

PTR Operating Conditions

Bay Area Air Quality District Odor Allocation Project

May 12-20, 2021 Test Program

The Proton Transfer Reaction Time of Flight Mass Spectrometer (Ionicon Model 6000/X3) was operated each day using the same set of operating conditions (Setting), denoted as "Odor" in this program. Screen shots presented here denote the initial day and final day of testing. As can be seen here, the PTR instrument operating parameters and conditions are very similar each day, which demonstrates overall consistency of day to day operations and determinations of ambient sample concentrations.

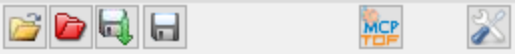
May 12, 2021 Initial Operating Parameters

The screenshot displays the initial operating parameters for the PTR instrument on May 12, 2021. The interface includes a top toolbar with icons for file operations and a main control area with various parameters and their values.

Parameter	Man/Ctrl	Ctrl		
Setting	Odor			
Primary Ion	H3O+			
Transmission	DC			
PC	353.3	353.34 mbar		
p Drift	2.30	2.29 mbar		
TofLens		4.81E-5 mbar		
TOF		5.85E-7 mbar		
E/N		120 Td		
Temps	80.10 °C	79.90 °C		
SrcValve	50.0			
H2O	6.0	6.00 sccm		
O2	0.0	0.00 sccm		
NO	0.0	0.00 sccm		
Ihc	4	4.0 mA		
	On/Off	On		
FCinlet	60.0	59.94 sccm		
U	FU	°C	↔	↔
Us	150			145.0 V
Uso	80			78.6 V
Udrift	525			526.1 V

Ion Production Settings

TPS ***Changed***



Lens 1	12.0	13.0 V	All on <input checked="" type="checkbox"/>	
Lens 2	30.0	30.0 V	Lenses <input checked="" type="checkbox"/>	
Lens 3	20.0	21.0 V		
Lens 4	76.0	76.0 V		
Lens 5	70.0	70.0 V		
Lens 6	60.0	60.0 V		
Lens 7	17.0	18.0 V		
Push L	16.5	16.0 V	<input checked="" type="checkbox"/>	3 mA
Push H	790.0	790.0 V	<input checked="" type="checkbox"/>	3 mA
Pull L	86.0	86.0 V	<input checked="" type="checkbox"/>	3 mA
Pull H	700.0	700.0 V	<input checked="" type="checkbox"/>	3 mA
Grid	2400.0	2283.0 V	<input checked="" type="checkbox"/>	1 μ A
Cage	5020.0	4768 V	<input checked="" type="checkbox"/>	100 μ A
Refl. Grid	665.0	632.0 V	<input checked="" type="checkbox"/>	76 μ A
Refl. Back	900.0	855.0 V	<input checked="" type="checkbox"/>	167 μ A
MCP F	5400	5134 V	<input checked="" type="checkbox"/>	17 μ A
MCP B	2550	2536 V	<input checked="" type="checkbox"/>	247 μ A

TOF Lens Voltages and Settings

Acquisition ACQ active

Single Spec Time (ms)

Extraction time (μ s)

max Flighttime(μ s)

Data Save Settings

Spec
 Trace
 Raw

Time Duration

Single File Duration

Number of Files To Store

Add File Count Extension

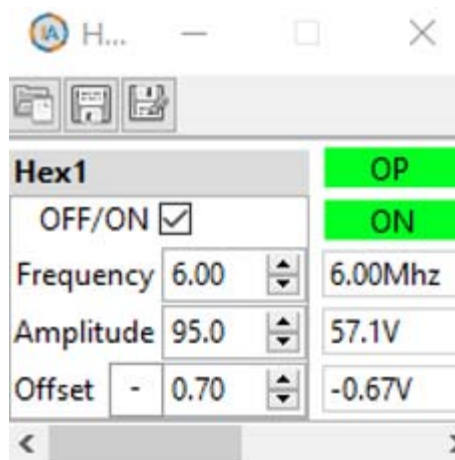
New ACQ for new file

Acquisition Settings

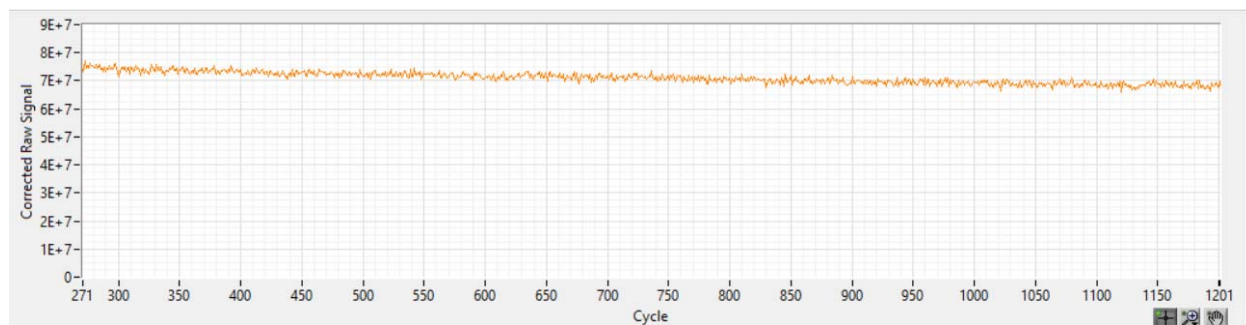
Mass Axis Calibration **AutoCAL done**

Mass	TimeBin			
21.0220	15965	<input type="button" value="Trash"/>	^	a <input type="text" value="15007"/>
203.9400	161478	<input type="button" value="Trash"/>		b <input type="text" value="-52835.8"/>
330.8500	220131	<input type="button" value="Trash"/>	v	

Mass Axis Calibration



Hex Settings



Hydronium Ion Isotope (21.022 amu) Stability Check

May 20, 2021 PTR Settings

Final Operating Parameters

The screenshot shows a software interface for PTR settings. At the top, there are icons for file operations and a refresh button. Below that, three dropdown menus are visible: 'Setting' set to 'Odor', 'Primary Ion' set to 'H3O+', and 'Transmission' set to 'DC'. Each dropdown has a pencil icon for editing. The main area is a table with two columns: 'Man/Ctrl' and 'Ctrl'. The parameters and their values are as follows:

	Man/Ctrl	Ctrl
PC	343.5	343.52 mbar
p Drift	2.30	2.30 mbar
TofLens		5.35E-5 mbar
TOF		7.91E-7 mbar
E/N		120 Td
Temps	80.00 °C	79.90 °C
SrcValve	50.0	
H2O	6.0	6.00 sccm
O2	0.0	0.00 sccm
NO	0.0	0.00 sccm
Ihc	4	4.0 mA
	On/Off	On
FCinlet	60.0	60.01 sccm
U	FU °C C→ C*	
Us	150	145.0 V
Uso	80	78.6 V
Udrift	525	526.1 V

Ion Production Settings

Component	Setting	Target Voltage	Checked	Current
Lens 1	12.0	13.0 V		
Lens 2	30.0	30.0 V		
Lens 3	20.0	21.0 V		
Lens 4	76.0	76.0 V		
Lens 5	70.0	69.0 V		
Lens 6	60.0	60.0 V		
Lens 7	17.0	18.0 V		
Push L	16.5	16.0 V	<input checked="" type="checkbox"/>	3 mA
Push H	790.0	790.0 V	<input checked="" type="checkbox"/>	2 mA
Pull L	86.0	86.0 V	<input checked="" type="checkbox"/>	3 mA
Pull H	700.0	700.0 V	<input checked="" type="checkbox"/>	3 mA
Grid	2400.0	2283.0 V	<input checked="" type="checkbox"/>	1 μ A
Cage	5020.0	4768 V	<input checked="" type="checkbox"/>	99 μ A
Refl. Grid	665.0	632.0 V	<input checked="" type="checkbox"/>	75 μ A
Refl. Back	900.0	855.0 V	<input checked="" type="checkbox"/>	167 μ A
MCP F	5400	5134 V	<input checked="" type="checkbox"/>	17 μ A
MCP B	2570	2479 V	<input checked="" type="checkbox"/>	235 μ A

TOF Lens Voltages and Settings

Acquisition ACQ active

Single Spec Time (ms)

Extraction time (μs) 372.7 amu

max Flighttime(μs) 31.25 kHz

Data Save Settings

Spec
 Trace
 Raw

Time Duration

Single File Duration

Number of Files To Store

Add File Count Extension

New ACQ for new file

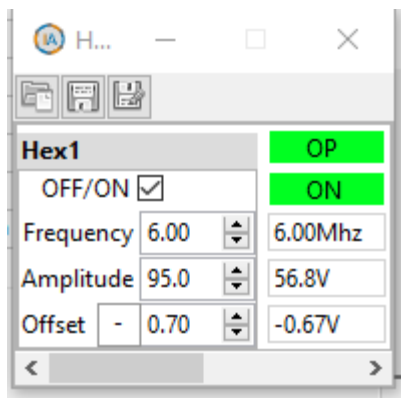
Acquisition Settings

Mass Axis Calibration

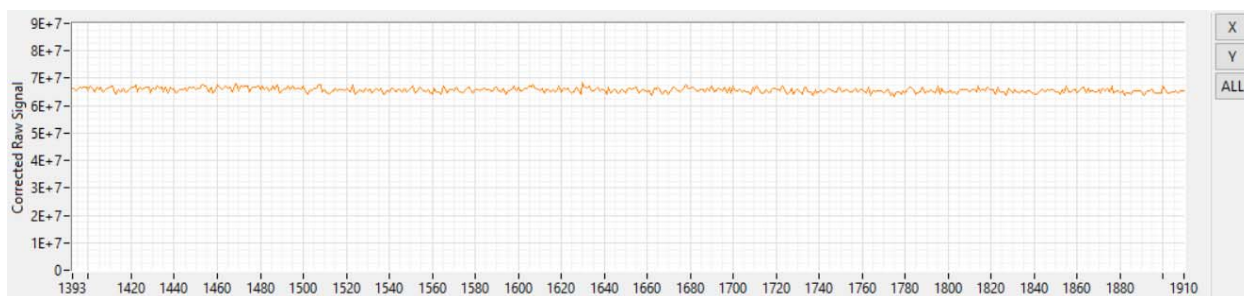
30 sec

Mass	TimeBin			
21.0220	15978	<input type="button" value="Trash"/>	^	a 15008.2
203.9400	161502	<input type="button" value="Trash"/>		b -52828.7
330.8500	220160	<input type="button" value="Trash"/>	v	

Mass Axis Calibration Values



Hex Settings



Hydronium Isotope (21.022 amu) Stability Check