

Preliminary Checklist

All users should read and become familiar with the setup procedures, instrument handling, and maintenance/cleaning information for their iC IR instruments. The information is in the iC IR Help file and Software User Guide.

This Quick Reference sheet assumes the following prerequisites:

- All hardware/software connections have been established.
- The following steps have been completed:
 - ✓ ReactIR system is ON and warmed up for the recommended amount of time. Start the iC IR software and check for communication.
 - ✓ Cool the MCT detector with liquid N₂, if applicable (iC10, 45m, 15).
 - ✓ For purged base units (iC10, 45m) or systems that use mirror conduit sampling technologies that require purge, ensure the system is under dry N₂ purge.

I. Tips for Obtaining Good Results

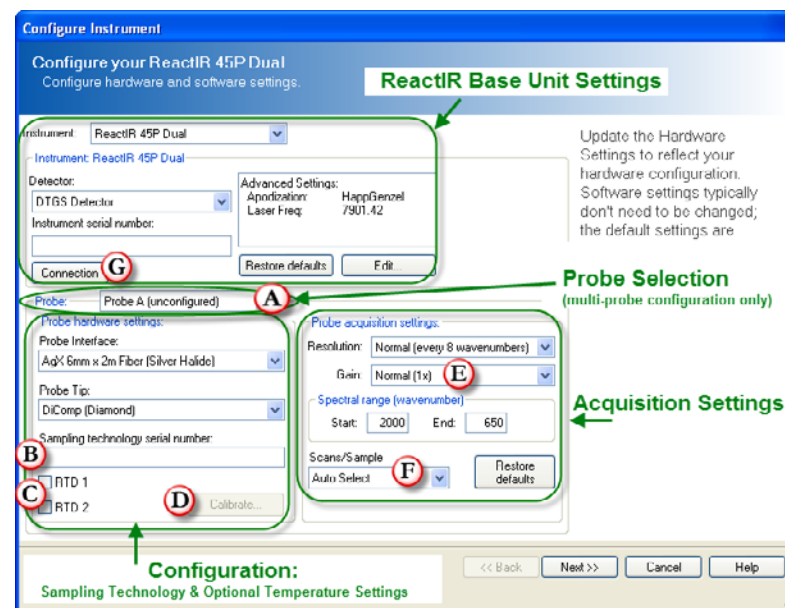
- Collect a “gold standard” background spectrum in the air with a clean sensor.
- Collect pure component spectra of solvent and major reagents.
- Start your reaction collection with just solvent in the reactor.
- Make sure no bubbles are trapped on the sensor, especially in aqueous systems.
- Check that the probe remains immersed in the solvent when stirring (not applicable with FlowIR instrument or DS Micro Flow Cell sampling technology).
- Add components one-at-a-time and collect at least four spectra between each addition.
- Please see “Best Practices” in the iC IR Help file for additional information on how to obtain good results.

II. New Experiment Setup

1. Click **New Experiment** on Start Page and follow the wizard to define your experiment.
2. Enter experiment name or accept default, specify the location where the experiment will be saved, and decide whether to use a previous experiment as a template.
3. Click **Configure Instrument** to change the default instrument or set up multiple probes. Options that appear are based on the selected instrument.

When setting up a multiprobe experiment—Configure each probe separately before starting an experiment. Multiprobe experiments only apply to Fiber MultiplexIR, MMIR45, or ReactIR 45P base units. Multiprobe experiments share the same detector and advanced settings established in the top section of the configuration window (see figure at the right).

- A Probe**—Define separate configurations for multiprobe experiments. In the Probe Interface and Probe Tip list boxes, specify the type of sampling technology being configured from a selection of applicable fibers, conduits, sentinels, flow cell, or FlowIR sensor.
- B Serial Number**—Record the sampling technology serial number for precise identification of the probe or flow sensor.



- C RTD 1 and RTD 2**—RTDs (Resistive Thermal Devices) enable temperature trending in the experiment with each spectrum collection. One or more RTD checkboxes appear depending on the specified instrument and sampling technology. Select the RTDs to be associated with the probe, if any.
- D Calibrate**—Click to calibrate the RTD temperature response.
- E Gain**—In a multiprobe experiment, this setting enables you to specify the gain (amplification) for each probe, independently.
- F Scans/Sample**—Accept the default or set the number of scans per sample.
- G Connection**—(only appears for ReactIR 45P, 247, and FlowIR instruments with Ethernet communication) Enter the connection parameter, such as an IP address or machine name; then test and initialize the connection.

4. Click **Next** and complete the following windows in the setup wizard:

Experiment Duration

Add/edit phases for an experiment. Phases are sequential and have a specific duration and measurement interval. Use a short interval during active portions of the experiment to capture fast changes. Use long intervals during less active phases to monitor long experiments while keeping file sizes small. Number of samples to be collected is based on interval and duration.

Add a phase—Click **Add** in the Experiment Duration window to define additional phases.

Edit Duration and Interval—Click the field and select a setting from the drop-down list. When you finish defining the phases, click **Next**.

Reference Spectra Needed?

- In the Select Reference Spectra Options window, choose one of the following options:
 - Collect reference spectra (recommended)**—Ensures that your reference spectra and reaction data share the same equipment and environmental conditions.
 - Load previously collected reference spectra**—Ideal for repeating experiments.
 - No reference spectra needed**—Load reference spectra during or after the experiment.
 - Just start the experiment**—Begin the experiment immediately.
- Click **Next**.

Position Probe

- Ensure the probe (or sensor in the case of FlowIR and DS Micro Flow Cell configurations) is only exposed to air—not immersed in any material.
- Click **Next**.

Align Probe

- Check the Peak Height and Contrast bars in the Align Probe window.

Green indicates proper alignment. If the colors are red, follow the alignment method for the sampling technology currently used with your ReactIR instrument.

FiberConduit—Rotate the fiber housing to adjust the alignment of the fiber to the system and adjust the detector x-y alignment. **NOTE:** DS Series FiberConduit probes are prealigned at the factory, so no rotation is required. Only DS Series configurations that use a Sentinel style probe require rotation.

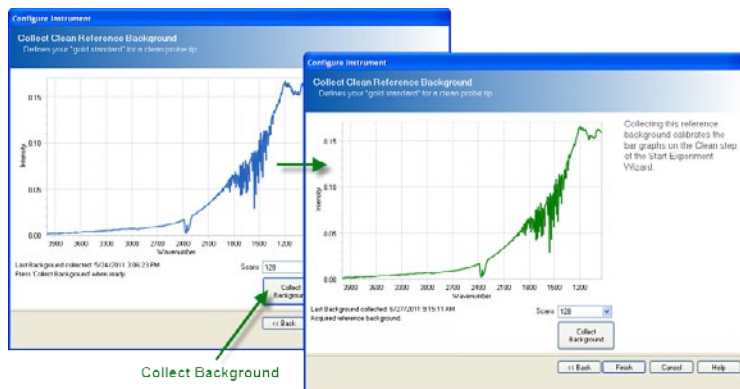
Mirror Conduit—Rotate the probe on the end of the conduit, adjust the three knurled knobs on the last mirror of the conduit, and adjust the detector x-y alignment, if applicable.
- Click **Next**.

Clean Probe

- Clean the probe tip (or FlowIR/DS Micro Flow Cell sensor) with acetone and a cleaning tissue.
- Ensure the base unit and mirror conduit (if applicable) are purged with instrument-grade air, nitrogen, or other suitable inert gas at a nominal purge pressure of 10psi (flow rate: 10scfh).
- Click **Next**.

Collect Background

- Click **Collect Background**. When the background spectrum turns to green, the background sample collection is complete.
- Click **Next**.



Collect Sample

- Collect a reference spectrum to aid your data analysis.

From the Collect Sample window:

 - Type the Name of the sample.
 - Select the Type of sample being collected from the drop-down list.
 - Select the prominent Functional Group to add a peak profile for that group.
 - Click **Collect Sample**.
- Repeat the above steps to collect all necessary reference spectra.
- Click **Next**.

Edit Reference Spectra

From the Edit Reference Spectra window, use the buttons to **Collect** additional spectra, **Load** previously collected spectra, **Delete**, or **View** existing reference spectra.

Clean Probe Tip

Follow the Clean Probe instructions earlier in this guide. Then, click **Next**.

Collect Background

It is highly recommended that you collect a new air background for each experiment. However, to reuse a background collected during the same session, click **Finish**.

V. Start Experiment

After your experiment appears, click the Play button on the Live Experiment toolbar to run the experiment.



NOTE: To reuse experiment settings in future experiments, click File > Save As Template.

VI. Notes about Optional Software Modules

- ConcIRT LIVE!** calculates relative concentration profiles for products, intermediates, and starting materials. While ConcIRT LIVE! is provided with iC IR, **ConcIRT Pro™** is an optional package that enables advanced post-processing analysis.
- iC Quant™** enables scientists to quickly and easily development quantitative models that predict actual concentrations of key reaction species in real time.
- iC Kinetics™** enables scientists to create kinetic models that simulate the effect of temperature and concentration parameters on the chemistry to optimize the reaction.

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