

Hardware Manual



November, 2010

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ReactIR 15™

Improve Chemistry Understanding

METTLER TOLEDO

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If you have any questions please contact the responsible authority or the distributor from which you purchased this device.

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Thank you for your contribution to environmental protection.

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Introduction

ReactIR 15™ is an automated laboratory spectrometer using Fourier Transform Infrared (FTIR) technology to optically measure and monitor changes in chemical species as they react over a period of time. Designed for the synthetic chemist to be easier to use than previous ReactIR products by virtue of no alignment (DS technology) and instrument purge requirement. Simplicity, reproducibility, and ergonomics meet the needs of routine reaction monitoring—all of which are key characteristics of the ReactIR 15 system.

This document contains instructions for site preparation, technical specifications, instrument installation and operational checklists, system configurations, routine operation, safety information, as well as care and maintenance information and troubleshooting tips.

Should you have questions that are not addressed in this document, please contact your local METTLER TOLEDO office or our Customer Care Department using the information under [“Service and Technical Assistance”](#) on page 8.

Related Documents

The following documents are included in the iC IR™/ReactIR product portfolio.

- “ReactIR Sampling Technology Guide” (MK-PB-0008-AC).
- Quick Reference—“Experiment Setup in iC IR” (MK-PB-0013-AC)
- Quick Reference—“Data Review and Analysis with iC IR” (MK-PB-00012-AC)
- “iC IR Installation Guide” (MK-PB-0020-AC)

If you are viewing this document electronically, click any blue-colored link to go to the related information and instructions.

General Policies

METTLER TOLEDO equipment is subject to the installation, repair, and computer service policies described below.

Installation Policy

Site preparation for the ReactIR 15 equipment is the user's responsibility. Structural installation details should be prepared and supervised by a certified and registered professional engineer who is properly qualified to assure a safe installation at your site.

1 ■ Introduction

Training Programs

Repair Policy

Mettler-Toledo AutoChem, Inc. warrants its products against defects in materials and workmanship for twelve months from the date of installation or fifteen months from the date of shipment. For details, please refer to the warranty provided with the instrument. For assistance, please contact your Technical and Applications Consultant (TAC) or send an email to **AutoChemCustomerCare@mt.com**.

It is recommended that you retain the original packing materials in the event you need to return the ReactIR 15. If factory service is required, your METTLER TOLEDO service engineer will issue you a Return Material Authorization (RMA) form.

Computer Service Policy

If a computer is included as part of your ReactIR 15 system, it will be from a major manufacturer such as Dell. In the U.S. and some European countries, the manufacturer will provide warranty service if required. METTLER TOLEDO can assist in diagnosing problems with computers, but the computer manufacturer will provide parts and labor for repairs under the service contract.

Training Programs

Training for ReactIR 15 systems is available from the AutoChem Community Web site and through your METTLER TOLEDO TAC. Contact **AutoChemCustomerCare@mt.com**. For information on training programs, see the users' Web site, <http://community.autochem.mt.com>. Access to the site requires a login and password that you can request at the site.

Software Upgrades

Contact your METTLER TOLEDO TAC for information or check the users' Web site for product information and availability of upgrades.

Service and Technical Assistance

METTLER TOLEDO has offices around the world. Contact the Mettler-Toledo AutoChem, Inc. headquarters in the USA for technical support or service. For specific application assistance at any time, contact a METTLER TOLEDO Technology and Applications Consultant (TAC) through the toll-free number below.

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Product Description

This chapter describes the ReactIR 15 system and the possible system configurations. A ReactIR 15 system consists of a base unit and sampling technology along with iC IR™ software. Designed to be simple and easy to use, the system comes in three overall configurations that differ only by the type of DS sampling technology.

- “DS FiberConduit Probe”
- “DS Micro Flow Cell”
- “DS Fiber-to-Sentinel or Fiber-to-Gas Cell”

Please refer to the “ReactIR Sampling Technology Guide” for details on specific DS technologies.

Definitions

ReactIR 15 systems use the following terminology:

iC IR—User interface software for the ReactIR 15. As a wizard-based application, iC IR guides a user through the experience of collecting, analyzing, and visualizing data important to gaining real time insight into reaction chemistry.

Sampling Technology—Any DS Series type of sensor and conduit combination or DS Micro Flow Cell placed on the ReactIR 15 system to monitor chemistry.

in situ—The term *in situ* refers to analyzing chemistry in the reaction mixture, in real time, under actual reaction conditions.

IQ/OQ—Abbreviation for the ReactIR 15 installation and operational qualification procedures performed by a METTLER TOLEDO Field Service Engineer in a non-regulatory environment.

FiberConduit™—A FiberConduit uses AgX (silver halide) fibers to transfer the infrared (IR) source light from the ReactIR to the probe in contact with chemistry, and then back to the detector.

Sentinel™—A Sentinel is a type of composite probe with a standard size of 1-inch diameter and 1-inch insertion depth. DS Fiber-to-Sentinel is one type of sampling technology available for a ReactIR 15 base unit.

Single Beam—A single beam is the energy profile of the ReactIR system with or without a sample in contact with the sensor. Single beam can refer to a background (without chemistry sample) or a sample (with chemistry).

2 ■ Product Description

DS FiberConduit Probe

DS FiberConduit Probe

DS FiberConduit Probe systems are suitable for monitoring chemistry in a reaction vessel of the customers' choice by insertion of the probe into the liquid-based reaction medium. Temperature monitoring of the reaction mixture is standard.

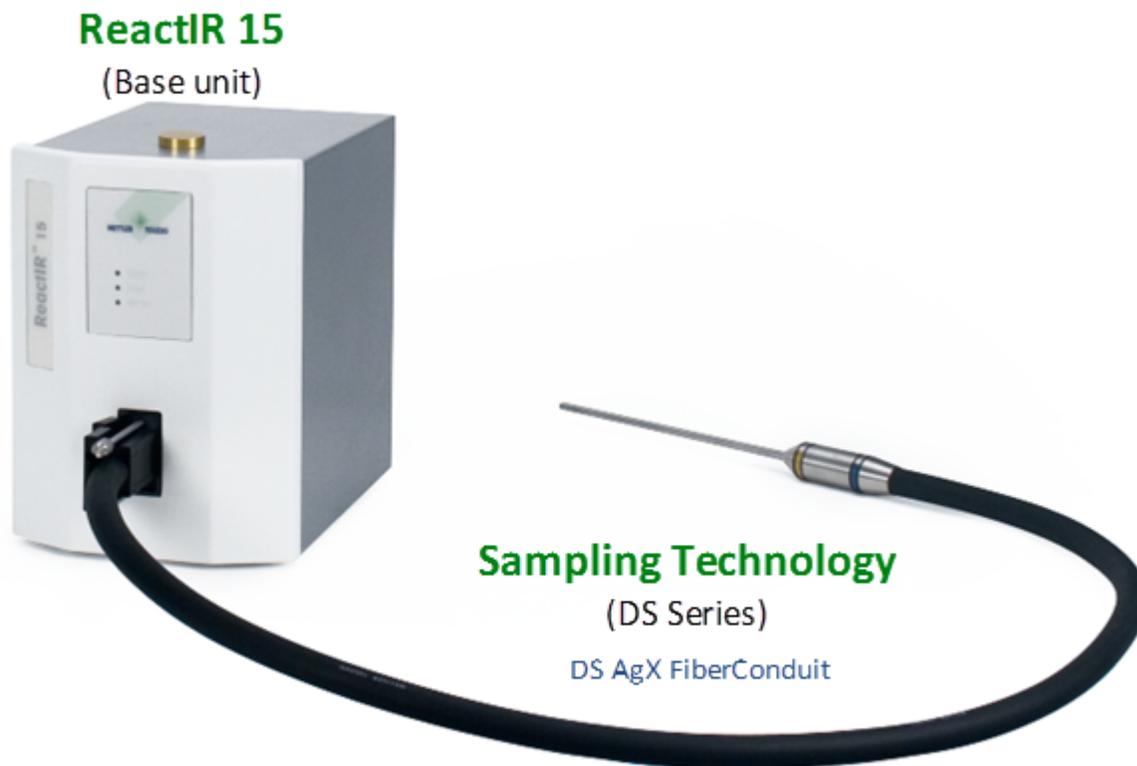


Figure 2-1 ReactIR 15 base unit with DS FiberConduit sampling technology

DS Micro Flow Cell

DS Micro Flow Cell systems are suitable for users who elect to flow their reaction chemistry through a specially designed cell to monitor chemical changes. Monitoring and control of the flow cell head temperature is available.



Figure 2-2 ReactIR 15 base unit with DS Micro Flow Cell (Heated)

[Figure 2-2](#) shows the heated model DS Micro Flow Cell which includes a heater controller and power supply (not shown).

DS Fiber-to-Sentinel or Fiber-to-Gas Cell

A DS Fiber-to Sentinel configuration is designed for customers who have a need for a sentinel in high pressure autoclaves, large volume circulation loops, or specialty reaction vessels. Customers who want to monitor gas phase reactions or head space can choose a DS Fiber-to-Gas Cell option in combination with a ReactIR 15 base unit. This type of configuration has a DS bell-style connector at the sampling technology end of the fiber. The bell-style connector attaches to a Sentinel ([Figure 2-3](#)) probe or to a gas cell ([Figure 2-4](#)).

2 ■ Product Description

DS Fiber-to-Sentinel or Fiber-to-Gas Cell

DS Fiber-to-Sentinel



Figure 2-3 ReactIR 15 base unit with DS Fiber-to-Sentinel sampling technology

DS Fiber-to-Gas Cell



Figure 2-4 ReactIR 15 base unit with DS Fiber-to-Gas Cell sampling technology

This remainder of this chapter includes the following sections:

- [“Overview of the ReactIR 15 System” on page 13](#)
- [“ReactIR 15 System Diagram” on page 14](#)

Overview of the ReactIR 15 System

The ReactIR 15 is an economical, practical FT-MIR based *in situ* reaction analysis system designed specifically for the synthetic chemist. Chemists can quickly and easily gather information that assists with what they want to do... study chemistry! No more spending time with an expert or a long setup to get valuable, data rich information about reaction initiation, progression and endpoint determination. With ReactIR 15 information, the synthetic chemist can reduce the time and number of experiments required to optimize reaction yield and purity. Additionally, the ability to measure *in situ* and real time offers immediate feedback on the synthetic chemist's theoretical reaction mechanism and pathway. Again more time to spend on the chemistry, especially for those reactions difficult to characterize otherwise.

Valuable characteristics of the ReactIR 15 include:

- Ergonomics—No obstruction to daily workflow, easier to monitor every reaction
- No purge—Improved data quality without external requirements/costs
- No alignment—Highest quality data assurance without user input
- Plug-n-Play sampling—Reproducible measurements
- Enhanced understanding of chemistry—Monitor reaction temperature simultaneously with chemical changes

Note: Sensor sampling technology interfaces are sold separately.

Standard items included with the ReactIR 15 base unit are:

- 24-hour cooling capacity, Mercury Cadmium Telluride (MCT) detector
- iC IR 4.2 or later software version
- 1.0 meter USB communications cable
- Replaceable desiccant cartridge

Not included but necessary for routine operation are,

- Workstation—Notebook: WIN XP (MTPN—14180610)
- DS AgX Fiber Probe and/or DS Micro Flow Cell (MTPN available upon request)
- One Year System Warranty (includes standard sampling technologies) purchased with system). System warranty ends one year after installation or fifteen months after shipment.

A ReactIR 15 system uses METTLER TOLEDO proprietary software, iC IR, to assure infrared data collection and analysis possible without the need for an expert. iC IR is the result of many years of evolution through valuable customer feedback that offers powerful reaction analysis functions with an easy-to-use user interface. As a wizard-based application, iC IR

2 ■ Product Description

ReactIR 15 System Diagram

guides you through the experience of collecting, analyzing, and visualizing data for real time insight into your chemistry. In essence, iC IR allows chemists to focus on solving chemistry problems instead of instrumentation and analysis procedures.

See [Chapter 3, "Safety"](#) for safety-related information.

ReactIR 15 System Diagram

The block diagram below identifies the components necessary to buildup a ReactIR 15 system, essentially what hardware the customer purchases from METTLER TOLEDO provides according to specifications to install and implement the system. Components include the base unit, computer, communication cables, power cable, sampling technology.

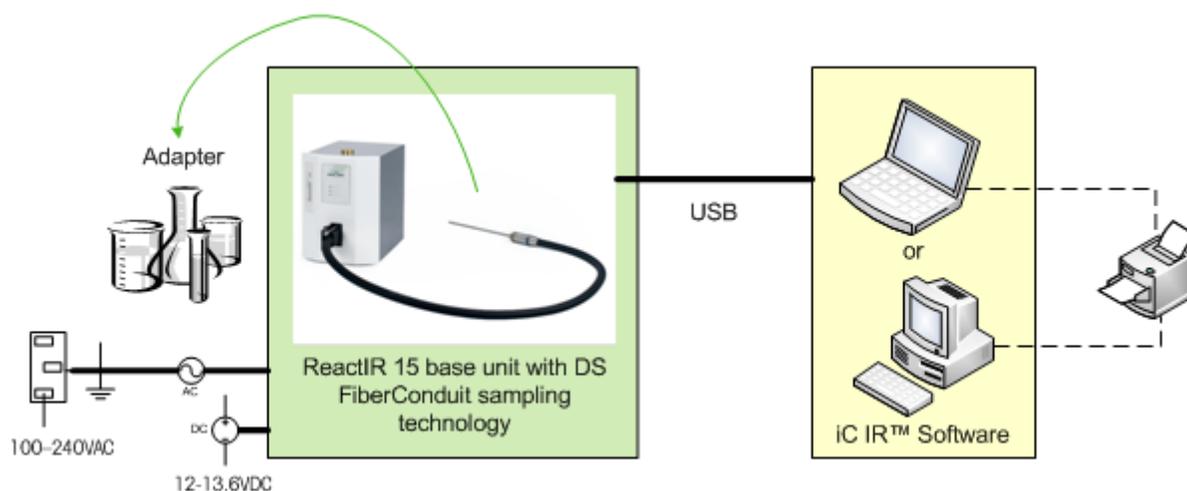


Figure 2-5 ReactIR 15 system diagram

The [Figure 2-1](#) describes the internal components of a ReactIR 15 base unit: We include the definitions for an understanding of the components that METTLER TOLEDO representatives discuss with you during initial training, follow-up service or potential repair. By design, the ReactIR 15 will not require the user to know the location for alignment or replacement of these components.

Table 2-1 ReactIR 15 Internal Components

Component	Description
MCT Detector	Senses the amount of infrared radiation after passing through a sample. Requires liquid nitrogen in the dewar to be operational. Includes a detector preamp.
Detector Preamp	Electronic board that assists the detector in reaching maximum operating performance. User adjustment may be necessary when changing sampling technology, for example from DS FiberConduit Probe to DS Micro Flow Cell.
IR Source	Supplies the infrared radiation to the sample
Midget Modulator	Mechanical device that affords full spectrum infrared measurements of high sensitivity in a shorter period of time than traditional dispersive spectroscopy methods. Also known as the interferometer or heart of the Fourier Transform Infrared (FTIR) measurement. Produces source radiation specific to the Fourier Transform Infrared Technology (FTIR).
Interferometer Control Board Module (ICBM)	Circuit board for controlling specific devices related to the interferometer (modulator).
Power supplies	Supplies electrical power to internal ReactIR 15 components.
Laser	Class 1 InGa/AsP/InP laser diode that is an integral component of the modulator.

2 ■ Product Description

ReactIR 15 System Diagram

Safety

Per the ISO 9001 procedures followed at METTLER TOLEDO, the ReactIR 15 system adheres to applicable regulations and standards in the area of intended use. Requirements for compliance with local regulations may be different. The end user of the equipment is responsible for compliance with all local, corporate, or other applicable regulations.



WARNING—Use of this product in a manner other than described in this manual may result in serious injury, damage to equipment, and/or void the warranty of the system.

Warnings, Cautions, and Notes

Three levels of information relate to equipment and user safety. To help you recognize information, the following symbols appear throughout this manual. Please pay particular attention to the sections marked by these symbols.

Table 3-1 Warnings, Cautions, and Notes

	Caution —Important information that tells you how to prevent damage to equipment, or to avoid a situation that may cause minor injury.
	WARNING —Important safety information—Failure to observe the warning may result in serious personal injury or equipment damage.
Note:	Information that you should pay attention to.

Product Safety

ReactIR 15 systems comply with the directives and laser classifications described below.

Compliance

- **EMC Directive 2004/108/EC**
IEC 61326-1: Electrical Equipment for Measurement, Control and Laboratory Use
- **Low Voltage Directive 2006/95/IEC**
EN61010-1: Safety requirements for electrical equipment for measurement, control, and laboratory use

3 ■ Safety

Product Safety

Laser Classification

All ReactIR 15 instruments are in compliance with the U.S Department of Health and Human Services (DHHS) Radiation Performance and in accordance with International Standards.

Class 1 Laser Product

Compliant with **21 CFR 1040.10** and **1040.11**

except for deviations per Laser Notice 50, dated June 24, 2007

and

Compliant with **IEC 60825-1**

Grounding the Power Supply



Make sure that you plug the power cable supplied with the ReactIR 15 system into power supply outlets that are grounded. A technical fault could otherwise result in death or serious injury.

Operational Safety



Connection of cables

Caution—Connect all cables (power and communications) of ReactIR iC10, 15, or 45m system to their respective inputs and outputs before you switch on the system. Do not disconnect any cables while the system is in operation as this may cause damage to internal electrical components.



Handling Liquid Nitrogen

Caution—Liquid Nitrogen is used with the ReactIR 15 system to cool the MCT detector for optimum detector performance. Liquid Nitrogen will cause severe burns to exposed skin. Ensure use of proper clothing (gloves) and eye protection before handling liquid Nitrogen.

NOTE: A caution label is located on the top of the ReactIR 15 base unit, next to the Liquid Nitrogen fill port.

**Liquid Nitrogen "Blow Off"**

Caution—When filling the MCT detector with Liquid Nitrogen there is a chance that the Liquid Nitrogen may "Blow Off" once sufficient pressure is reached inside the detector cooling chamber. It is recommended to add liquid Nitrogen slowly to allow sufficient time for entrained pressure to release from the cooling chamber and prevent "Blow Off."

**Cold Surfaces (Liquid Nitrogen Spills)**

Caution—Spills will most likely occur when filling the MCT cooling chamber with Liquid Nitrogen. Normal Liquid Nitrogen spillage (i.e. Blow Off) will not damage components of the ReactIR iC10, 15, or 45m system BUT will create COLD surfaces. Avoid touching these cold surfaces without proper protective clothing. These cold surfaces typically warm to room temperature within a few minutes (~15min).

**Lithium Battery**

Caution—The ReactIR 15 base unit includes a CR-2032 3V manganese dioxide lithium coin battery for the real-time clock. Battery is not user-replaceable.

**Service**

Caution—Never open the enclosure of the ReactIR 15 system or any of its components. These items are serviced only by a qualified METTLER TOLEDO AutoChem Service Engineer.

**General Caution**

Exclude the following environmental influences:

- powerful vibrations
- direct sunlight
- atmospheric humidity greater than 60%
- temperatures below 15°C and above 40°C
- powerful electric or magnetic fields

System Handling



Caution—The system can be awkward when handling. Follow the basic safety steps outlined below

3 ■ Safety

Product Safety

- When moving the ReactIR 15 system, it is highly recommended to use a cart or similar type device. The system can be hand-carried by using the integrated handle on the rear of the system. The ReactIR 15 does not have a front sampling attachment port, so lift using the handle in the rear and support the front from the underside of the enclosure.
- DO NOT hand-carry the system with the fiber optic or mirror conduit attached to the system. Remove the conduit first before moving the unit.
- ONLY move the system with the conduit attached by using a cart or similar device. This will prevent any possible damage to the unit or personnel.
- ONLY lift the system using the handle in the rear while supporting the front underside of the ReactIR 15 base unit. Lifting the unit in other manner may cause damage to the system or personal injury should the cover unexpectedly become detached.
- Position the ReactIR 15 base unit to enable easy disconnection of the DC power cable.

Specifications

This chapter provides specifications for the ReactIR 15 system in the following sections:

- [“Materials of Construction” on page 21](#)
- [“ReactIR 15 System” on page 22](#)
- [“Purge \(if applicable\)” on page 23](#)
- [“iC IR Computer Specifications” on page 23](#)

Specifications include those provided by METTLER TOLEDO and those that are your responsibility as the customer.

Manufacturer Name—METTLER TOLEDO AutoChem, Inc.

Manufacturer’s Address—7075 Samuel Morse Drive Columbia, Maryland USA 21046

Product—ReactIR™

Model No—A15

Trademark—METTLER TOLEDO

Intended Use—The use of this product is to provide unattended, *in situ* data collection and simultaneous data analysis of chemical reactions. This product is designed to be used in a ventilated fume hood. Alternatively, this system can be used on a bench top with the flexible fiber optic conduit positioned inside the fume hood where the reactor is located.

Materials of Construction

ReactIR 15 has the materials of construction specified in the upcoming table. Refer to [“ReactIR 15 System Diagram” on page 14](#) as a visual aid to identify items below:

Table 4-1 ReactIR 15 Materials of Construction

Specification	Details
Material	Aluminum Alloy 5052-H32
Desiccator	Plug —Aluminum Desiccant —Silica Gel
Enclosure finish	Iridite and Paint Polane-T
Labels	Poly carbonate
Pressure Seals	Alloy C-276 spring-energized graphite-filled PTFE

4 ■ Specifications

ReactIR 15 System

ReactIR 15 System

Table 4-2 ReactIR 15 System Specifications

Specification	Details
Power	AC: 100–240VAC, 50–60Hz, 1.2A (max) DC (supplied): <ul style="list-style-type: none">■ 12-13.6VDC, 6A■ 5A Mini Fuse (Fast Acting, internal)■ BATTERY: CR-2032 3V manganese dioxide lithium coin battery for real-time clock
Temperature Range	Operating: 19 to 25°C (recommended range for proper system stability) Ambient (max): 40°C (invalidates performance specification)
Humidity	Ambient: <60% non-condensing
Communications	USB 2.0 communications cable between base unit and computer, 10m
Detector	24-Hour Cooling Capacity, Mercury Cadmium Telluride (MCT) Detector
Resolution	4cm ⁻¹ maximum
Optical Range	4000 to 650 cm ⁻¹ maximum
Weight	9.0 kg (19.8 lbs)
Dimensions (W x H x D)	180 x 249 x 274 mm (see Figure 4-1) [7.1 x 9.8 x 10.8 in]

Purge (if applicable)

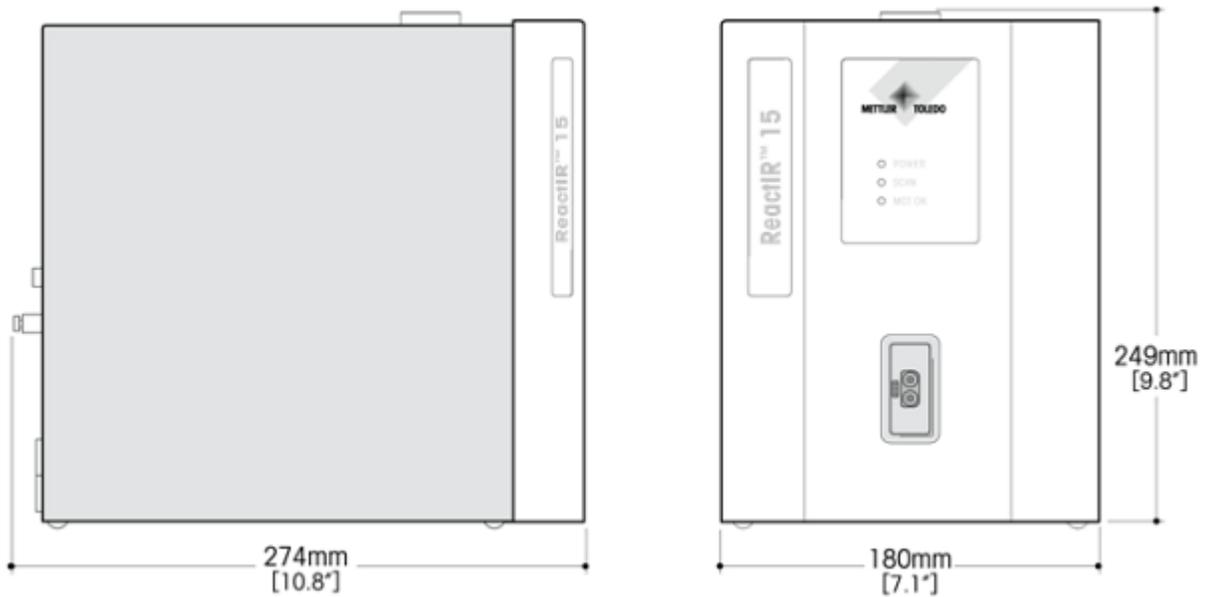


Figure 4-1 ReactIR 15—Dimensions in mm [inches]

Purge (if applicable)

If you use the DS Fiber-to-Sentinel sampling technology (page 34), a purge connection is required. Clean, dry, instrument grade air, nitrogen, or equivalent gas is recommended.

Table 4-3 Purge Specifications for Fiber-to-Sentinel Sampling Technology

Specification	Details
Purge	Instrument grade air, nitrogen, or equivalent gas
Particulate	< 0.1ppm CO ₂
Dew Point	< 1ppm water vapor at -100° F/-73.3° C
Pressure	10psig/0.69barg and 10SCFH/4.7LPM

iC IR Computer Specifications

System requirements for the PC or laptop that runs iC IR software for the ReactIR 15 system are in the beginning of the “iC IR Installation Guide.” Since requirements can change with new software releases, please refer to the current installation guide.

4 ■ Specifications

iC IR Computer Specifications

Installation

This chapter provides procedures on how to install or reinstall a ReactIR 15 system. An Installation Qualification (IQ) checklist is provided for installations in **non-regulatory** * environments.

* **Note:** **IPac for Regulatory Environments**—METTLER TOLEDO offers an Instrument Qualification Package (IPac) service at a nominal fee. IPac service delivers comprehensive test procedures and verification records on installation and operation to assist you in meeting regulatory requirements. When applicable, the IPac replaces the Installation Qualification (IQ) procedure.

Basic installation includes site preparation performed by you and installation performed by a METTLER TOLEDO Field Service Engineer. The scope covers the following actions with steps documented in the Installation Qualification (IQ) form available on [page 79](#):

- Site requirements verification (“[Site Preparation \(Customer Responsibility\)](#)” on [page 26](#))
- System inspection and setup
- Document software version and revision level
- System configuration
- Installation summary checklist
- Document test results for ongoing comparison
- System Acceptance

Installing ReactIR 15 in a Non-Regulatory Environment

As stated in the note above, METTLER TOLEDO provides installation of the ReactIR 15 at no charge to the customer in a non-regulatory environment—one that requires minimal qualification of installation and operation. Otherwise the customer can separately order a service that assists in meeting the requirements of the organization to comply with a regulatory environment.

In a non-regulatory environment, a METTLER TOLEDO Field Service Engineer will go through the ReactIR 15 system Installation Qualification (IQ) checklist (copy form from [page 79](#)) after confirmation that the site is ready for installation. The checklist includes the steps necessary to install and start up the system in a non-regulatory environment. In addition to verifying the site preparation and receipt of ordered parts (including service agreements/programs), the checklist covers all aspects of the final stages of system installation. The checklist ensures that the ReactIR 15 meets the manufacturing specifications and quality assurance in a non-regulatory environment.

5 ■ Installation

Site Preparation (Customer Responsibility)

Acceptance Criteria

The "ReactIR 15 Installation Qualification (IQ)" form requires approval signatures from the METTLER TOLEDO AutoChem Field Service Engineer and your Company Project Leader after completion of the checklist procedures.

Note: Place the signed Installation Qualification checklist in a readily accessible location for reference during system service or maintenance.

Site Preparation (Customer Responsibility)

Permanent or temporary installation site for a ReactIR 15 must include the following items:

- Electrical supply
- Space preparation
- Environment preparation

Table 5-1 describes the site requirements for a ReactIR 15 system installation. Refer to Chapter 4 on page 21 for detailed system specifications.

Table 5-1 Site Preparation

Site Preparation Description	System	Requirement	Status
Electrical	Computer	iC IR Workstation	See specific computer manual for voltages
	PC		(dedicated circuit)
	Instrument	ReactIR 15 with power supply	100-240VAC +/- 7%, 50/60Hz, 1.2A. Rated DC input: 12-13.6 VDC, 6A (dedicated circuit)
	Note: Power requirements do not include any additional device. We recommend the use of an AC line conditioner in areas where noisy power is known to exist. Line conditioner should have a power rating of at least 800 VA.		
Space Requirement *	ReactIR 15	180 x 249 x 274 mm (W x H x D)	Yes
		7.1 x 9.8 x 10.8 inches	No
	Power supply	76 x 447 x 130 mm (W x H x D)	Yes
		3.0 x 1.7 x 5.1 inches	No
Purge *	ReactIR 15	No purge system required	Yes
			No
	Note: Gauge and pressure regulators are NOT supplied with the equipment.		

-
- Notes:**
- * Purge for sampling technology—If you use the DS Fiber-to-Sentinel sampling technology, a purge connection is required. Clean, dry, instrument grade air, nitrogen, or equivalent gas is recommended.
Clean: < 0.1 ppm CO₂
Dry: < 1 ppm water vapor at –100° F/–73.3° C dewpoint).
Pressure: 10psig/0.69barg and 10SCFH/4.7LPM.
 - * Space requirement (location)—System can be installed either on bench top or inside fume hood.
 - Overall system dimensions will also vary depending on the sampling technology.
-

A METTLER TOLEDO Field Service Engineer will install the ReactIR 15 system upon completion of the site preparation. To facilitate rapid completion of installation and operation testing at the time of installation, please make a copy of the following checklists:

"[ReactIR 15 Installation Qualification \(IQ\)](#)" (IQ) on [page 79](#)

"[ReactIR 15 Operational Qualification \(OQ\)](#)" (OQ) on [page 80](#).

Then, complete the site preparation requirements section at the top of the Installation Qualification checklist.

Installation Instructions

This section describes the procedures for installing the ReactIR 15.

- "1. Confirm Site Readiness" on [page 27](#)
- "2. Verify Hardware Configuration/Order Validation" on [page 28](#)
- "3. Install iC IR Software and Confirm Hardware Service Agreement" on [page 29](#)
- "4. Establish System Connections" on [page 29](#)
- "5. Remove Shipping Constraint from MCT Fill Port" on [page 31](#)
- "6. Connect Sampling Technology" on [page 32](#)
- "7. Establish the Sampling Technology Conduit Purge (if applicable)" on [page 34](#)
- "8. Start Up System" on [page 34](#)

1. Confirm Site Readiness

A METTLER TOLEDO Field Service Engineer (FSE) will check the ReactIR 15 installation site in accordance with the product requirements, and complete the first section of the Installation Qualification (IQ) form ([page 79](#)). Customers can speed this process by assuring the site is ready prior to arrival of the FSE. The critical elements are power, environmental temperature,

5 ■ Installation

Installation Instructions

and space. A purge utility is only necessary when the system configuration includes the DS Fiber-to-Sentinel sampling technology. Otherwise the ReactIR 15 base unit requires no purge utility, as is required with the ReactIR 45m.

Proceed to the next step only after confirming the site is ready.

2. Verify Hardware Configuration/Order Validation

Using the Installation Qualification (IQ) form ([page 79](#)), perform a visual inspection of the shipment for the items on the checklist.

Sampling Technology

Although unusual, the possibility exists that a customer only orders a base unit. In that case draw a single line through the section and write N/A (not applicable). Otherwise, find the section that applies to the customer order for sampling technology. Complete the corresponding section with the information specific to the type of technology ordered. In the absence of a AgX FiberConduit probe or DS Micro Flow cell order, complete the other section with the description of the sampling technology. Enter N/A (not applicable) for sections that do not apply to the customer order. Record the 'wetted materials' and 'pressure/temperature' specifications for the sampling technology. Any items that are missing should be entered into the non-conformances section of the form with an action plan to resolve.

Hardware and Software

All items in this section of the Installation Qualification form should be with the order. Check the items that are with shipment. Any items that are missing should be entered into the non-conformances section of the form with an action plan to resolve.

Optional Software

Check the items with the shipment that cross reference to the customer order. Enter N/A in the check box if the customer did not order that item. Any items that are missing should be entered into the non-conformances section of the form with an action plan to resolve.

Documentation

All items in this section of the Installation Qualification form ([page 79](#)) should be with the order, with the exception of the Certificate of Conformity for Sampling Technology as the customer may not order this item with the base unit. Check the items that are with the shipment. Any items that are missing should be entered into the non-conformances section of the form with an action plan to resolve.

3. Install iC IR Software and Confirm Hardware Service Agreement

Before setting up the communications between a computer and the ReactIR 15, verify that the PC meets the specifications under “[iC IR Computer Specifications](#)” on [page 23](#). You will need iC IR Instrument License, included with your order, to operate the ReactIR 15 instrument.

1. Insert the iC IR installation CD in the PC and click **Install iC IR #.# (setup.exe)** from the welcome page.
2. Install the software according to the wizard-guided steps.
Refer to the “iC IR Installation Guide” for additional installation information on administering preferences, licensing, and sharing data between iC/iControl software applications.
3. Confirm the following information on the Installation Qualification form ([page 79](#)).
In the **Software Install** section of the form, enter the version number for the iC IR software shipped with the ReactIR 15 order.
In the **Hardware Service Agreement** section of the form, record the ReactIR 15 and Sensor coverage the customer ordered. Otherwise enter the standard warranty coverage information.

4. Establish System Connections

Complete the System Connections checklist in the Installation Qualification ([page 79](#)) while progressing through these instructions that will assure all ReactIR system hardware is in the proper location with connectivity to utilities, computer, and sampling technology.

Note: DO NOT proceed with the 'System Start Up' section until all applicable check boxes are complete.

Locate ReactIR 15 Base Unit and Computer at Site

1. Place the base unit in the predetermined customer location per the site preparation requirements.
2. In addition, place the computer in a suitable work location that allows connectivity through a USB cable.

5 ■ Installation

Installation Instructions

Connect power

Power connections as well as USB communications connections to the computer are made at the back of the ReactIR 15 base unit.

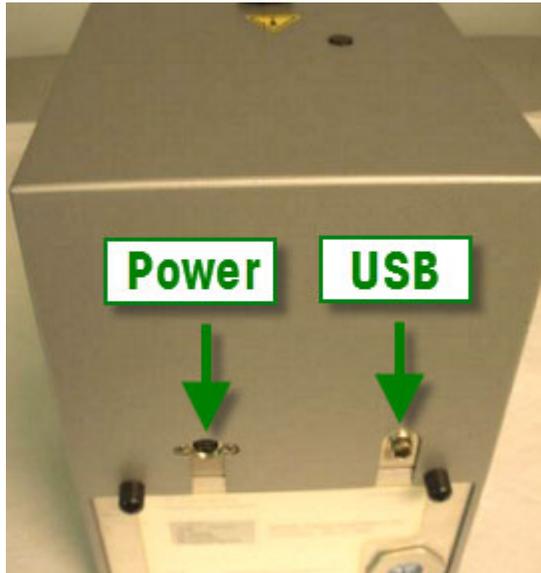


Figure 5-1 Connection points at back panel of ReactIR 15

1. Ensure that your power supply meets the specifications under the electrical specifications section.
2. Connect the supplied power cord to the left-most unique connector on the back panel of the ReactIR 15.



Figure 5-2 ReactIR 15 power cord connection on back panel (inset shows transformer)

3. Connect the opposite end into a power supply source using the country-specific power cord. Power supply must meet specifications on [page 22](#).
4. Connect power to the computer.

Connect USB Cable

1. Connect the supplied USB communications cable to the right-most unique connector on the back panel of the ReactIR 15.

[Figure 5-3](#) shows the ReactIR 15 back panel where you connect supplied communications cable and then with the cable connected.



Figure 5-3 ReactIR 15—Communications cable connection on back panel

2. Connect the opposite end of the USB communications cable to any available USB port on the computer where the iC IR software will be installed. Ensure that your power supply meets the specifications in [Table 4-2](#) on [page 22](#).
3. If the Found New Hardware wizard appears, point to the folder where the drivers were installed during software installation.
Default installation folder: Program Files > METTLER TOLEDO > iC IR #.# > Installation folder > FTIR Device Driver > icbm.

5. Remove Shipping Constraint from MCT Fill Port

The ReactIR 15 ships with restraining hardware for the MCT fill port. Remove this hardware by twisting the locking nut counter-clockwise. Save the locking nut in the event the unit needs to be shipped for service in the future.

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6. Connect Sampling Technology

Connect the sampling technology ordered to the factory DS SIM on the front panel of the ReactIR 15. The procedure differs slightly depending on the type of sampling technology, as described below.

DS AgX FiberConduit Probe or Fiber-to-Sentinel



Figure 5-4 Connecting DS FiberConduit sampling technology

1. Orient the DS end with the retractable cover to the left.
2. Pull back on the retractable cover that exposes the optical connection and insert the end into the DS SIM to align the unique connector.
3. Secure the sampling technology with the two knurled screws.

To install the Fiber-to-Sentinel sampling technology:

1. Connect the Sentinel sensor to the opposite end of the FiberConduit.
2. Orient the DS end with the retractable cover to the left.
3. Pull back on the retractable cover that exposes the optical connection and insert the end into the DS SIM to align the unique connector.
4. Secure the sampling technology with the two knurled screws.

DS Micro Flow Cell

Figure 5-5 Connecting DS Micro Flow Cell sampling technology

1. Orient the DS end with the retractable cover to the left.
2. Pull back on the retractable cover that exposes the optical connection and insert the end into the DS SIM to align the unique connector.
3. Secure the sampling technology with the two knurled screws.

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Installation Instructions

7. Establish the Sampling Technology Conduit Purge (if applicable)

The ReactIR 15 system is sealed and requires no purge. However, if you use the Fiber-to-Sentinel or Fiber-to-Gas Cell sampling technology, a purge is required

1. Attach a filtered, pressure-controlled air supply to the sampling technology.

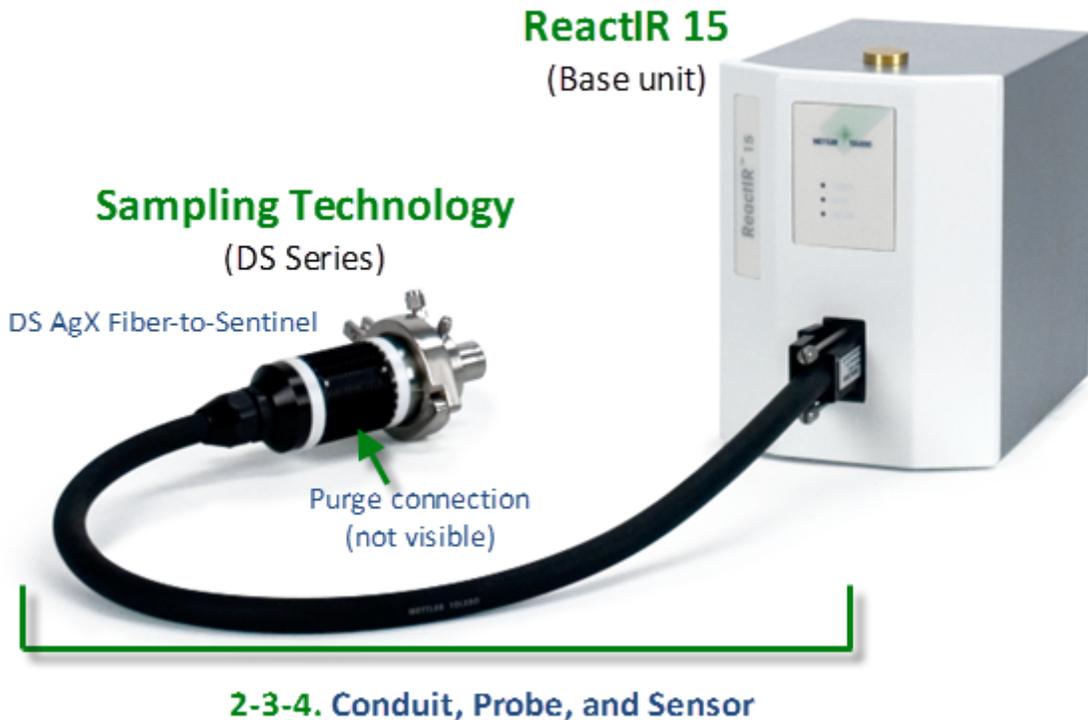


Figure 5-6 ReactIR 15 with DS Fiber-to-Sentinel sampling technology

2. Set the purge pressure to nominal 10psig (0.69barg) and 10SCFH (4.7lpm) flow rate.

8. Start Up System

Now that the ReactIR 15 connections are complete, the last step is to confirm the system is capable of reaching a state of readiness for operational testing or implementation. Use the checklist in the Installation Qualification form ([page 79](#)) to assess readiness as you proceed with the following instructions. Record any non-conformances with an action plan to resolve.

1. **Confirm the Power LED** illuminates on the base unit front panel. This event will happen after connecting the power cord to the unit and supply line. Also confirm the computer turns ON.



Figure 5-7 Power LED

2. **Confirm the Scan LED** illuminates and flashes repeatedly. The flashing occurs after connection of the USB cable between the base unit and computer, and when both devices are ON.



Figure 5-8 Power and Scan LEDs

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3. **Confirm the MCT Detector LED** illuminates after filling the dewar with liquid nitrogen. Go to the [“C. Fill the Detector Dewar”](#) on page 41 to find the procedure for filling the dewar.



Figure 5-9 Power, Scan, and MCT OK LEDs

4. **Confirm iC IR software launches.** Using the computer mouse, point to the iC IR icon on the Windows desktop and double-click on the icon.



You will see the Start Page for iC IR software.

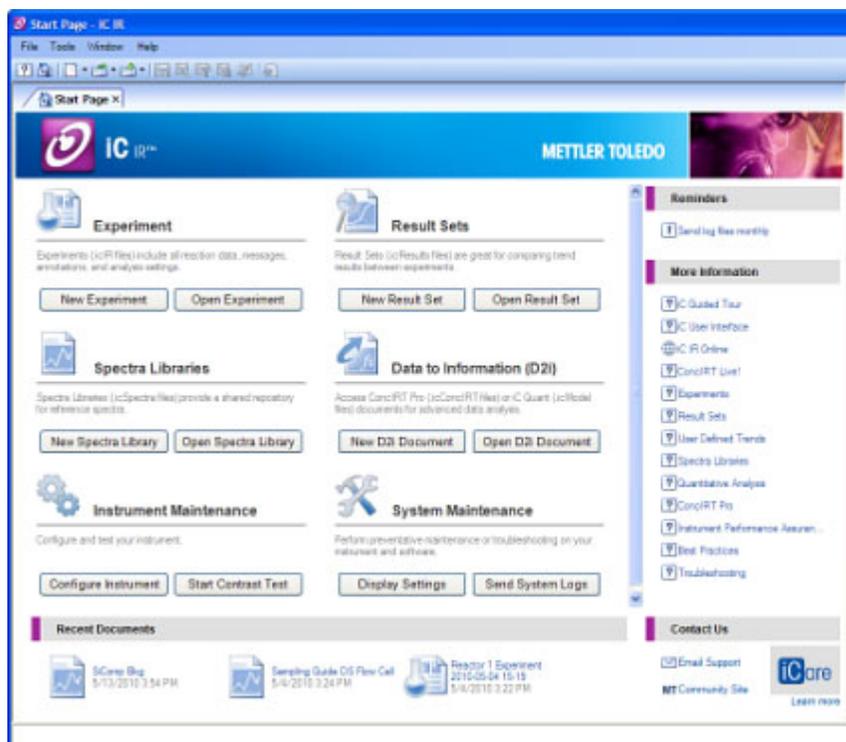


Figure 5-10 iC IR Start Page

5. **Confirm any optional software add-ons launch**, such as iC Kinetics, iC Quant or ConciRT Pro. iC Quant and ConciRT PRO appear as Data-to-Information documents from the iC IR Start Page. iC Kinetics is a separate software application with its own Start Page.

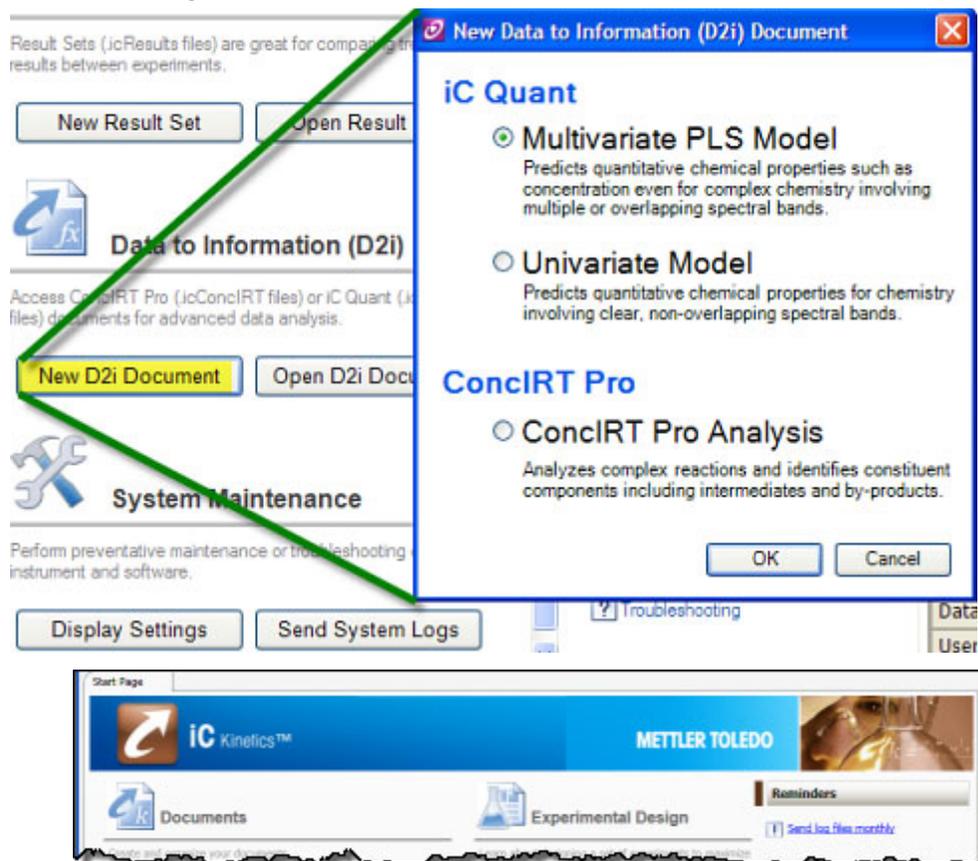


Figure 5-11 Optional add-on software

Implementation Readiness

At this point all items in the Installation Qualification form (page 79) should be complete, including resolution of any non-conformances. Users can always use the form or any portion therein to check readiness after placing in service following storage, relocation, or lengthy downtime. In either case, the ReactIR 15 will be ready for operational testing to verify high level system capability that then leads to running experiments with confidence the data and information reflect changes in chemistry.

A qualified Mettler-Toledo AutoChem, Inc. Field Service Engineer will sign and date the Installation Qualification form to confirm completion of the process in due and proper manner. The customer who witnesses the process and is responsible for the ReactIR 15

5 ■ Installation

Implementation Readiness

within their organization will then sign and date the Installation Qualification form as confirmation of the Field Service Engineer execution. This record is copied by the Field Service Engineer for delivery to the customer while on site, and the original put on file in the Service Department of Mettler-Toledo AutoChem, Inc.

The Field Service Engineer may now proceed to the Operational Qualification process that this manual covers in the Operations Chapter. In the event that the ReactIR 15 is returning to service following storage, relocation, or lengthy downtime, the customer can follow the same process or call Mettler-Toledo AutoChem, Inc Service for assistance in performing the service at a nominal fee. Check your service contract, if purchased, for inclusion of this service.

Complete the "[ReactIR 15 Installation Qualification \(IQ\)](#)" (see form on [page 79](#)) and proceed to [Chapter 6, "Operation"](#) for instructions on how to perform ReactIR 15 operational checks.

Operation

This chapter describes two areas of operation:

- **Operational Qualification (OQ)** that METTLER TOLEDO provides as a courtesy service with the purchase of a ReactIR 15. The service occurs at time of initial installation and is performed by a METTLER TOLEDO Field Service Engineer. Operational Qualification tests the ReactIR 15 installation by performing specific procedures to verify operational readiness (see [“Operation Instructions” on page 40](#)).

Note: **IPac for Regulatory Environments**—METTLER TOLEDO offers an Instrument Qualification Package (IPac) service at a nominal fee. IPac service delivers comprehensive test procedures and verification records on installation and operation to assist you in meeting regulatory requirements. When applicable, the IPac replaces the Operational Qualification (OQ) procedure.

Operational qualification scope covers the following actions with steps documented in the Operational Qualification (OQ) form available on [page 80](#):

- System identification
- Alignment/adjustment at installation location
- Functional Testing
- Operation summary checklist
- Document test results for ongoing comparison
- System Acceptance

Operational tests can also be performed periodically, according to your standard operating procedure. At any time, the user can duplicate the Operational Qualification form on [page 80](#) to independently verify product functionality. We recommend this process following storage, relocation, or months of infrequent use.

- **Routine Operation** that provides steps you follow to easily implement the product. Instructions include the most efficient way to use the ReactIR 15 to monitor chemistry.
 - [“Simple Steps to a Successful Experiment”](#) starting on [page 57](#)
 - [“Best Practices”](#) beginning on [page 68](#)).

Acceptance Criteria

The [“ReactIR 15 Operational Qualification \(OQ\)”](#) (see form on [page 80](#)) requires approval signatures from the METTLER TOLEDO AutoChem Field Service Engineer and your Company Project Leader after completion of the checklist procedures. The ReactIR 15 warranty and service contracts officially start at this point.

Note: Place the signed Operational Qualification checklist in a readily accessible location for reference during system service or maintenance.

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Operation Instructions

Upon completion of the system installation, a METTLER TOLEDO AutoChem Field Service Engineer will go through the ReactIR 15 system “[ReactIR 15 Operational Qualification \(OQ\)](#)”. The checklist includes the steps necessary to test the system in a non-regulatory environment and includes a place to record the results. To facilitate rapid completion of operation testing at the time of installation, print a copy of the OQ form from [page 80](#).

Note: Please follow the test procedures completely to ensure the comprehensive results.

This section describes the procedures for operational qualification in the following sections:

- “1. Identify the ReactIR 15 System” on [page 40](#)
- “2. Prepare ReactIR 15 System for Use” on [page 40](#)
- “3. Configure Instrument in Software” on [page 42](#)
- “4. Align the System” on [page 43](#)
- “5. Perform Functional Testing” on [page 52](#)

1. Identify the ReactIR 15 System

Complete the first two sections of the Operational Qualification form that documents the owner and serial number of the system under test.

2. Prepare ReactIR 15 System for Use

Proceed through the checklist in the System Readiness section of the Operational Qualification form to record actions necessary to prepare for alignment. By this point the unit should be ON for four (4) hours and the iC IR software ready to use on the computer.

A. Confirm the ReactIR 15 is ON for Four Hours

1. Ensure the Installation Qualification checklist is complete ([page 79](#)).

Note: For startup immediately following installation, this step will not be necessary unless you are relocating the product.

2. Apply power to the ReactIR 15 analyzer, if not already powered.

IMPORTANT / CRITICAL! **FROM A COLD START:** You must allow a minimum of **four (4) hours warm-up time** before you can proceed to make any alignment adjustments to the system. **DO NOT PROCEED** until the unit has been allowed to warm up.

3. If using DS Fiber-to-Sentinel sampling technology, apply 10psig of dry air to the inlet on the Sentinel (see [Figure 5-6](#) on [page 34](#)).
4. Turn on the computer and start the iC IR software, if not already done in the Installation Qualification procedure.

B. Launch the iC IR Software



Start the iC IR software from the Start menu or by clicking the desktop icon.

C. Fill the Detector Dewar

The ReactIR 15 uses a Mercury Cadmium Telluride (MCT) detector for collecting infrared absorbance by the reaction mixture components. This highly sensitive detector offers the user a means to detect analyze component concentrations as low as 0.1 weight percent for strong infrared absorbers. To render the detector functional, you must fill the MCT dewar with liquid nitrogen. At this temperature the detector operates to maximum performance for up to 24 hours without refilling.

Liquid nitrogen must be handled in accordance with applicable safety procedures.



Caution—Liquid Nitrogen must be handled in accordance with applicable safety procedures. Liquid Nitrogen will cause severe burns to exposed skin. Ensure use of proper clothing (gloves) and eye protection before handling liquid Nitrogen.

NOTE: A caution label is located on the top of the ReactIR 15 base unit, next to the Liquid Nitrogen fill port.

1. Remove the plug from the top of the ReactIR 15 system and insert supplied funnel into the opening.



Figure 6-12 Liquid nitrogen fill port on ReactIR 15—Plug removed

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2. Pour liquid nitrogen into funnel.



Figure 6-13 Filling Dewar with liquid nitrogen to cool the detector

- a. Add several funnels full of liquid nitrogen.
-
- Note:** At some point the nitrogen may blow back, creating a jet of nitrogen vapor and possibly liquid.
-
- b. After blow back subsides, add several more funnels full of liquid nitrogen.
3. Once liquid nitrogen spills from the top of the detector, replace the plug.
 4. Record the action as complete in the Operational Qualification form.

3. Configure Instrument in Software

Specific settings in iC IR software drive the ReactIR 15 to collect data in a manner appropriate for the product configuration and chemistry monitoring objective. You can then be confident that the infrared fingerprints are accurate representations of chemical changes. The software provides recommended default settings to speed the process.

A. Establish Instrument and Probe Settings

1. Click **Configure Instrument** on the Start Page.
2. Set the following parameters to match the configuration of the ReactIR 15, if not already done at the factory. Record these settings in the Operational Qualification form.
 - Instrument—Select **ReactIR 15**
 - Detector—**MCT Detector**
 - Probe Interface—Specify the type of DS sampling technology in use.
 - Probe Tip—**SiComp** or **DiComp**

B. Establish Acquisition Settings

1. Click **Configure Instrument** on the Start Page.
2. Set the following parameters in the 'Probe acquisition' section to the 'normal' selection. Record these settings in the Operational Qualification form

- Resolution—Normal (8 wavenumbers)
 - Spectral Range—Preset with the probe interface and probe tip settings
 - Gain Adjustment—Normal (1x)
3. Set the Scan/Sample parameter to **128 scans**.
 4. Set the Apodization Method to Happ-Genzel through the **Edit** button in the 'Instrument' section.

4. Align the System

By design the alignment process for the ReactIR 15 is quick and easy to enable the rapid implementation of the system. As a result, you get to monitoring the data and information about your chemistry without spending significant time preparing the reaction analysis instrument.

The purpose of alignment is to assure the energy of the system (source) properly travels from the origin to the sample and then to the detector. Maximum energy reaching the detector through this optical pathway will yield an infrared fingerprint characteristic of the chemistry in contact with the sampling interface (sensor). Over time these fingerprints accurately represent the chemistry dynamics that assist you in understanding the reaction mechanism and pathway.

Proceed through the checklist in the alignment section of the Operational Qualification form to record actions necessary to reach functional testing.

Note: By this point, the unit should be ON for 2 hours and the iC IR software ready to use on the compute (see [“2. Prepare ReactIR 15 System for Use” on page 40](#)). Remember that use of the form is optional after installation by a METTLER TOLEDO Field Service Engineer.

A. Sampling Technology Alignment

The ReactIR 15 is factory aligned for the sampling technology ordered with the base unit (if applicable). For the DS AgX FiberConduits and DS Micro Flow Cells, there is no rotational alignment required, so skip this section and proceed to the detector alignment.

With DS Fiber-to-Sentinel sampling technology, rotation of the Sentinel might be necessary to maximize peak height and contrast values.

If you have the DS Fiber-to-Sentinel, the Sentinel can be rotationally aligned as follows:

1. Before beginning the Sentinel rotation adjustment, select the **Test Instrument** task pane from the iC IR Toolbox.
2. Verify the appropriate fiber, probe, and MCT detector options in the Instrument Settings and Probe Settings section of the task pane. (These settings should reflect the instrument configuration settings established on [page 60](#).)
3. Select **Contrast and Align** from the 'Test mode' section and click **Start**.
4. Loosen the clamp around the Sentinel and slowly rotate the Sentinel.

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5. While rotating the Sentinel, maximize the contrast and peak height.
6. Once the contrast and peak height have been maximized, retighten the clamp.
7. Record the action as complete in the Operational Qualification form.
Record the values for contrast and peak height in a log book if performing a routine alignment after initial installation.

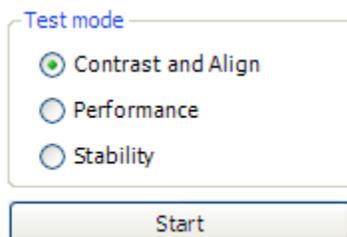
B. Detector Alignment

Factory alignment of the ReactIR 15 detector eliminates adjustment of this hardware.

C. Detector Preamp Adjustment

The MCT detector uses a preamplifier to maximize energy at the detector for a variety of sampling technologies. Adjustment may be necessary to reach factory-recommended peak height counts when changing from one sampling technology to another. In particular, the high energy throughput of a DS Micro Flow cell in comparison to the AgX FiberConduit Probe or AgX Fiber-to-Sentinel will require this adjustment.

1. In the iC IR Toolbox, click on the **Test Instrument** task pane.
2. Verify that the appropriate instrument configuration settings appear for fiber, probe, and MCT detector.
3. Select **Contrast and Align** and click **Start**.



- Adjust the gain pot on the preamp with a small flat head screwdriver, either clockwise or counterclockwise, until the peak height measures between 20,000-25,000.



Figure 6-14 Preamp adjustment on ReactIR 15

- Switching from a DS Micro Flow Cell to a AgX FiberConduit Probe or AgX Fiber-to-Sentinel, the gain pot on the preamp will need to be turned up (clockwise)
 - Switching from an AgX FiberConduit Probe or AgX Fiber-to-Sentinel to a DS Micro Flow Cell the gain pot on the preamp will need to be turned down (counterclockwise)
- Record the action as complete in the Operational Qualification form. Record the values for contrast and peak height in a log book, if performing a routine alignment after initial installation.

D. Fixed Mirror Alignment

Fixed mirror alignment may be necessary after shipment or relocation of the ReactIR 15. To assure the mirror position is in an optimal position, follow the short procedure that checks the position and if necessary aligns the fixed mirror.

- Launch the fixed mirror test program in iC IR software Toolbox, **Test Instrument** task pane. Click on the Advanced tab located in the lower-left corner of the contrast screen to open the fixed mirror adjustment panel.

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2. Using the toggle buttons (N, S, W and E,) verify/optimize proper alignment of the fixed mirror for maximum peak height and contrast levels.
3. Verify the shape of the single beam is consistent with the sampling technology using the images below.

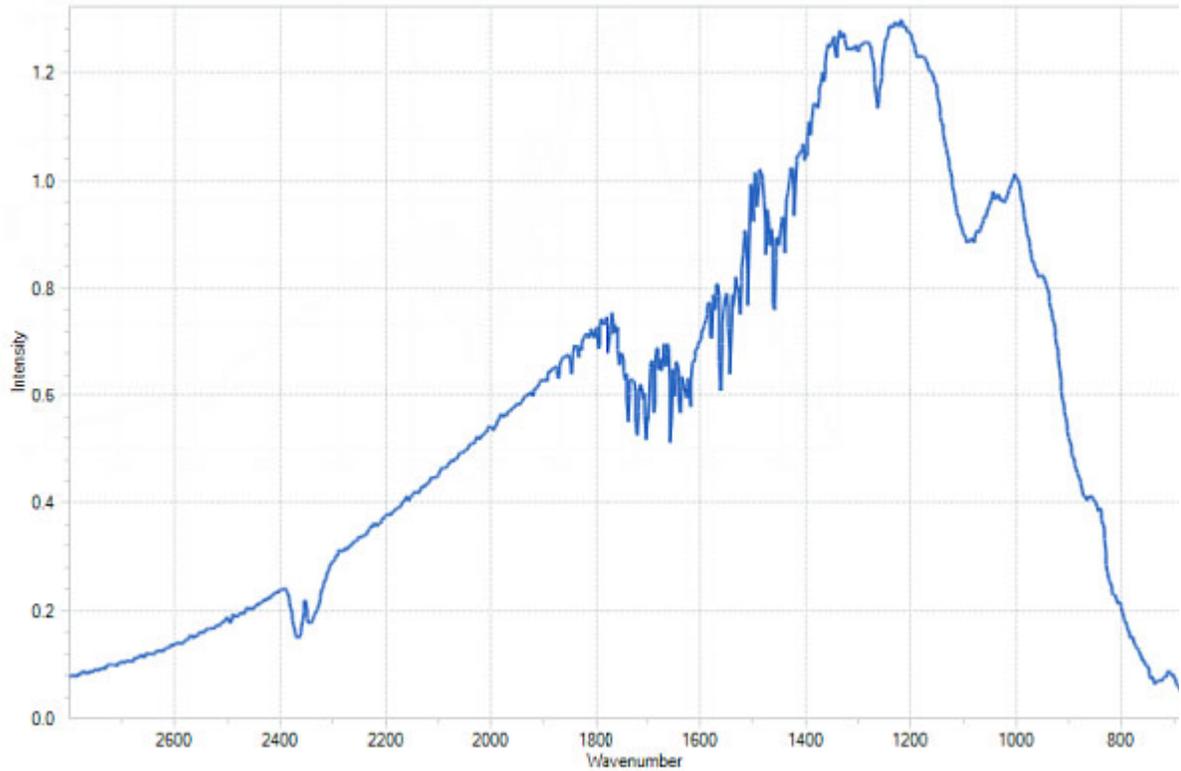


Figure 6-15 SiComp AgX FiberConduit probe (6.3mm)

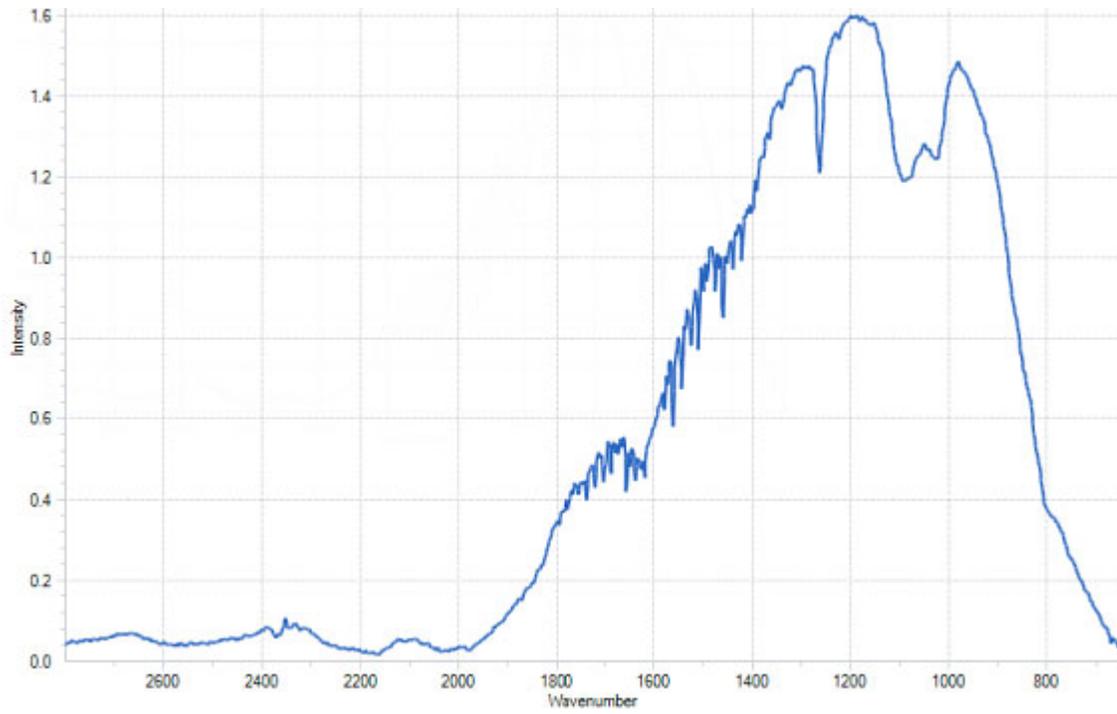


Figure 6-16 DiComp AgX FiberConduit probe (9.5mm)

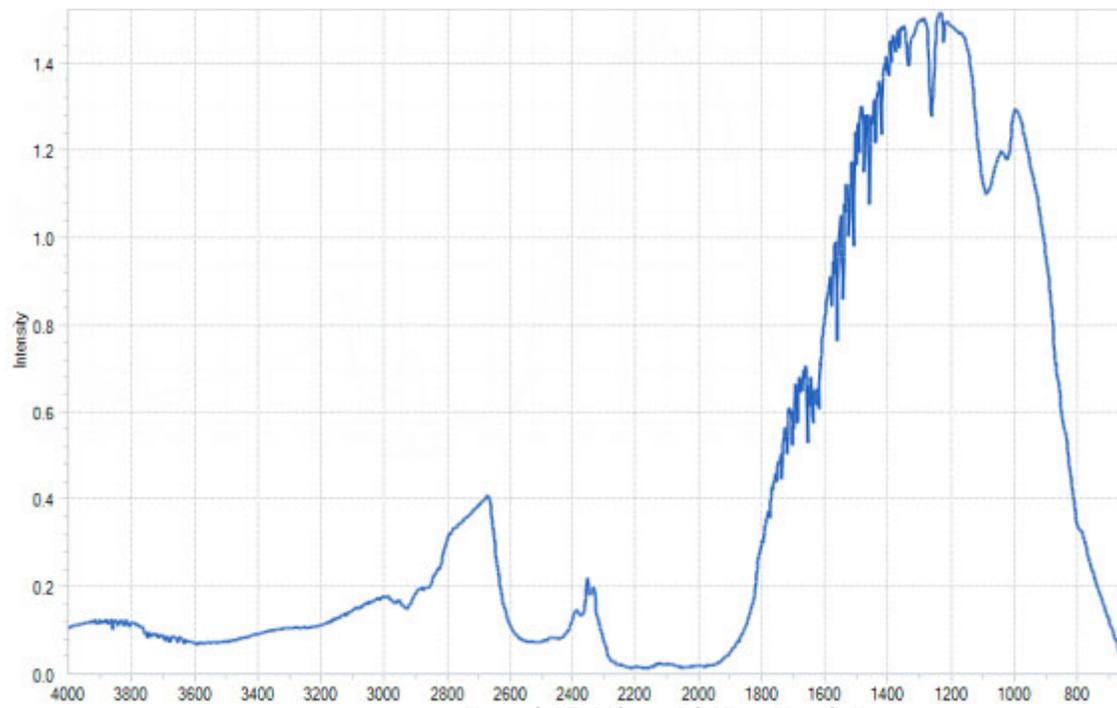


Figure 6-17 DiComp DS Micro Flow Cell

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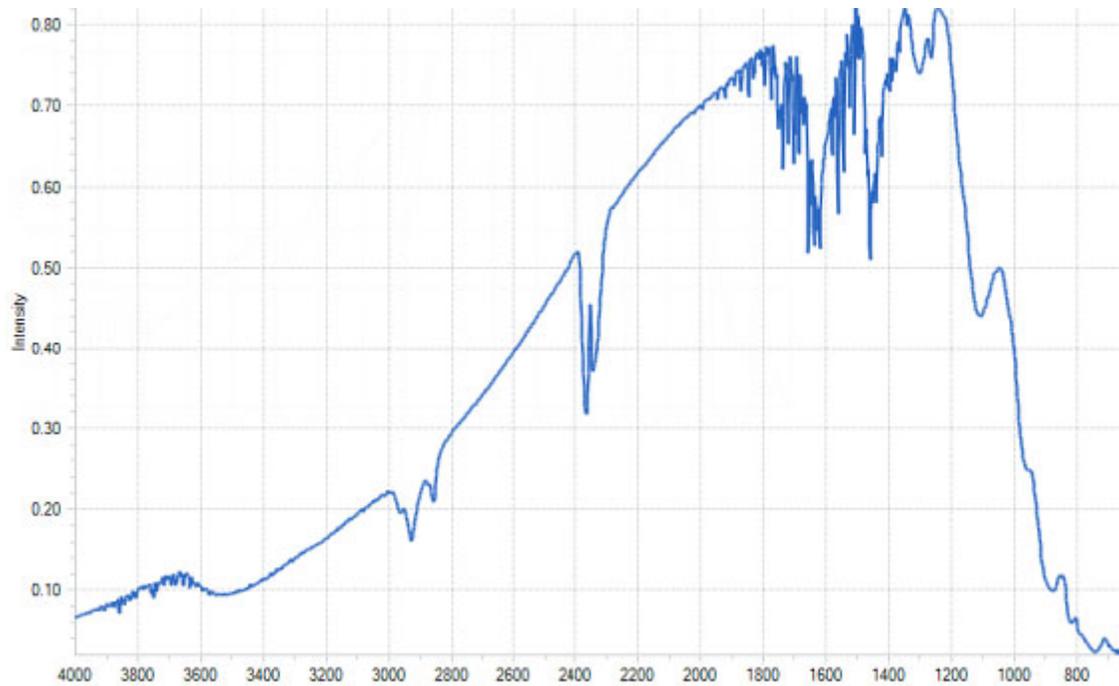


Figure 6-18 SiComp DS Micro Flow Cell

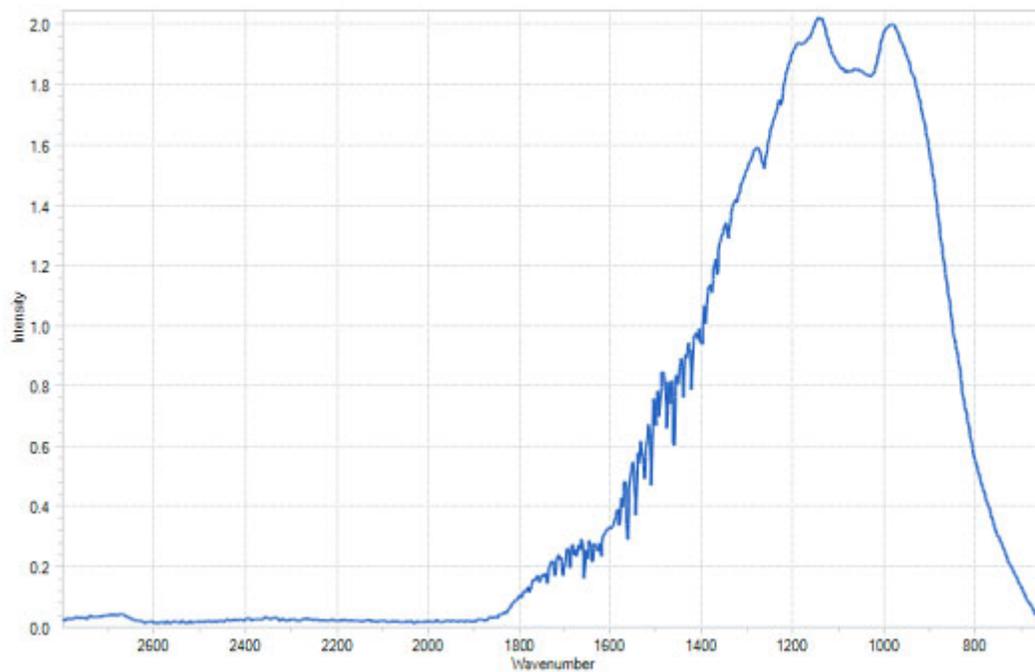


Figure 6-19 DiComp Fiber-to-Sentinel

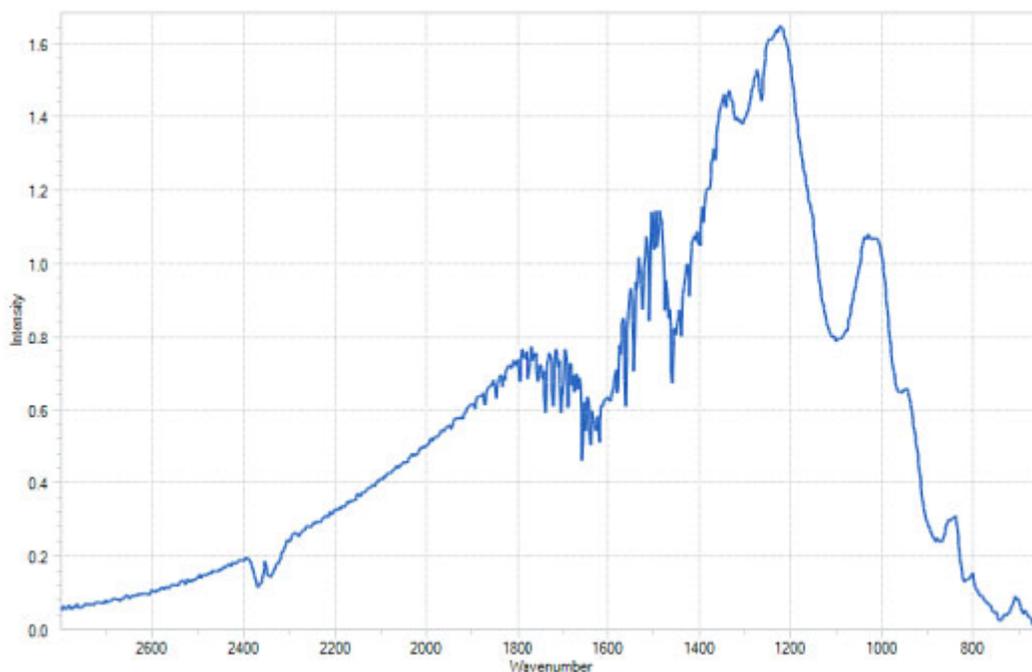


Figure 6-20 SiComp Fiber-to-Sentinel

- Record the action as complete in the Operational Qualification form.
Record the values for contrast and peak height in a log book, if performing a routine alignment after initial installation.

E. Clean the Sensor

The probe tip and DS Micro Flow Cell contain a diamond or silicon composite sensor that samples the reaction mixture to produce infrared fingerprints of the molecular composition. Cleaning the probe or DS Micro Flow Cell eliminates any chance of observing infrared fingerprints from a previous reaction or sample measurement, thus assuring an accurate representation of the reaction of interest. A simple process of cleaning the sensor, and checking cleanliness using an iC IR software assists to that end.

Note: Ensure the probe is not in contact with any chemicals (exposed only to air) before proceeding.

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Clean the probe or DS Micro Flow Cell from the previous experiment using the most appropriate solvent(s) to dissolve the reaction species. A final cleaning with reagent grade acetone is recommended. A virgin cotton swab on a wooden stick makes an ideal cleaning tool for the sensor tip in the case of probe cleaning.

Note: Q-tips and similar type swabs have lubricants and are not a great choice for a cleaning tool!

1. Clean the probe, as described above.
2. Click **Configure Instrument** on the iC IR Start Page
3. Proceed through the wizard by clicking **Next** until you reach the 'Collect Clean Reference Background.'
4. Click **Collect Background** to collect a reference background to prepare the wizard for a sensor cleanliness check and click **Next**.
5. Click **Finish**. This action skips the 'water vapor' collection and exits the wizard.
6. Click **New Experiment** on the iC IR Start Page.
7. Click **Next** and click **Next** again to reach the 'Reference Spectra Needed?' wizard window.
8. Select 'Collect reference spectra (recommended)' and click **Next**.
9. Click **Next** and click **Next** again to reach the 'Clean Probe' wizard window.

10. Observe the two colored bars that indicate if the sensor is clean or dirty.

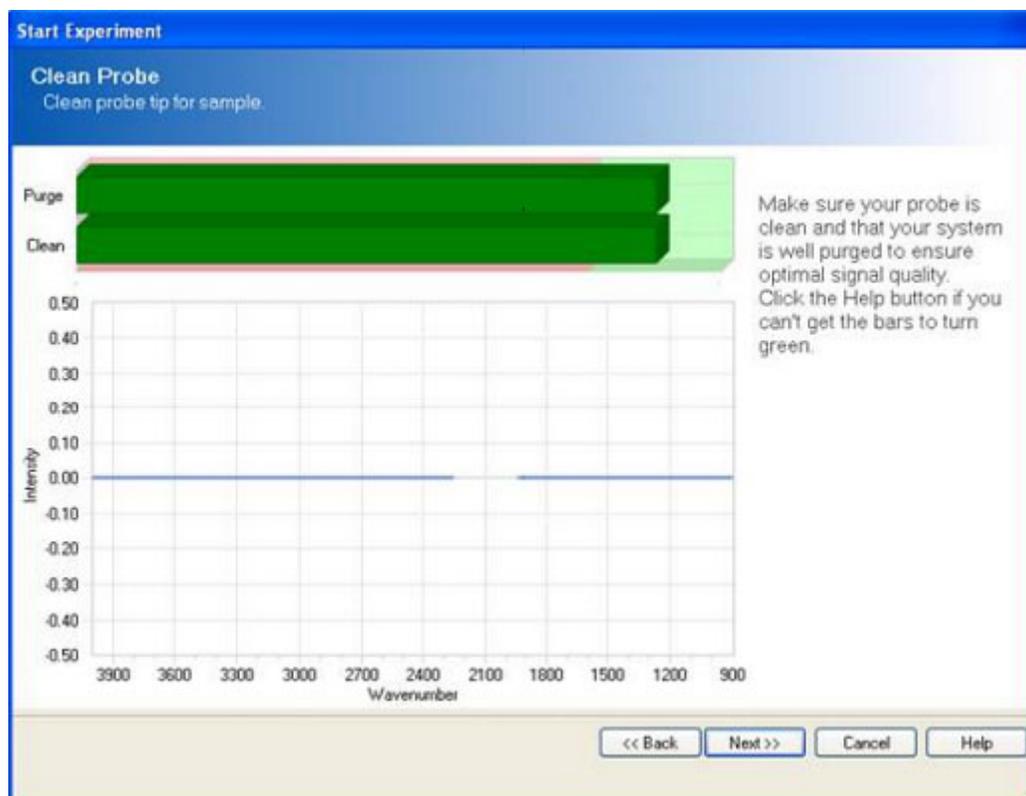


Figure 6-21 Collect Clean Reference Background in iC IR

- If the bars are green, the sensor is ready for monitoring chemistry.
- If the bars are red and in the red area of the purge and clean zone, the probe surface or DS Micro Flow Cell need further cleaning.

Note: The Intensity versus Wavenumber image will appear as a relatively flat line when the sensor is clean and the indicator bars are green.

11. If the clean sensor check indicates the probe is not ready, repeat the clean procedure and take another 'Background' until the bars turn green. At this point the sensor is ready for monitoring chemistry.
12. Click **Finish**.
13. Check off this action in the Operational Qualification form if performing an initial installation, or using the form to requalify the performance.

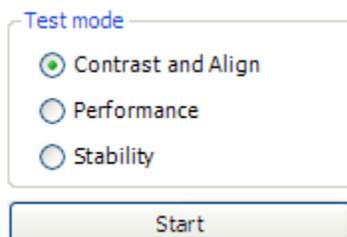
6 ■ Operation

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F. Record Final Align and Contrast

To complete the ReactIR 15 alignment in the Operational Qualification process, follow the instructions below to record a final peak height and contrast. These values serve as a reference point to attain as assurance of a fully functional product.

1. In the iC IR Toolbox, click on the **Test Instrument** task pane.
2. Verify that the appropriate instrument configuration settings appear for fiber, probe, and MCT detector.
3. Select **Contrast and Align** and click **Start**.



4. Record the Peak Height and Contrast values in the Operational Qualification form.

Note: These values should be maximized after performing all the preceding steps of alignment and configuration. If not, repeat any step that will maximize these values.

5. Perform Functional Testing

This section addresses the performance and stability of the ReactIR 15 base unit and sampling technology. Measurements are recorded in the Operational Qualification form where space is provided for up to two sampling technologies at time of purchase. Below is a list of standard sampling technology available for use with the ReactIR 15. In the IQ form, record the type of sampling technology used in the functional test.

Table 6-2 Sampling Technologies

Sampling Technology
DS AgX Fiber DiComp
DS AgX Fiber SiComp
DS Fiber-to-Sentinel DiComp
DS Fiber-to-Sentinel SiComp
DS Micro Flow Cell DiComp
DS Micro Flow Cell SiComp
DS Fiber-to-Gas Cell

A. Performance Test—Record Signal-to-Noise Ratio (SNR)

A good measure of ReactIR 15 performance is the Signal-to-Noise Ratio (SNR). This value represents a specific method of measurement at METTLER TOLEDO that historically defines performance according to the original design specification. Recording the value in the Operational Qualification form (printed from [page 80](#)) will define the reference point for verification of ReactIR 15 performance when executing the test at anytime in the future.

Note: The IPAC service includes pass/fail criteria for the SNR. Purchase the service product if your organization requires this criteria when qualifying the ReactIR 15.

Before proceeding, be sure the system has been properly configured and aligned.

1. In the iC IR Toolbox, click on the **Test Instrument** task pane. The performance test window will appear.
2. Enter **10** for the number of runs.
3. Set the Start/End region to the values that correspond to your sampling technology in [Table 6-3](#). For example, in the case of a DS AgX FiberConduit DiComp Probe, the start value is 1142 and the end value is 1042 cm^{-1} .

Note: The Start/ End region is defined by the type of sampling technology that is configured in the Configure Instrument wizard.

Table 6-3 Wavenumber Region by Sampling Technology

Sampling Technology	Wavenumber Region for SNR
DS AgX Fiber DiComp	1142–1042 cm^{-1}
DS AgX Fiber SiComp	1250–1150 cm^{-1}
DS Fiber-to-Sentinel DiComp	1142–1042 cm^{-1}
DS Fiber-to-Sentinel SiComp	2600–2500 cm^{-1}
DS Micro Flow Cell DiComp	1142–1042 cm^{-1}
DS Micro Flow Cell SiComp	2600–2500 cm^{-1}

4. Click **OK**.
The system will collect 10 background / sample pairs. The parameters used for collection are 1 minute scan time and 4 cm^{-1} resolution.

Note: A corrected root mean square calculation is performed on each sample spectrum over the selected wavenumber region. The SNR is then calculated from the inverse of the corrected RMS.

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5. Proceed to the ["B. Performance Test—Record Acetone Peak Height"](#) section for instructions on the performance wizard window that appears immediately after the SNR test completion. Recording the SNR values will occur at the end of the next section.

B. Performance Test—Record Acetone Peak Height

Another good measure of ReactIR 15 performance is the Acetone Peak Height. This value indicates sensor integrity in a probe or Micro Flow Cell by measuring the absorbance of neat acetone with your sampling technology. Recording the value in the Operational Qualification form will define the reference point for verification of ReactIR 15 performance when executing the test at anytime in the future.

Note: The Acetone Peak Height window will appear immediately following completion of the SNR test described starting on [page 53](#).

1. Enter **4** in the number field for the number of tests. This step instructs the system to collect four acetone spectra.
2. Ensure the sensor is clean and dry, and void of any potential contact with solvent or reaction mixture.
3. Select **OK** at the next message reminding you to have a clean, dry sensor (probe). The system will collect a background (16 scans at 4 cm⁻¹).
4. Dip the probe into a vessel, vial, or beaker that contains neat acetone, making sure the liquid completely covers the sensor surface. In the case of a DS Micro Flow Cell, flow neat acetone through the cell.

Note: Check the sensor surface for any air bubbles that can cause an inaccurate measurement of acetone peak height. To remove a bubble, gently sweep a swab or other small picking tool across the sensor surface.

5. Select **OK**. The system will collect the requested number of acetone spectra. The Acetone Peak Height is calculated automatically by the following equation:

$$\text{Absorbance}_{1092 \text{ cm}^{-1}} - \text{Absorbance}_{1018 \text{ cm}^{-1}} = \text{Acetone Peak Height}$$

6. Locate the SNR and Acetone Peak Height values in the 'PerfSNR<date><time>Results' tab on the iC IR Start Page.
7. Record the Average SNR and Average Acetone Peak Height in the Functional Testing section of the Operational Qualification form.

Note: For future reference, the software saves the results in a default "test data" folder on the computer or the location specified in Preferences (Tools > Preferences).

The default location is:

C:\Documents and Settings\[*username*]\My Documents\iC IR experiments,

C. Performance Test—Record Acetone-to-Noise Ratio (ANR)

Holistic measurement of ReactIR 15 performance comes from the Acetone-to-Noise Ratio through a calculation using Signal to Noise and Acetone Peak Height. Knowing the energy throughput of the system (Signal to Noise) and sensor path length (Acetone Peak Height), we can calculate a value that best represents the performance across all ReactIR 15 base units and applicable sampling technology. What the value actually gives you is assurance of chemistry monitoring that affords detection of reaction start, progress, and end-point. Infrared fingerprints (data) over time will yield absorbance trends of key reaction species (information) at concentrations possible with the ANR value. The higher the ANR, the lower the detection limit of the ReactIR 15. You can purchase a variety of sampling technologies for attaining an ANR that fits the concentration levels to monitor in your chemistry.

Recording the value in the Operational Qualification form will define the reference point for verification of ReactIR 15 performance when executing the test in the future.

1. Locate the SNR and Acetone Peak Height values in the 'PerfSNR<date><time>Results' tab on the iC IR Start Page.
2. Record the Average SNR and Average Peak Height.
ANR is an automatic calculation in the software using the following formula:

$$\text{(Acetone Peak Height)} \times \text{(Signal to Noise)} = \text{ANR}$$

3. Record ANR value in the Functional Testing section of the Operational Qualification form.

D. Stability Test—Record System Stability as a Function of Time

ReactIR stability is a measure of performance consistency over a period of time. Regular infrared measurements as a function of time, in the same manner as monitoring a reaction, reveal stability information through % Transmittance trends at specific wavenumber locations. This test uses the variation in the absorbance trends to measure ReactIR 15 stability.

1. Confirm the MCT dewar contains enough liquid nitrogen to complete this four-hour test. If necessary, completely fill the MCT dewar with liquid nitrogen and then wait for approximately 30 minutes before beginning the stability test.
2. Verify the probe is NOT in contact with any chemicals, only air.
3. Verify the probe is clean and dry.
4. In the iC IR Toolbox, click on the **Test Instrument** task pane. A window will appear prompting you to define the duration of the test and interval between data points.
5. Enter **240** in the Duration field and **60** in the Interval field. These parameters correspond to a 240-minute test that collects a spectrum every 60 seconds.
6. Click **OK** in the Stability window.
The stability test will start by collecting a background and then successive sample spectra over the 240-minute period. The software automatically measures and plots

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Operation Instructions

the %Transmittance value at the wavenumbers corresponding to the sampling technology.

7. Record the average %Transmittance values in the Operational Qualification form at the conclusion of the test. The values appear in the 'Stability Test Results' tab under the 'Summary Results.'

E. Calibrate Resistive Temperature Device (RTD)

Calibration of the Resistive Temperature Device (RTD) within the AgX FiberConduit Probes and DS Micro Flow Cells is a necessary step at installation to assure an accurate reading of the reaction temperature. ReactIR 15 hardware will read the RTD and relay the value to the iC IR software for trending with other chemical information.

-
- Notes:**
- Fiber-to-Sentinel and Fiber-to-Gas Cell sampling technology would not require this step.
 - The calibration process will require the use of an external calibrated temperature monitoring device such as a thermocouple, which serves as the reference of absolute temperature.
-

1. Verify that the hardware and software are properly communicating.
2. Open the **Configure Instrument** wizard.
3. Select RTD 1 and click **Calibrate** to launch the RTD calibration wizard.
4. Select the RTD1 row and highlight the RTD Device.
 - a. Select 'new' using the drop down arrow and create a new name for the RTD.
 - b. Click **Next**.
 - c. Select the two-point calibration and click **Next**.
5. Cool the AgX FiberConduit probe tip OR DS Micro Flow Cell, along with the calibrated temperature monitoring device, to as close to 0°C as possible.
6. Wait for the system to stabilize by observing a constant value at the calibrated temperature monitoring device.
7. Enter the actual value from the calibrated temperature monitoring device in the Reference Temperature section. Click **Next**.
8. Heat the AgX FiberConduit probe tip OR DS Micro Flow Cell, along with the calibrated temperature monitoring device, to as close to 100°C as possible.
9. Wait for the system to stabilize by observing a constant value at the calibrated temperature monitoring device.
10. Click **Save** to record the calibration.
11. Record the action as complete in the Operational Qualification form.

Implementation Readiness

At this point all items in the Operational Qualification form should be complete, including resolution of any non-conformances. A qualified METTLER TOLEDO Field Service Engineer will sign and date the Operational Qualification form to confirm completion of the process in due and proper manner. The customer who witnesses the process and is responsible for the ReactIR 15 within their organization will then sign and date the Operational Qualification form as confirmation of the Field Service Engineer execution. This record is copied by the Field Service Engineer for delivery to the customer while on site, and the original put on file in the Service Department of Mettler-Toledo AutoChem, Inc.

In the event that the ReactIR 15 is returning to service following storage, relocation, or lengthy downtime, you can follow the same process or call Mettler-Toledo AutoChem, Inc. service for assistance in performing the service at a nominal fee. Check your service contract, if purchased, for inclusion of this service.

ReactIR 15 is now ready for routine use with confidence the data and information accurately reflect changes in chemistry. Proceed to the next section to learn the steps to a successful ReactIR 15 experiment.

Simple Steps to a Successful Experiment

Getting the most out of your ReactIR 15 requires simple steps that lead to the monitoring of your chemistry. The data will then be of the highest quality for easy conversion to chemical information that you can use for better understanding of the reaction dynamics. All of the actions center around gaining maximum performance of the ReactIR 15 through the iC IR software tools. Once complete, you can be certain that the infrared fingerprints accurately reflect chemical changes pertinent to your chemistry.

Below are the steps:

["1. See An Overview of the Process" on page 57](#)

["2. Interface Sampling Technology with Your Chemistry" on page 58](#)

["3. Align the Probe" on page 60](#)

["4. Clean the Sensor" on page 61](#)

["5. Collect a Background" on page 64](#)

["6. Set the Data Collection Parameters" on page 67](#)

Refer to ["Best Practices" on page 68](#) for additional guidelines.

1. See An Overview of the Process

The following useful references are available to help you learn more on this subject:

"Experiment Setup in iC IR" (DCN - MK-PB-0013-AC)—Included in your product documentation portfolio available through iC IR Help > Show Documentation Portfolio. This

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Simple Steps to a Successful Experiment

is a Quick Reference guide that provides instructions on the basics of ReactIR 15 hardware and iC IR software for starting an experiment.

“iC IR Guided Tour”—A link to the tour is in the More Information section of the iC IR software Start Page. The tour is a video that provides a concise overview of the software with special attention to efficiently collecting data and converting it to information. To review a specific part of the tour, click the small ‘Jump to’ link above the tour window and select from the drop-down list.

▶ Jump to:

Figure 6-22 Guided Tour segment selection link

2. Interface Sampling Technology with Your Chemistry

Interfacing the sampling technology with your chemistry will lead to data and information about the reaction, thus meeting the purpose behind your purchase of the ReactIR 15. Start by placing the reaction vessel within reach of the probe end of the sampling technology or flow distance of the Micro Flow Cell.

DS FiberConduit Probe

A short procedure will establish the correct orientation of the probe tip in the reaction vessel before adding solvent and reagents. You will need an adaptor to assure a secure fit of the probe in one of the vessel ports. Check with your Technical Applications Consultant (TAC) to make sure you have the appropriate adaptor for your specific vessel.

1. Once you have the right adapter, simply insert the probe through the adaptor and secure with the plastic compression fitting. This step can be done prior to or after inserting the adaptor into the reaction vessel.



Figure 6-23 DS FiberConduit with adapter in common reaction vessels

- Adjust the insertion depth of the probe into the vessel to assure complete coverage of the tip throughout the experiment. The vessel contents should be empty at this point to collect an 'air background'

DS Micro Flow Cell

Monitoring reaction chemistry requires injection of solvent and reagents or flow of the liquid solution into the DS Micro Flow Cell. Establish connections to the cell using the specified Omnifit-style fittings (not provided). Mate the opposite end to the reaction chemistry to allow continuous flow. Alternately, create a shorter length of tubing to afford easy injection of solvent and reagents.

For additional instructions on the subject please read the Quick Reference Guide: "Connecting a DS Micro Flow Cell" that ships with the DS Micro Flow Cell product and is included in the ReactIR and iC IR documentation portfolio.

Note: Be sure to collect an 'air background' before introducing liquid reaction chemistry into the DS Micro Flow Cell.

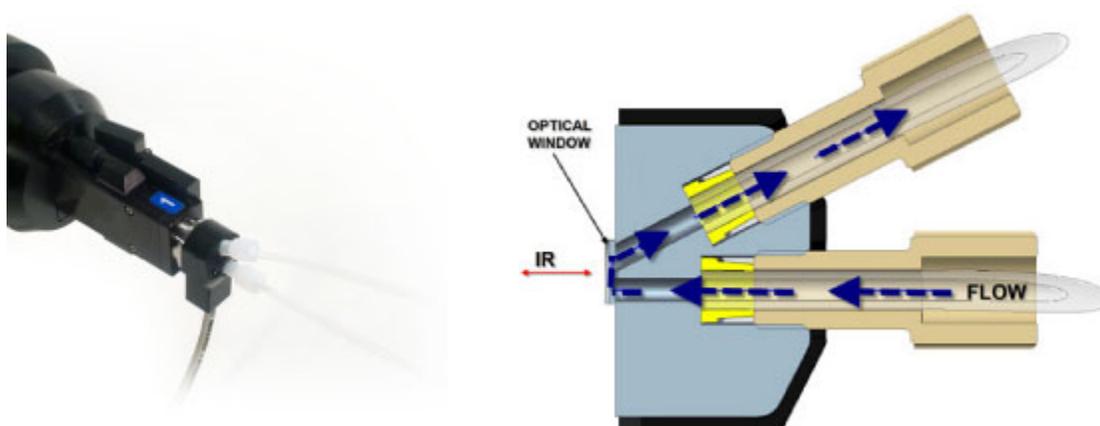


Figure 6-24 DS Micro Flow Cell (heated) and Omnifit-style fittings

DS Fiber-to-Sentinel

Reaction vessels (large volume flow cells, high pressure autoclaves) with a proprietary connection design are necessary to insert and secure a Sentinel probe in contact with liquid chemistry. Each Sentinel comes with the hardware and liquid seal to safely secure the connection. Check with your Technical Applications Consultant (TAC) to make sure you have the appropriate vessel and fitting to safely secure the connection.

Note: Be sure to collect an 'air background' before introducing liquid reaction chemistry into the DS Fiber-to-Sentinel.

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Simple Steps to a Successful Experiment

DS Fiber-to-Gas Cell

Monitoring reaction gases requires connection to the Gas Cell through 1/8" input and output ports. You supply the gas sample and hardware to adjust flow and pressure.

Note: Be sure to collect an 'air background' before introducing gas samples into the Gas Cell.

3. Align the Probe

We recommend checking alignment before each experiment using a simple software wizard. The purpose is to assure the energy of the system (source) properly travels from the origin to the sample and then to the detector. By aligning maximum energy through this optical pathway, the ReactIR 15 will yield an infrared fingerprint characteristic of the chemistry in contact with the sampling technology (sensor).

A successful Operational Qualification sets the stage for routine use of the Align Probe wizard prior to an experiment. Use the following steps to access and implement the wizard.

1. Click **Configure Instrument** on the iC IR Start Page.
2. If necessary, configure the instrument per the instructions in [“3. Configure Instrument in Software”](#) on page 42.
3. Proceed through the wizard by clicking **Next** until you reach the 'Align Probe' window.

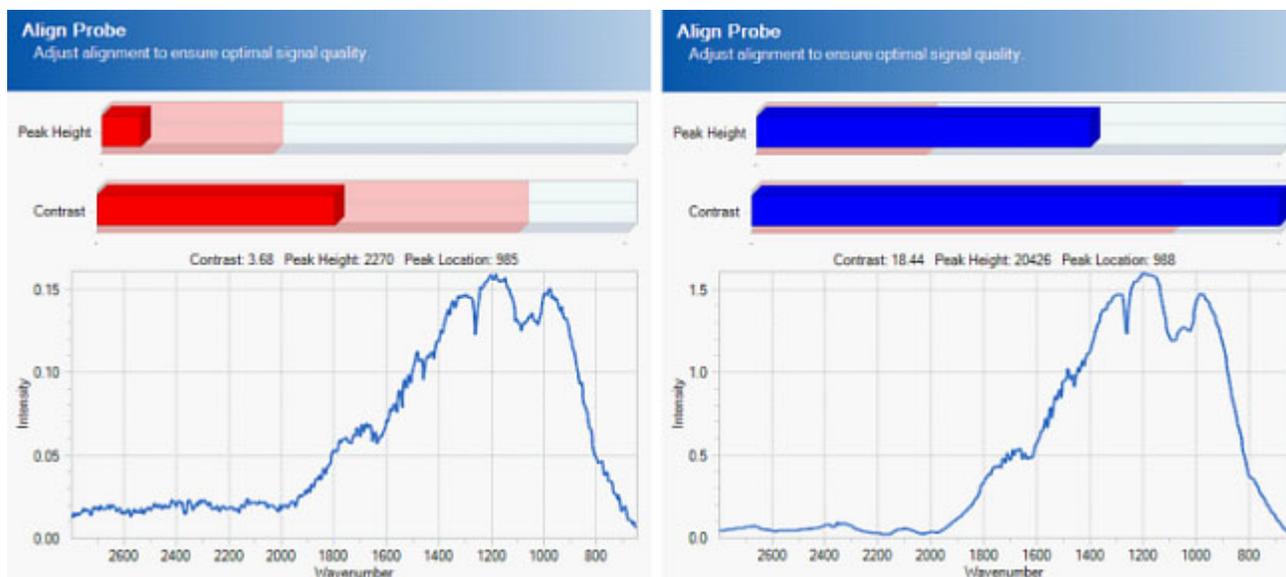


Figure 6-25 Align Probe wizard—From red to blue bars

4. Check the Peak Height and Contrast bars at the top of the Align Probe window.
 - If the indicator bars are both Blue, then alignment is OK.

- If the indicator bars are Red, exit and return to the alignment procedures starting under [“4. Align the System” on page 43](#) to adjust the following:
 - DS Fiber-to-Sentinel**—This step is not necessary for DS FiberConduit Probe, Micro Flow Cell, or Fiber-to-Gas Cell.
 - Detector Preamp**—Refer to adjustment steps on [page 44](#).

Note: Only use the instructions that relate to hardware adjustments, not the software steps to view peak height and contrast. The Align Probe wizard will react to any adjustments to the hardware.

5. If the indicator bars are still Red after sampling technology and/or detector preamp adjustment, exit the wizard to adjust the fixed mirror per the instructions under [“D. Fixed Mirror Alignment” on page 45](#).

4. Clean the Sensor

Cleaning the probe or DS Micro Flow Cell is recommended after each experiment. This action eliminates any chance of observing infrared fingerprints from a previous reaction or sample measurement, thus assuring an accurate representation of the reaction of interest. Follow the instructions under [“4. Clean the Sensor” on page 61](#) to properly clean either type of sampling technology.

Although you will clean the 'wetted' surfaces of the probe or DS Micro Flow Cell, the most important part is the sensor (DiComp or SiComp in most cases) since it is the true sampling surface when measuring reaction chemistry. The sensor is at the tip of a probe and inside the cavity volume of a DS Micro Flow Cell. Both sampling technology types are accessible for liquid and physical cleaning.

The iC IR 'Clean Probe' wizard dramatically speeds the cleaning process. Once in the wizard, you can quickly determine whether cleaning is necessary, as well as observe the impact of the clean method. The following images show possible types of 'dirty' sensors and the desirable end result.

Peaks pointing in the positive direction indicate one of two situations.

- **Sensor has materials present on the surface** relative to the last background measurement, likely taken immediately after cleaning the sensor. This is a common occurrence if the probe has not been cleaned following an experiment. Enough residual reaction mixture is on the sensor to yield an infrared fingerprint. If you do not clean before the next experiment the residue can cause inaccurate measurement of reaction component trends.
- **Residual cleaning solvent is present on the sensor surface.** Wait for the solvent to dry, assuming no residue will result, or wipe with a clean kimwipe. If a residue persists, choose another solvent for a final rinse.

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Simple Steps to a Successful Experiment

Dirty Sensor Examples

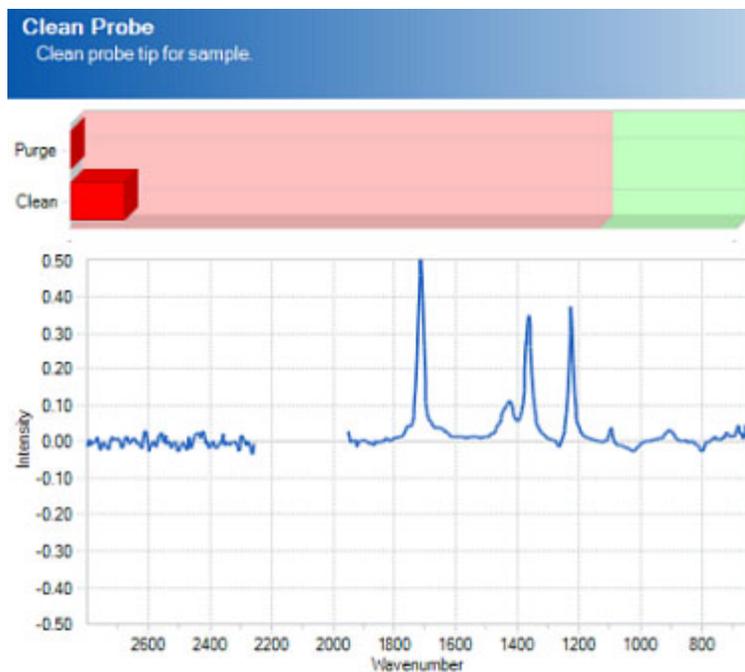


Figure 6-26 'Dirty' sensor—Prior reaction mixture or insufficient drying time of cleaning solvent



Figure 6-27 'Dirty' sensor—Poor cleaning method and subsequent collection of new background

Peaks pointing in the negative direction are a result of cleaning a residue off the sensor relative to the last background measurement. For example, not cleaning the residue from the a previous experiment (as above) and collecting a new air background will essentially include the residue in the background spectrum. When you finally clean the sensor, the negative peaks will appear since the residue is no longer present on the sensor relative to the original background spectrum.

When the sensor is 'dirty,' repeat the following steps until you see green indicator bars and a flat spectral line:

1. Clean the sensor free of any visible residue.
2. Check sensor cleanliness using 'Clean Probe' wizard.



Figure 6-28 'Clean' sensor—Green indicator bars and flat spectral line

- If positive peaks are present, repeat the cleaning process until green indicator bars appear and a flat spectral line is present, proceed through the wizard.
- If negative peaks are present:
 - a. Collect a new background by clicking **Back** in the New Experiment wizard until you reach the 'Name Experiment File' page.
 - b. Click **Configure Instrument**.
 - c. Click **Next** to reach the 'Collect Clean Reference' page.
 - d. Click **Collect Background** to apply the new background to the 'Clean Sensor' wizard.

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Simple Steps to a Successful Experiment

- e. Click **Next** and then **Finish** to return to New Experiment wizard.
- f. Proceed to 'Clean Probe' page.
- g. If negative peaks persist then repeat the process or change cleaning solvent until green indicator bars appear and a flat spectral line is present.

5. Collect a Background

The collection of an air background prior to each experiment is the single-most important step in getting high quality infrared data out of a fully functional ReactIR 15. Every sample measurement following this step will use the background to 'ratio out' all infrared absorbing materials in the optical path and the source intensity profile. The end result is an infrared fingerprint of absorbance versus wavenumber of only the reaction mixture components. A flat baseline will appear at whatever wavenumbers are non-absorbing by the chemistry.

For example, water vapor will always be present in the ReactIR 15 at a very small and constant concentration, and the air background will show the characteristic fingerprint. Subsequent collection of air samples will also contain the water vapor in the raw single beam (intensity versus wavenumber). However, subsequent ratio of sample to background single beam eliminates the water vapor to produce a flat zero absorbance in air. Note in [Figure 6-29](#) that all other absorbing features (sensor, AgX, source energy profile) also ratio out of the sample spectrum. This processing is a routine step in an infrared spectroscopy measurement that the software performs automatically.

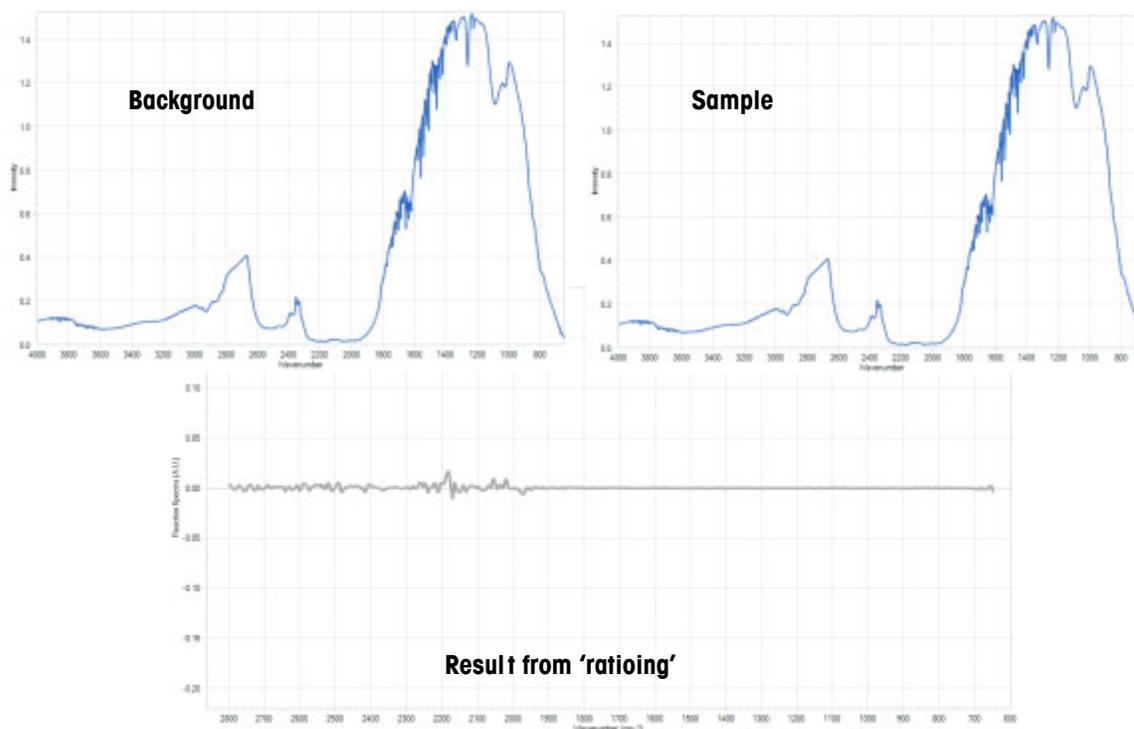


Figure 6-29 Water Vapor in background and sample (plus the result of 'ratioing')

Results from Infrequent Background Collection

Infrequent collection of air backgrounds will produce infrared fingerprints that lack the peak definition to properly trend reaction components. You can identify these cases by observing the shape of the infrared fingerprints, specifically in the baseline.

The following images show common examples of baseline 'wag,' negative peaks, and abnormal peaks:

Figure 6-30 shows baseline 'wag' due to change in optical alignment or no collection of air background from experiment to experiment. This normally occurs when you start a new experiment without collecting a new background

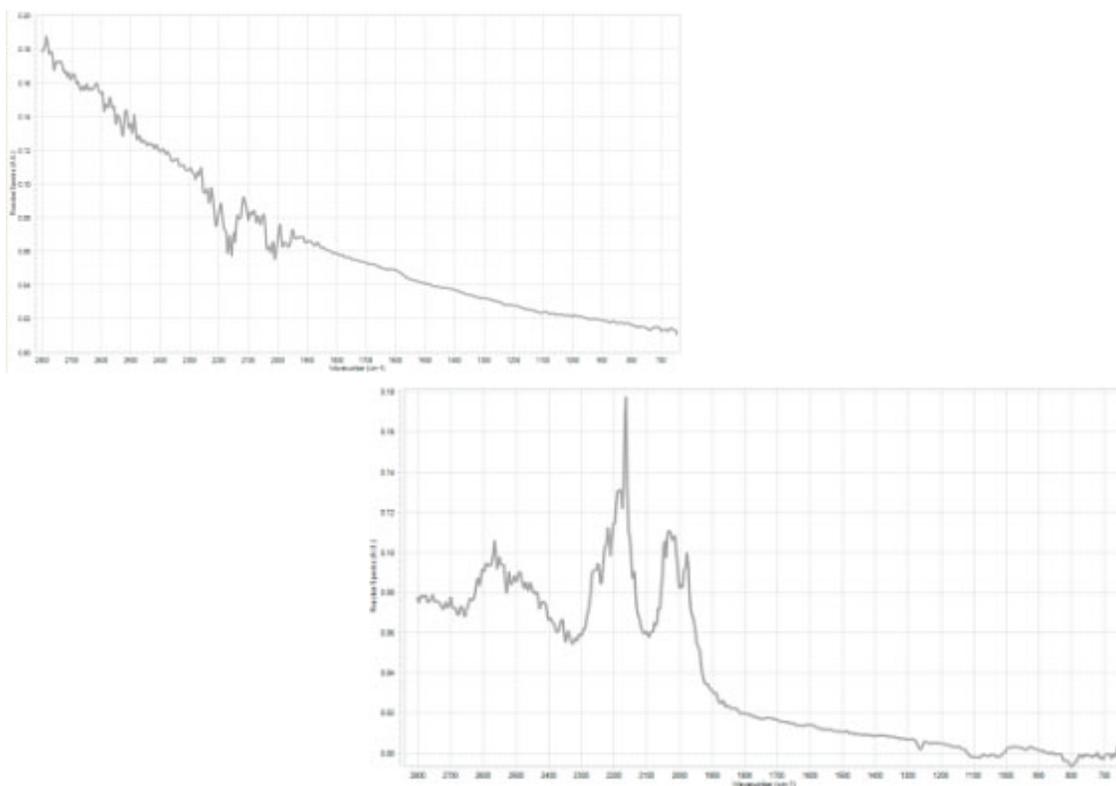


Figure 6-30 Baseline 'wag'

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Simple Steps to a Successful Experiment

Below is an example of negative peaks that result from an unclean sensor.

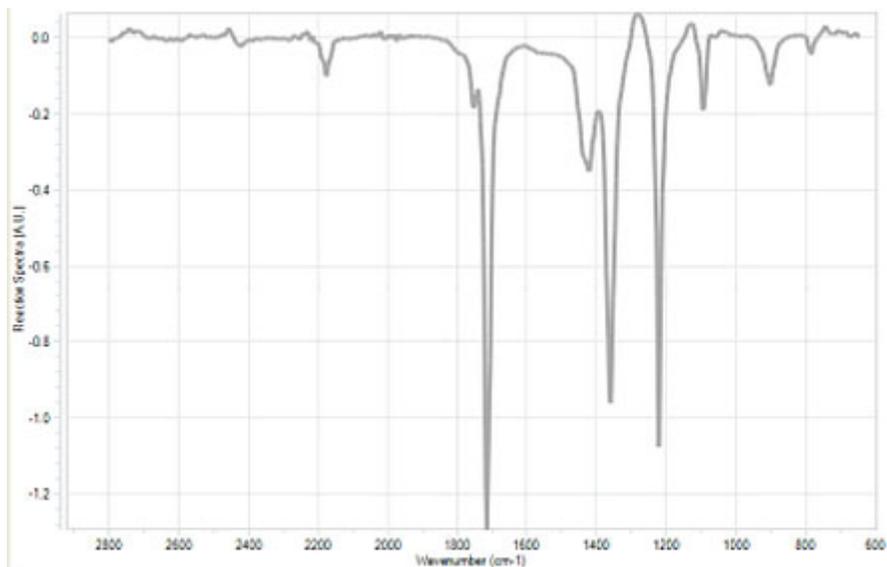


Figure 6-31 Negative peaks due to unclean sensor

The following example shows abnormal peaks due to a change in the type of sensor (DiComp to SiComp) without collecting a new air background:



Figure 6-32 Abnormal peaks from changed sensor without new background

Background Collection Procedure

1. Collect a new background prior to each experiment by clicking the **Collect Background** button in the New Experiment wizard. The button is located on the Collect Background wizard window.

- When the background spectrum turns green, the background sample collection is complete.

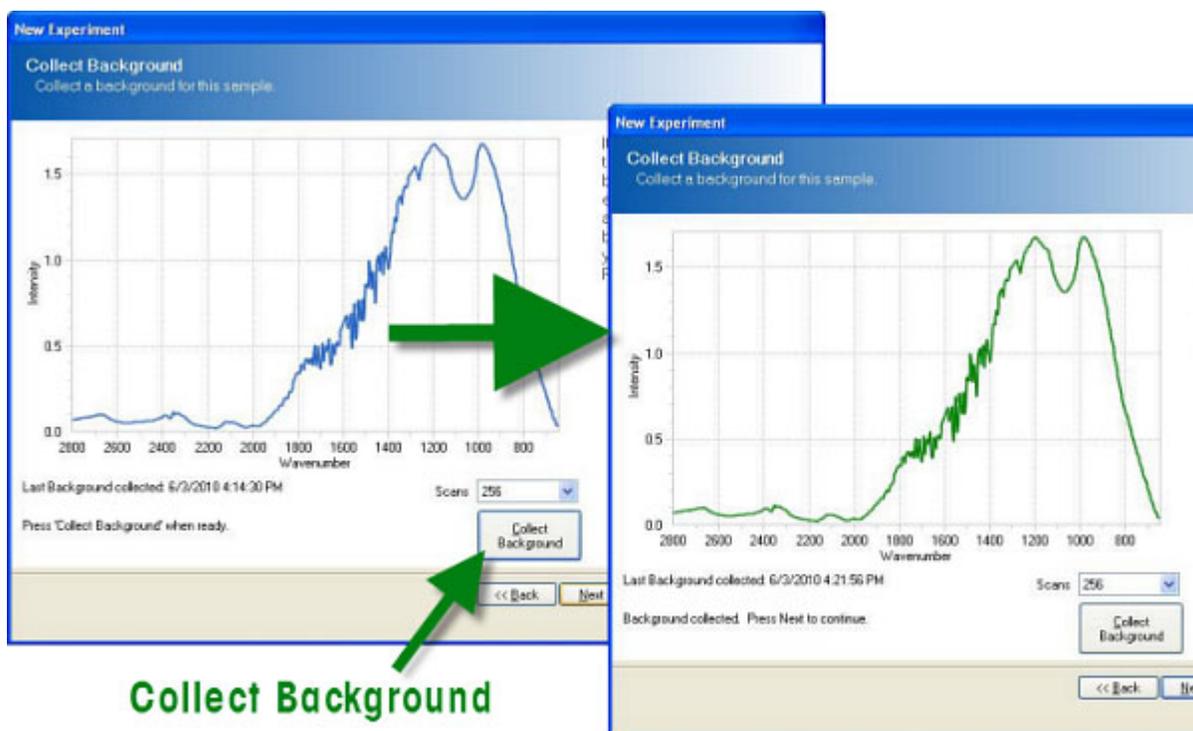


Figure 6-33 Reference background

6. Set the Data Collection Parameters

There are a number of data collection parameters worthy of user intervention and understanding to potentially maximize infrared measurement sensitivity and chemical trend information. Keep in mind that iC IR establishes default parameters that account for the most common applications to speed the experiment collection workflow, but you can choose to adjust the settings. Here are the more common parameters and how they impact the infrared measurements during an experiment. The software prompts you for these parameters in New Experiment process.

Scans/Sample

The number of scans per sample is an automatic setting depending on your choice of Interval and Resolution. Users can alter the parameter to a maximum allowable setting to gain the best contrast of infrared fingerprints, which leads to the best possible identification of peaks to trend reaction components.

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Best Practices

Phases

Add and edit phases for the experiment. Define each phase with a specific duration and measurement interval. Phases enable you to vary the sampling interval at different times throughout the experiment. Phases will execute in sequence.

Collection Interval

You may choose to shorten or lengthen the collection interval to match the chemistry kinetics. Use a short interval during active portions of the experiment to capture fast changes. With this feature, you can monitor long experiments while keeping file sizes small.

Experiment Duration

Choose the total time for the experiment or each phase with this parameter. We recommend extending the total time for the experiment beyond normal expectations during the investigation of new chemistry to gain maximum information. Data is cheap!

Best Practices

- **Identify Correct Sampling Technology**—Make sure concentration of the species of interest is within the detection limits of the ReactIR 15 system and sampling technology with your system. A good rule of thumb for a ReactIR 15 and standard sampling technology is a detection limit of 0.1wt% for a moderate infrared absorber.
- **Measure Pure Reaction Components**—Whenever possible, measure the infrared fingerprints of pure reagents and products. This action speeds the identification of specific peaks in the reaction mixture that allow accurate trending of a particular component over time. An alternate approach is to add reagents one-at-a-time (see below).
- **Check Sensor Coverage**—After adding the solvent, make sure no bubbles appear on the sensor, especially in aqueous systems. Otherwise the detection limit will be higher than expected due to incomplete coverage of the sensor. Remove the bubbles with a sweeping motion across the sensor using a spatula or wooden end of a cotton swab. Rapid stirring can sometimes remove the bubbles as well.
- **Check Probe Immersion**—The probe must remain in the reaction mixture at all times to properly measure infrared fingerprints. Check for immersion before starting the experiment, and include stirring if applicable.
- **Begin Experiment with Solvent Only**—After collecting an air background, add the solvent only and begin the measurement of infrared fingerprints. Wait for several measurements before adding reagents to get a clear identification of fingerprints for solvent and distinguishable peaks for reagents.

- **Add Annotations**—Label the beginning and end of additions, results from grab samples, modifications in reaction parameters, and observations regarding the physical changes in the reaction mixture. Any one or all of these events help explain the infrared fingerprint changes for a better understanding of the chemistry.
- **Add Reagents One-at-a-Time**—The addition of reaction components should occur in sequence whenever possible. Collect at least four spectra between each addition to clearly identify infrared fingerprint features specific to the component that will later help define peak trends.
- **Correlate Offline Analysis**—ReactIR 15 produces infrared fingerprints that show component absorbance, which is proportional to concentration. This fact offers correlation to offline analysis of grab samples to create concentration trends for component peaks that are isolated. Full quantitative analysis is also an option for overlapping peaks with the use of iC Quant, a methods development software tool.

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Best Practices

Care and Maintenance

The ReactIR 15 system care and maintenance chapter includes the following sections:

["Service Contracts" on page 71](#)

["Maintaining the ReactIR 15 System" on page 71](#)

["Replacing the Desiccator" on page 72](#)

["ReactIR 15 Relocation, Packaging, and Storage" on page 74](#)

Service Contracts

METTLER TOLEDO offers service contracts for your ReactIR 15 product to assist you with maintaining maximum functionality and performance. Contact your Mettler-Toledo AutoChem, Inc. representative anytime to discuss the details using the METTLER TOLEDO part number below for the one- or two-year service agreement.

14690082—One (1) year service agreement

14690083—Two (2) year service agreement

Maintaining the ReactIR 15 System

Follow the cleaning instructions below for ReactIR 15 base units.

- Ensure the unit is powered off before doing any cleaning.
- Clean all exterior surfaces only with water and mild detergent.
- Do not use any alcohols, acids, bases or any flammable material to clean any part of the system.
- Be careful not to submerge any parts of the system with washing liquid.
- Be certain to dry all surfaces of the system after washing to avoid pooling of any liquid.
- Leave system powered off for at least 30 minutes after washing to avoid accidental short circuit of the electronics.

The customer assumes responsibility for maintaining a logbook to record and monitor the operation and performance of the ReactIR 15. Reproduce the checklist forms in [Appendix A on page 77](#) as needed.

7 ■ Care and Maintenance

Replacing the Desiccator

Customer-Replaceable Parts

Table 7-5 contains all the available customer-replaceable parts. Should you need to replace the desiccator, please read the instructions that follow. Contact METTLER TOLEDO to order any of these items.

Table 7-4 Customer-Replaceable Parts

Item	Part Number	Part
1	14104084	Desiccator
2	14170398	AC Power Cord
3	14170394	External USB Cable

Replacement Parts

Table 7-5 contains all replaceable parts with the normal replacement period. METTLER TOLEDO qualified Field Service Engineers should replace these items. This information is useful for planning potential cost of ownership.

Table 7-5 Parts replacement schedule

Item	Part Number	Part	Lifetime
1	14147003	IR Source	2-3 years
2	14166487	MCT Detector	1-2 years
3	14800000	MCT Preamplifier	2-3 years
4	14147012	Laser Diode	2-3 years
5	14147004	ICBM Board	> 5 years
6	14170412	Midget Modulator	> 5 years
7	14120145	Power Supply—ReactIR 15	> 5 years

Replacing the Desiccator

Periodic checking of the desiccant status is necessary to assure a dry optical environment inside the base unit. Otherwise the infrared data begins to show an increase of water vapor that can conflict with important chemical species you track during reactions. Some water vapor will always exist but as long as the amount is consistent per the capacity of the desiccant then the standard process of ratioing a sample measurement to the background reference will remove this component from the infrared data.

The desiccant cartridge is on the lower right side of the ReactIR 15 rear panel. Observe the color of the center portion of the cartridge to identify whether replacement is necessary.

- Blue is OK.
- Pink means replace the cartridge.

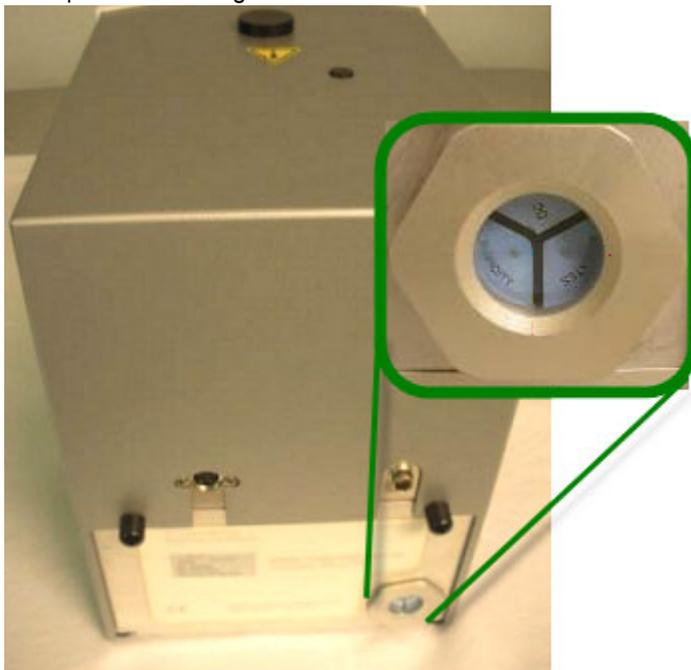


Figure 7-34 Desiccant location and status check (Blue is OK)

Follow these steps to replace the cartridge.

1. Turn the cartridge counter-clockwise until loose from the base unit.
2. Remove the cartridge from the base unit.



Figure 7-35 Desiccant cartridge removed

7 ■ Care and Maintenance

ReactIR 15 Relocation, Packaging, and Storage

3. Insert the new cartridge into the base unit.
4. Tighten the cartridge by turning clockwise. Finger tight is sufficient to compress the o-ring and secure the cartridge in place.

ReactIR 15 Relocation, Packaging, and Storage

To prevent and minimize damage to the ReactIR 15, follow the instructions below to prepare the base unit and sampling technology for relocation, shipment, or storage.

Shutdown

1. Close the iC IR software application and shutdown the computer according to normal operating procedures.
2. Disconnect the power cord and USB communications cable from the rear panel of the base unit as well as from the wall socket and computer. Store with the base unit.
3. Check the desiccator condition to assure an active state (blue color). This is particularly important in a humid environment or for long-term storage.
4. Secure the MCT dewar cap with tape to avoid falling out of the base unit.
5. Remove the sampling technology from the front of the unit and store it with the base unit in the factory-supplied box.
6. Transport for relocation or storage taking precautions similar to any electronic device to avoid damage to the base unit and sampling technology.
7. For long-term storage, choose a secure, cool, dry location.

Reinstalling the ReactIR 15

Follow the "[Installation Instructions](#)" beginning on [page 27](#).

Troubleshooting

This section highlights the most common troubleshooting issues for the ReactIR 15 system.

Table 8-1 Troubleshooting

Problem	Cause	Solution
Power LED light is OFF	■ Power cable disconnected	■ Connect power cable.
	■ Power cable faulty	■ Contact METTLER TOLEDO
Scan LED light is OFF	■ USB cable disconnected from base unit or computer	■ Connect USB cable.
	■ USB cable faulty	■ Contact METTLER TOLEDO
iC IR not communicating with base unit	■ USB cable disconnected	■ Connect USB cable
	■ USB cable faulty	■ Contact METTLER TOLEDO
MCT OK LED light is OFF	■ MCT is warmer than liquid nitrogen temperature	■ Fill MCT dewar with liquid nitrogen
	■ MCT dewar is faulty	■ Contact METTLER TOLEDO
MCT OK LED light is OFF in less than 21 hours after complete fill of dewar with liquid nitrogen.	■ MCT dewar is faulty	■ Contact METTLER TOLEDO
Align bars are RED	■ Using an 'old' background	■ Clean probe tip and take a new background
Negative peaks present in infrared data	■ Unclean sensor surface	■ Clean probe tip and take a new background
User manipulation of 3D Surface Viewer in iC IR is slow to respond	■ Video graphics card driver insufficient to support action	■ Verify graphics card meets System Requirements shown in "iC IR Installation Guide."
		■ Set Surface Viewer Preference to "Use alternate rendering" in iC IR Tools >

Refer to "Best Practices" on page 68 for useful tips.

IQ/OQ Checklists

This appendix includes checklist forms for use during installation and operation. Installation instructions begin on [page 27](#) and operation instructions begin on [page 40](#).

Installation and Operation

Use the following forms to check the installation and operation of the ReactIR 15 system in a non-regulatory environment:

- [“ReactIR 15 Installation Qualification \(IQ\)” on page 79](#)
- [“ReactIR 15 Operational Qualification \(OQ\)” on page 80](#)

Copy the checklist forms as often as needed, such as if you move the system or want to perform operational tests. The two forms are designed to print back-to-back on a single sheet.

Note: Retain the completed forms in a readily accessible location for reference during system service or maintenance.

ReactIR 15™ Installation Qualification (IQ / Non-regulatory)



Company:	Order Number:
Department:	Contact:
Address:	
Phone:	Email:

ReactIR 15 Serial No: _____

SITE REQUIREMENTS

Power: 100-240VAC +/- 7%, 50/60Hz, 1.2A dedicated circuit. Rated DC input: 12-13.6 VDC, 6A _____	Environmental Temperature: 19 to 25°C, <60% Relative Humidity _____
DS Fiber-to-Sentinel sampling technology Purge: Instrument grade air, nitrogen or equivalent gas, 10psi (0.7bar), 10.0scfh (4.7L/min), < 1ppm water vapor at -100°F (-73.3°C), < 0.1ppm carbon dioxide _____	
Space Requirement: 180 x 249 x 274 mm (W x H x D) _____	

HARDWARE CONFIGURATION / ORDER VALIDATION

Sampling Technology:	AgX FiberConduit Probe: Probe Diameter _____ Probe Length _____ Fiber Length _____ Sensor Type _____
	DS Micro Flow Cell: Volume _____ Sensor Type _____ Temperature Controller (Y/N) _____
	Other: _____
	Wetted Materials: _____ Pressure/Temperature Rating: _____
Hardware and Software:	<input type="checkbox"/> ReactIR 15 Base Unit <input type="checkbox"/> Computer and Accessories <input type="checkbox"/> iC IR Software CD <input type="checkbox"/> USB Cable <input type="checkbox"/> Funnel
	<input type="checkbox"/> Power Supply <input type="checkbox"/> Country-Specific AC Power Cord <input type="checkbox"/> Desiccator Cartridge (spare)
Optional Software:	<input type="checkbox"/> iC Quant <input type="checkbox"/> iC ConcIRT Pro <input type="checkbox"/> iC Kinetics
Documentation:	<input type="checkbox"/> Certificate of Conformity for Sampling Technology <input type="checkbox"/> Declaration of Conformance for ReactIR 15 <input type="checkbox"/> Product Documentation CD <input type="checkbox"/> Engineering Training Certificate

SOFTWARE CONFIGURATION AND SERVICE AGREEMENT

Software Configuration:	iC IR Version: _____	Service Agreement:	ReactIR 15 Coverage: _____	Expiration Date: ____/____/____
	_____		Sensor Coverage: _____	Expiration Date: ____/____/____

SYSTEM CONNECTIONS

<input type="checkbox"/> ReactIR 15 base unit in hood or benchtop	<input type="checkbox"/> Shipping restraint from MCT fill port removed
<input type="checkbox"/> Computer located in a suitable work location	<input type="checkbox"/> Sampling technology connected to ReactIR 15
<input type="checkbox"/> USB communications connected to base unit and computer	<input type="checkbox"/> Purge line connected to sampling technology (if applicable)
<input type="checkbox"/> Power connected at base unit and computer	<input type="checkbox"/> iC IR installed

SYSTEM STARTUP

<input type="checkbox"/> Power at base unit and computer is ON	<input type="checkbox"/> Detector LED lights
<input type="checkbox"/> Power LED lights	<input type="checkbox"/> iC IR launches
<input type="checkbox"/> Scan LED flashes	<input type="checkbox"/> Software Add-ONs installed and successfully launch (optional)
<input type="checkbox"/> MCT dewar filled with liquid nitrogen	

Non-conformances (include action to resolve):

Mettler-Toledo AutoChem, Inc. Field Service Engineer: Completed in due and proper manner	Responsible ReactIR 15 User: Copy of this check record received
Name: _____	Name: _____
Date: ____/____/____ Signature: _____	Date: ____/____/____ Signature: _____

ReactIR 15™ Operational Qualification (OQ / Non-regulatory)



Company:	Order Number:
Department:	Contact:
Address:	
Phone:	Email:

ReactIR 15 Serial No: _____

SYSTEM READINESS

<input type="checkbox"/> System ON for more than four (4) hours	<input type="checkbox"/> MCT dewar filled with liquid nitrogen	<input type="checkbox"/> iC IR software launched
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SYSTEM CONFIGURATION IN SOFTWARE

<input type="checkbox"/> Establish and Record Hardware Settings Instrument _____ Detector _____ Probe Interface _____ Probe Tip _____	<input type="checkbox"/> Establish and Record Software Settings Resolution _____ Spectral Range _____ Gain Adjustment _____ Apodization _____ Scans/Sample _____
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ALIGNMENT

<input type="checkbox"/> Sampling technology aligned (if necessary)	<input type="checkbox"/> Preamp gain adjusted (if necessary)	<input type="checkbox"/> Fixed mirror aligned
<input type="checkbox"/> Verify the probe is clean	<input type="checkbox"/> Record the following values in Align Mode Peak Height _____ Contrast _____	

FUNCTIONAL TESTING

Record Performance Values for Sampling Technology 1: Sampling Technology Type _____ <input type="checkbox"/> Signal to Noise (SNR) _____ <input type="checkbox"/> Acetone Absorbance (AA) _____ Acetone to Noise Ratio (ANR) _____	Record Performance Values for Sampling Technology 2: Sampling Technology Type _____ <input type="checkbox"/> Signal to Noise (SNR) _____ <input type="checkbox"/> Acetone Absorbance (AA) _____ Acetone to Noise Ratio (ANR) _____
<input type="checkbox"/> Record Stability Test Results DS Micro Flow Cell _____ DS FiberConduit, or Fiber-to-Sentinel, or Fiber-to-Gas Cell _____ @ 1000 cm-1 _____ @ 800 cm-1 _____ @ 3000 cm-1 _____ @ 1300 cm-1 _____	<input type="checkbox"/> RTD Calibrated – AgX FiberConduit Probe 1 <input type="checkbox"/> RTD Calibrated – AgX FiberConduit Probe 2 <input type="checkbox"/> RTD Calibrated – Micro Flow Cell

Non-conformances (include action to resolve):

Mettler-Toledo AutoChem, Inc. Field Service Engineer: Completed in due and proper manner	Responsible ReactIR User: Copy of this check record received
Name: _____	Name: _____
Date: ___/___/_____ Signature: _____	Date: ___/___/_____ Signature: _____

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