



Watson's Notes

Innovative Solutions
for Difficult Problems

**"You have recently been in
Afghanistan, I perceive"**

With these words was born the most famous team in detective fiction; Sherlock Holmes and his trusted comrade and biographer, Dr. John H. Watson.

In the spirit of Watson, who chronicled the exploits of Holmes, we have created this newsletter named "Watson's Notes".

In the pages of "Watson's Notes", modern day scribes document the discoveries, unusual cases and other news of Investigative Science Incorporated, our scientific consulting firm in Burlington, Ontario, Canada.

Please contact us if you have comments, and please read on.

ISI INVESTIGATIVE
SCIENCE
INCORPORATED

Scientists and Technical Consultants

1050 Cooke Blvd., Unit 2

L7T 4A8

(905)634-4200

mail@investigativescience.com

www.investigativescience.com

Direct Photolysis OECD 316

Introduction

OECD 316 is part of the New Substance Notification (NSN) Regulations for the Canadian Environmental Protection Agency (CEPA).

OECD 316 is a test to determine the effects of solar irradiation on chemicals or chemical pollutants in water. It can help to determine the possible fate of a chemical if it were spilled into our natural waterways. It provides guidance for conducting phototransformation studies to determine the potential effects of solar irradiation on chemicals, or chemical mixtures in water.

These types of studies when used in conjunction with other physical/chemical properties such as OECD 111 (hydrolysis), and OECD 106 (soil adsorption desorption) can help to assess the overall impact of the chemical pollutant in the environment.

ISI has the capability to conduct OECD 316. The test is comprised of three components in two tiers. Tier 1 is a theoretical screen based on the Ultraviolet (UV) absorbance spectrum of the test Substance in water or buffer to establish if the chemical has a photolytic half life of less than 30 days. Tier 2 is the experimental study to determine the photolysis rate constant when the test substance is exposed to the equivalent of 30 days of summer sunlight. A second part to Tier 2 is the identification of the major transformation products and determination of the quantum yield.

Methods

Tier 1 involves dissolving the Test substance in the appropriate buffer or water to produce a clear solution. One can estimate a maximum direct photolysis rate constant for a specific latitude by using the absorbances obtained from solution on a UV spectrophotometer. If the half-life is less than 30 days, Tier 2 must be conducted.

Tier 2 is used to determine the actual photolysis rate constant when a Test Substance is exposed to sunlight. OECD 316 allows for the use of direct sunlight

from the sun or a light source capable of simulating natural sunlight in the 290 – 800 nm range. The method suggests a xenon arc lamp. ISI uses a solar climatic chamber with a metal halide lamp to simulate natural sunlight and to control temperature. The metal halide lamp closely approximates the wavelength of natural sunlight. Samples are placed in the chamber and exposed for a period equivalent to 30 days of natural sunlight. At appropriate time points samples are removed from the chamber and analyzed to determine if degradation has occurred. Figure 1 is a proposed scheme for direct photolysis.

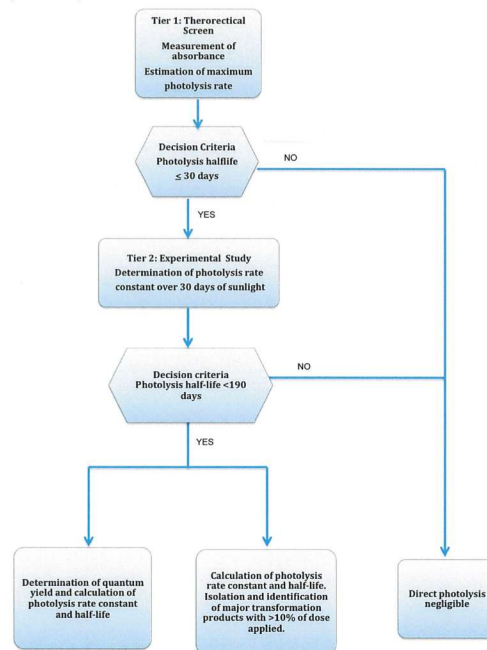


Figure 1: Proposed test Scheme for Direct Photolysis

The method of analysis is dependent on the type of chemical being tested. Samples may have to be extracted into a solvent to isolate the chemical from the water.

Sample Preparation

In Tier 1 the photolysis rate constant and associated half life are determined using the solar irradiation data from tables at various latitudes (EPA OPPTS 835.2210) and the decadic absorbance data from the UV scans. Figure 2 shows the results of a typical Tier 1 analysis.

**ELEMENTARY
MY
DEAR
WATSON**

Uncertain About
Heisenberg?:

! Werner Heisenberg was a German physicist known as the father of quantum mechanics. He is best known for his uncertainty principle, which states that one can not simultaneously know the velocity and position of an electron with certainty.

! There is a sign in Munich which states: "Heisenberg might have slept here"

! Earlier today Dr. Heisenberg stated unequivocally that he may or may not have been responsible for the Uncertainty Principle.

! The Heineken Uncertainty Principle:
You can never be sure how many beers you had last night.

! Heisenberg is out for a drive when he's stopped by a traffic cop. The cop says: " Do you know how fast you were going? Heisenberg replies: "No, but I know exactly where I am".

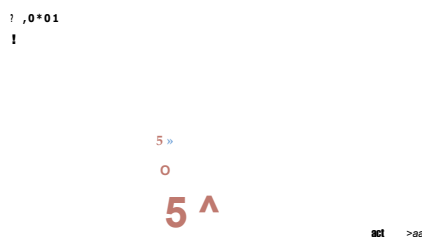


Figure 2: UV/Vis Absorbance vs Wavelength

For Tier 2, the strategy used at ISI is based on sacrificial samples at each time point. The test substance is dissolved in water or buffer depending on whether or not the test substance is ionizable. The solution is then transferred to quartz tubes and capped. Quartz tubes are useful for substances absorbing below 340 nm. Half the tubes are covered in foil and are used as dark controls. The dark control is to control for changes that may occur in the sample such as hydrolysis over the time period of the test. Both the samples and control samples are placed in the solar climatic chamber as pictured in Figure 3. Blank controls are also used to ensure no changes have occurred in the buffer or water used.

Figure 3: Dark controls and Samples in solar climatic chamber

Dark controls and samples are removed at specified time points with a minimum of five time points. The samples from each time point are analyzed using an appropriate instrument such as High pressure liquid chromatography (HPLC) or Gas chromatography/mass spectrometry (GC/MS).

The time points chosen are dependent on how quickly the degradation is occurring. A preliminary test can be conducted with a

couple of time points to determine an initial rate of breakdown. This information can be used to establish ideal sampling times.

The samples and dark controls are prepared in duplicate. This helps to determine variability and reduces uncertainty in the determination of the kinetic parameters. The test is conducted between 23 - 27 °C.

The analytical data obtained from the analysis of samples and controls can be plotted to determine degradation rates. Figure 4 below is an example of an irradiated sample and a dark control sample. This particular test substance was composed of several components. The graph shows the degradation of an individual peak at 3 minutes and the total area. The dark controls show no degradation occurred over the same period of the exposure.

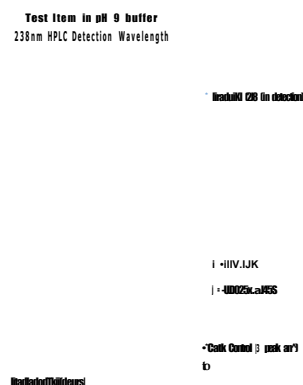


Figure 4: Irradiated Sample vs Control Sample (140 hours of exposure)

The photolysis rate can be determined using the rate constant from the above plots and the photon irradiance from the metal halide lamp. If photolysis is determined, OECD 316 requires that the major products be identified.

OECD 316 is a complicated test requiring experience with photochemistry, analytical chemistry and structural determination. ISI has all of these capabilities under one roof.