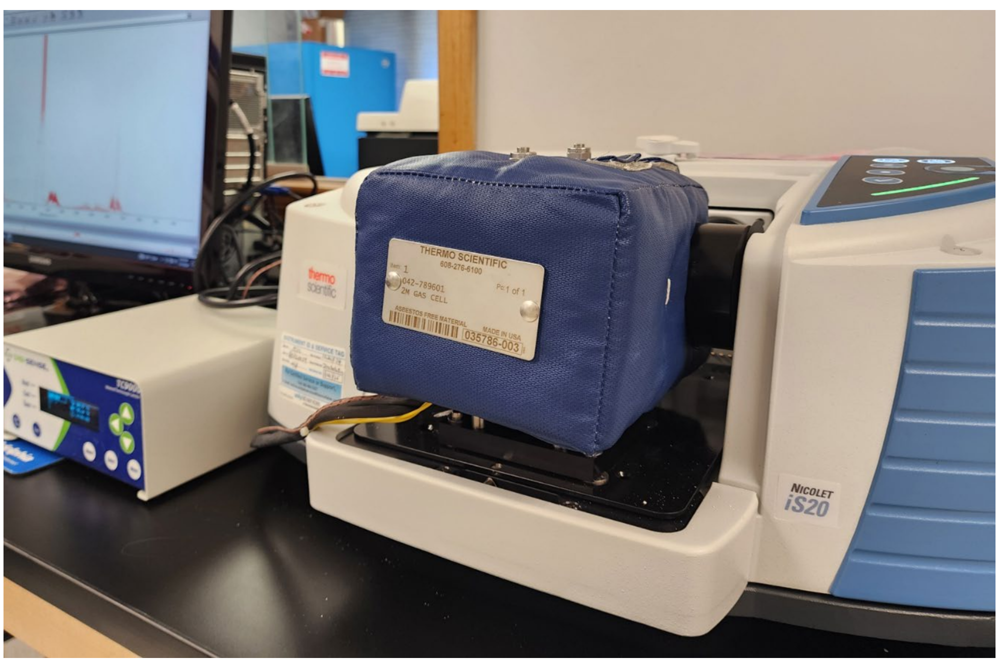
ASTM E2550, Standard Test Method for Thermal Stability by Thermogravimetry. This test method covers the assessment of material thermal stability through the determination of the temperature at which the material starts to decompose or reacts and the extent of mass change using thermogravimetry.

Figure 1: TG 209 F3 Tarsus Thermogravimetric Analyzer manufactured by Netzsch™ Group of Selb, Germany

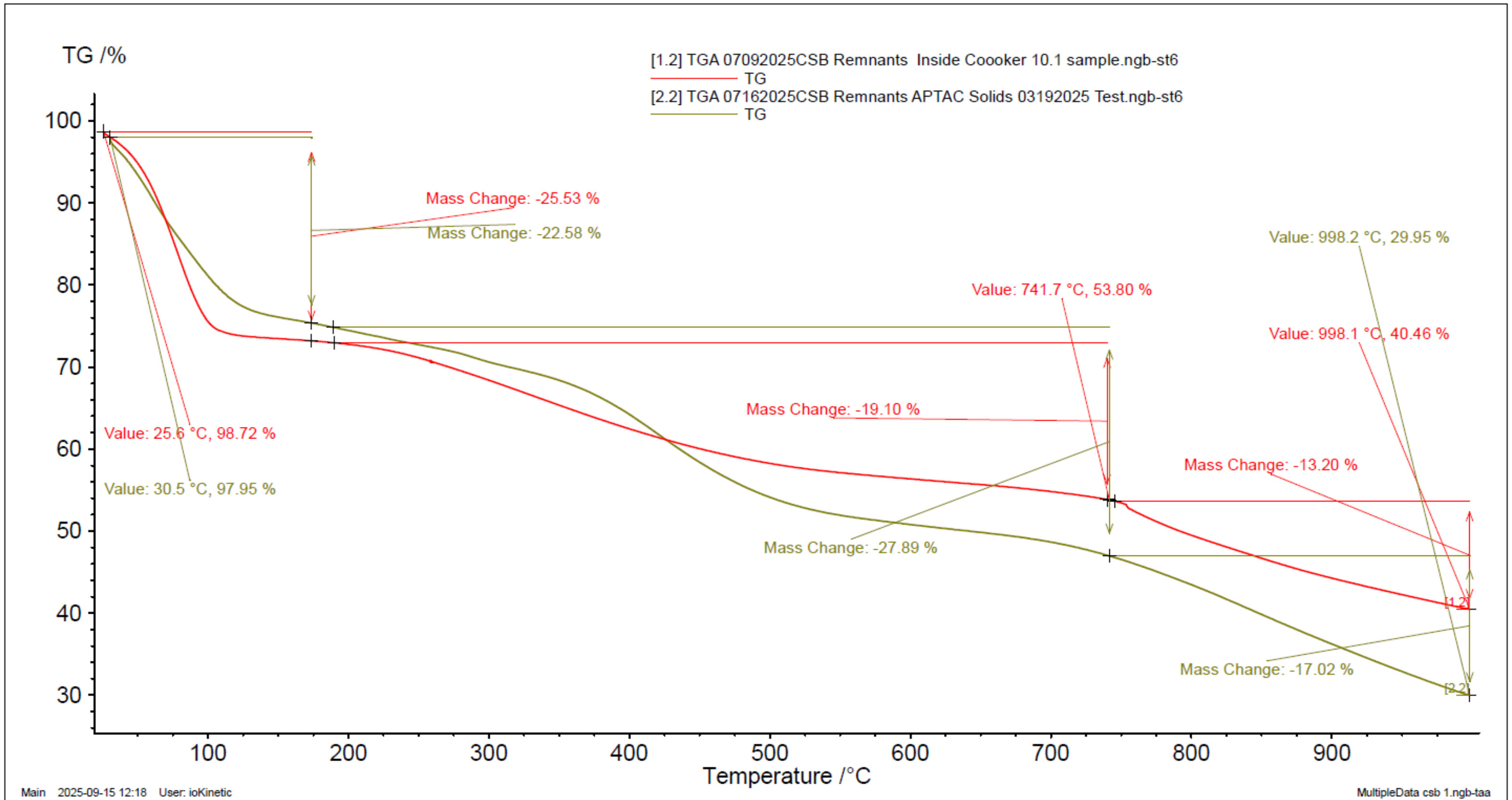


https://analyzing-testing.netzsch.com/

Figure 2: Thermo Scientific Nicolet iS20 FTIR with heated 2m gas cell accessory.

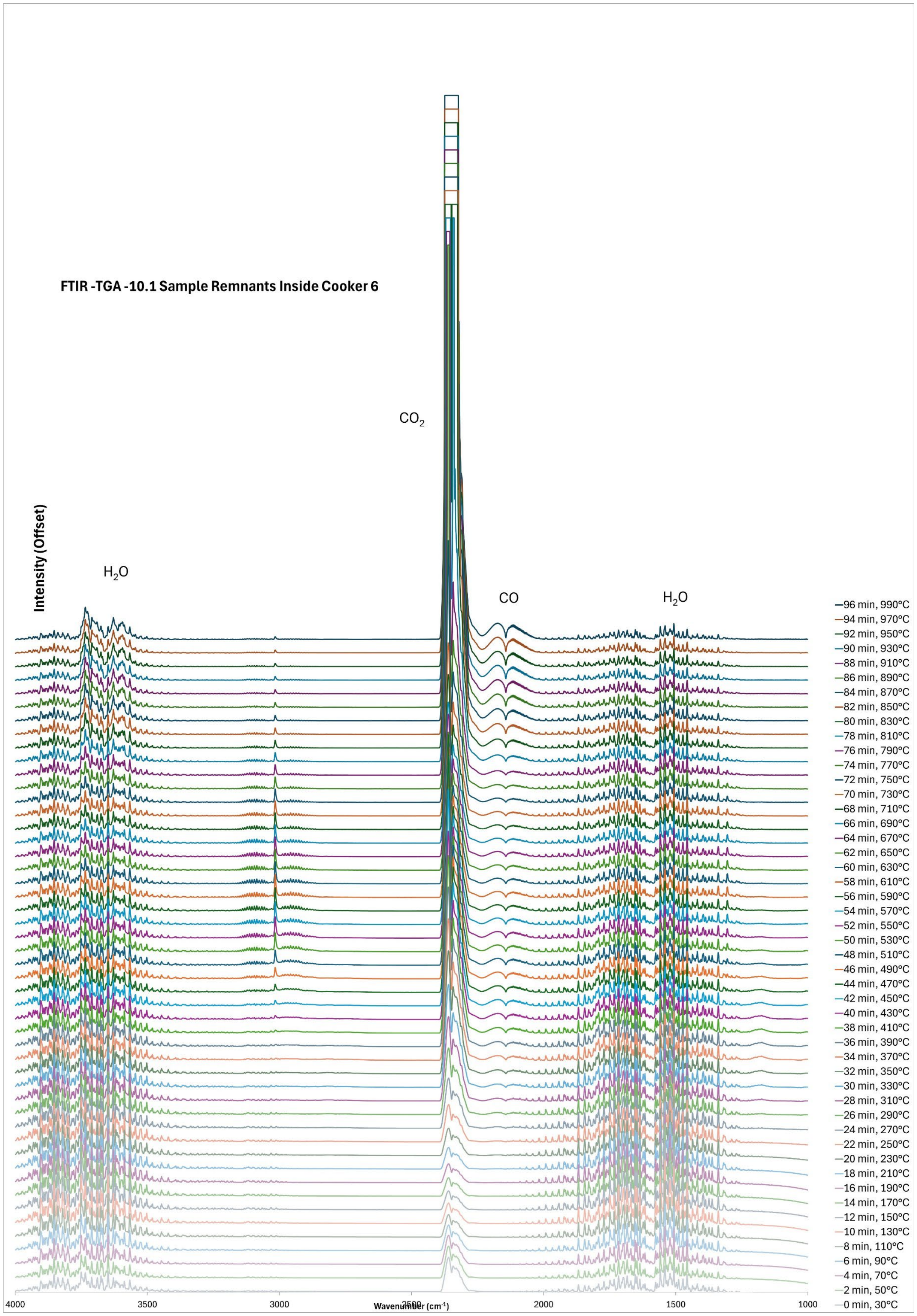


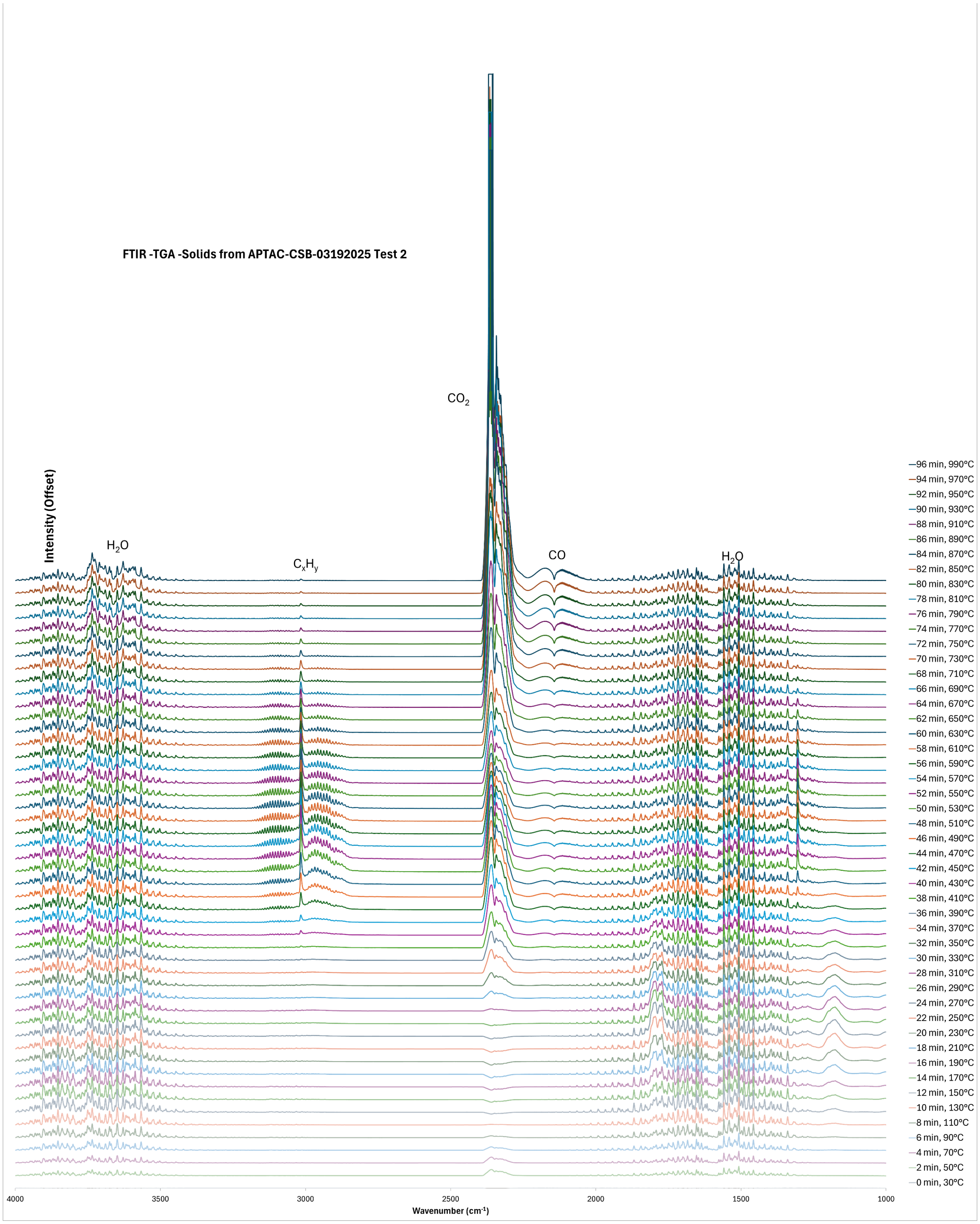
Appendix B: Test Data Reports

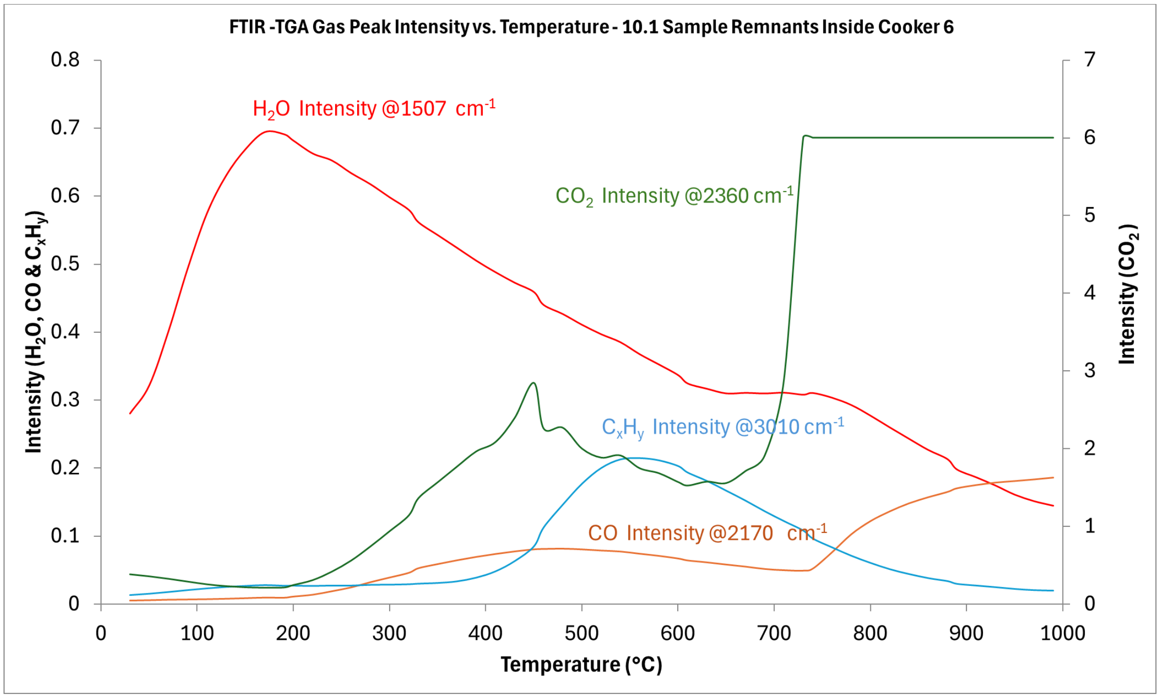


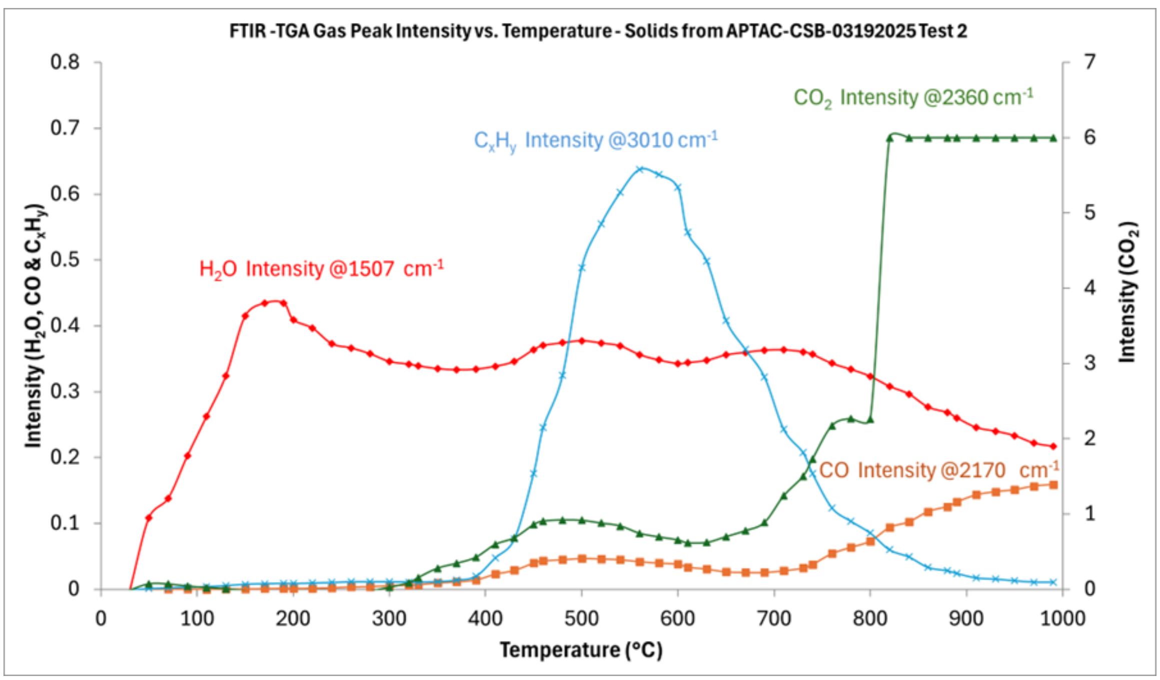
[#] Instrument	File	Date	Identity	Sample	Mass/mg	Segment	Range	Atmosphere	Corr.
[1.2] TG 209F3	TGA 07092025CSB Remnants Inside Coooker 10.1 sample.ngb-st6	2025-07-09	CSB	10.1 Sample Inside Coooker 6.	28.2	2/2	30°C/10.0(K/min)/1000°C	N2, 20.0ml/min	---
[2.2] TG 209F3	TGA 07162025CSB Remnants APTAC Solids 03192025 Test.ngb-st6	2025-07-16	CSB	APTAC solids 03192025test	15	2/2	30°C/10.0(K/min)/1000°C	N2, 20.0ml/min	---

Created with NETZSCH Proteus software

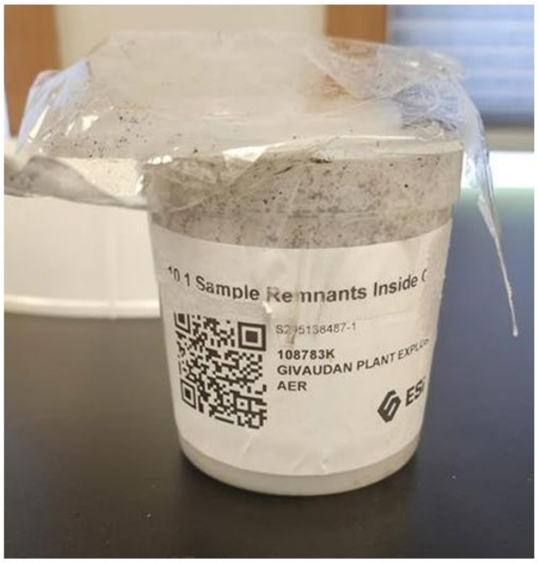

FTIR -TGA -10.1 Sample Remnants Inside Cooker 6
Intensity (Offset)
Wavenumber (cm-1)
CO_2
H_2O
CO
H_2O
4000
3500
3000
2500
2000
1500
1000
96 min, 990°C
94 min, 970°C
92 min, 950°C
90 min, 930°C
88 min, 910°C
86 min, 890°C
84 min, 870°C
82 min, 850°C
80 min, 830°C
78 min, 810°C
76 min, 790°C
74 min, 770°C
72 min, 750°C
70 min, 730°C
68 min, 710°C
66 min, 690°C
64 min, 670°C
62 min, 650°C
60 min, 630°C
58 min, 610°C
56 min, 590°C
54 min, 570°C
52 min, 550°C
50 min, 530°C
48 min, 510°C
46 min, 490°C
44 min, 470°C
42 min, 450°C
40 min, 430°C
38 min, 410°C
36 min, 390°C
34 min, 370°C
32 min, 350°C
30 min, 330°C
28 min, 310°C
26 min, 290°C
24 min, 270°C
22 min, 250°C
20 min, 230°C
18 min, 210°C
16 min, 190°C
14 min, 170°C
12 min, 150°C
10 min, 130°C
8 min, 110°C
6 min, 90°C
4 min, 70°C
2 min, 50°C
0 min, 30°C


FTIR -TGA -Solids from APTAC-CSB-03192025 Test 2
Intensity (Offset)
H2O
CxHy
CO2
CO
H2O
96 min, 990°C
94 min, 970°C
92 min, 950°C
90 min, 930°C
88 min, 910°C
86 min, 890°C
84 min, 870°C
82 min, 850°C
80 min, 830°C
78 min, 810°C
76 min, 790°C
74 min, 770°C
72 min, 750°C
70 min, 730°C
68 min, 710°C
66 min, 690°C
64 min, 670°C
62 min, 650°C
60 min, 630°C
58 min, 610°C
56 min, 590°C
54 min, 570°C
52 min, 550°C
50 min, 530°C
48 min, 510°C
46 min, 490°C
44 min, 470°C
42 min, 450°C
40 min, 430°C
38 min, 410°C
36 min, 390°C
34 min, 370°C
32 min, 350°C
30 min, 330°C
28 min, 310°C
26 min, 290°C
24 min, 270°C
22 min, 250°C
20 min, 230°C
18 min, 210°C
16 min, 190°C
14 min, 170°C
12 min, 150°C
10 min, 130°C
8 min, 110°C
6 min, 90°C
4 min, 70°C
2 min, 50°C
0 min, 30°C
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)


FTIR -TGA Gas Peak Intensity vs. Temperature - 10.1 Sample Remnants Inside Cooker 6
H2O Intensity @1507 cm-1
CO2 Intensity @2360 cm-1
CxHy Intensity @3010 cm-1
CO Intensity @2170 cm-1
Intensity (H2O, CO & CxHy)
Intensity (CO2)
Temperature (°C)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
1
2
3
4
5
6
7
0
100
200
300
400
500
600
700
800
900
1000


FTIR -TGA Gas Peak Intensity vs. Temperature - Solids from APTAC-CSB-03192025 Test 2
CO2 Intensity @2360 cm-1
CxHy Intensity @3010 cm-1
H2O Intensity @1507 cm-1
CO Intensity @2170 cm-1
Intensity (H2O, CO & CxHy)
Intensity (CO2)
Temperature (°C)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
1
2
3
4
5
6
7
0
100
200
300
400
500
600
700
800
900
1000

Appendix C: Sample Photos



10.1 Sample Remnants Inside Cooker 6

Solids from APTAC-CSB-03192025 Test 2

CHO Elemental Analysis Report

10.1 Sample Remnants Inside Cooker 6, and Solids from APTAC-03192025 Test 2

Report to:
U.S. Chemical Safety and Hazard Investigation Board
470 L'Enfant Plaza SW
Suite 604 #23278
Washington, DC 20026

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ANAB ACCREDITED ISO/IEC 17025 TESTING LABORATORY AT-1922

95 Stiles Road | Salem, New Hampshire 03079
www.ioKinetic.com | P: 603.893.7009 | F: 603.386.6522

Revisions

Rev.	Date	List of Changes	Prepared by	Approved by
0	08/05/2025	First Release	E. Shaaban, PhD	A. Iskandar, PhD
1	08/07/2025	Include full sample name as 10.1 Sample Remnants Inside Cooker 6	E. Shaaban, PhD	A. Iskandar, PhD
2	09/15/2025	Final Report	E. Shaaban, PhD	A. Iskandar, PhD

Table of Contents

List of Tables

Appendices

1 Study Overview

This report provides a detailed account of the elemental analysis for carbon (C), hydrogen (H), and oxygen (O) in solids from sugar decomposition experiments. The analysis covers two samples:

1. 10.1 Sample Remnants Inside Cooker 6
2. Solids from APTAC-03192025 Test 2

Each sample was dried under vacuum overnight at 100 °C to eliminate moisture, ensuring accurate quantification of hydrogen and oxygen within the organic matrix by preventing interference from adsorbed water.

Carbon & Hydrogen Determination: Performed using PerkinElmer 2400 Series II CHNS/O Analyzer. Samples were combusted at 920–980°C in an oxygen atmosphere. CO_2 and H_2O measured by thermal conductivity detection

Oxygen: Measured on the Thermo Finnigan FlashEA 1112 Elemental Analyzer. Sample material is pyrolyzed under an inert atmosphere and passed over a nickelized carbon catalyst, converting organic oxygen species to carbon monoxide. The carbon monoxide is then separated by chromatographic column, analyzed by thermal conductivity detector, and then calculated as oxygen content based on external calibration.

A detailed test description is provided in Appendix A.

2 Test Results and Discussions

The results of the sample CHO analysis are summarized in the table below.

Table 1: Summary of CHO Analysis Test Results

Sample	Carbon (C) %	Hydrogen (H) %	Oxygen (O) %
Solids from APTAC-03192025 Test 2	66.56%	5.34%	22.93%
10.1 Sample Remnants Inside Cooker 6	49.60%	4.40%	32.36%

The following observations were made:

1. During caramelization and thermal decomposition of sucrose, the material becomes increasingly carbon-rich as volatile species like H_2O and CO_2 (high in H and O) are released from the matrix. Theoretical CHO values reflect this shift:

   Theoretical CHO of Sucrose ($C_{12}H_{22}O_{11}$) = 42.11% C, 6.48% H, 51.41% O;

   Theoretical CHO of Caramelan ($C_{24}H_{36}O_{18}$) = 47.06% C, 5.93% H, 47.01% O

   ,demonstrating increased carbon and reduced oxygen with progressive caramelization.

2. So, the CHO profiles reflect the extent of decomposition between the three measured samples:
   a. 10.1 Sample Remnants Inside Cooker 6 (subjected to a max temperature of ~196.1 °C, the maximum recorded reactor temperature before rupture): Moderate carbon (49.60%), intermediate oxygen (32.36%) — indicating partial decomposition.
   b. APTAC Solids (Test 2) (subjected to a max temperature of ~275 °C): Lowest oxygen (22.93%), highest carbon (66.56%) — indicating more decomposition and carbonization.

Appendix A: Test Description

CHN Determination using PerkinElmer 2400 Series II CHNS/O Analyzer

This instrument burns a sample in pure oxygen at 920 – 980°C under static conditions to produce combustion products of CO_2, H_2O, and N_2. The PE-2400 automatically separates and analyzes these products in a self-integrating, steady-state thermal conductivity analyzer. An extended combustion time may be employed for difficult-to-combust samples.

Procedure

Samples, standards, and blanks are sealed in tin capsules. System suitability is verified using blanks and conditioners. The instrument is calibrated using acetanilide standards. Analytical runs include quality control (QC) standards every ten samples to ensure consistent accuracy. Final results are normalized to the mass of the sample used.

Accuracy and Precision (Based on Acetanilide, 1–3 mg)

Element	Mean Recovery (%)	Uncertainty (2s)
Carbon	100.05%	±0.49%
Hydrogen	100.22%	±3.37%
Nitrogen	100.11%	±0.99%

Determination of Oxygen Content

This method quantifies oxygen in powdered organic materials by converting organic oxygen species to carbon monoxide via pyrolysis over a nickelized carbon catalyst under inert atmosphere. The CO is separated chromatographically and detected by thermal conductivity, with oxygen content calculated based on external calibration.

Samples are sealed in silver capsules, leak-checked, and analyzed with bracketing QC standards every 10 runs. The instrument used is the Thermo Finnigan FlashEA 1112, with weekly six-point calibration using standards like acetanilide and benzoic acid.

Accuracy may be affected by high halogen, sulfur, phosphorus, or metal content. The method is unsuitable for primarily inorganic samples.

The quantitation limit is 0.5 wt%. Acetanilide recovery averages 100.22% ±5.10%. Results are reported as weight percent