Highly-Efficient Sulfonated UiO-66(Zr) Optical Fiber for Rapid Detection of Trace Levels of Pb$^{2+}$

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Abstract: Lead detection for biological environments, aqueous resources, and medicinal compounds, rely mainly on either utilizing bulky lab equipment such as ICP-OES or ready-made sensors, which are based on colorimetry with some limitations including selectivity and low interference. Remote, rapid and efficient detection of heavy metals in aqueous solutions at ppm and sub-ppm levels have faced significant challenges that requires novel compounds with such ability. Here, a UiO-66(Zr) metal-organic framework (MOF) functionalized with SO$_3$H group (SO$_3$H-UiO-66(Zr)) is deposited on the end-face of an optical fiber to detect lead cations (Pb$^{2+}$) in water at 25.2, 43.5 and 64.0 ppm levels. The SO$_3$H-UiO-66(Zr) system provides a Fabry–Perot sensor by which the lead ions are detected rapidly (milliseconds) at 25.2 ppm aqueous solution reflecting in the wavelength shifts in interference spectrum. The proposed removal mechanism is based on the adsorption of [Pb(OH$_2$)$_6$]$^{2+}$ in water on SO$_3$H-UiO-66(Zr) due to a strong affinity between functionalized MOF and lead. This is the first work that advances a multi-purpose optical fiber-coated functional MOF as an on-site remote chemical sensor for rapid detection of lead cations at extremely low concentrations in an aqueous system.

Keywords: nano-bio detectors and sensors; nano-bio systems; aqueous quality; nanobiotechnology; optical fiber vesicle; sulfonated MOFs

1. Introduction

Lead (Pb$^{2+}$) and other small-scale substances (e.g., soot aerosol, ammonia, and arsenic) [1,2] are known as deadly widespread toxic pollutants in the environment at macro- to nano-scale due to recent industrialization and agricultural activities [3,4]. A serious concern has raised for Canadian [5], the U.S. [6], and old European mega-cities [7] with high amounts of lead nano-substances found in drinking water which are originated from old pipes or chemical reactions occurred in corroded plumbing components [8].

According to American Academy of Family Physicians (AAFP), any level of detectable lead in human blood is abnormal [9]. Recurring exposure to low levels of Pb creates serious health issues for infants and children such as slow development and permanent intellectual disability [10,11]. In addition to various sources, lead can be taken up by fishes and other aquatic organisms from water accumulating in humans tissues after consumption [12].
and then resulting in neurological [13], hematopoietic [14], musculoskeletal [15], cardiac function [16] and reproductive damages [17,18]. Despite the detrimental properties of lead to living objects, there is yet a significant gap to efficiently and abruptly detect and characterize lead at extremely small levels in bioactive compounds [19,20].

Methodologically, atomic absorption spectroscopy (AAS), atomic emission spectroscopy (AES), X-ray fluorescence (XRF), and inductively coupled plasma-optical emission spectrometry (ICP-OES) are the commonly used laboratory techniques for measuring lead contents in drinking water [21]. To use the above expensive and complicated equipment, water samples should be collected on-site, transported to a laboratory, and tested by trained professionals. This process for a large-scale determination of lead concentration is costly, time-consuming, and effortful. As yet, there are considerable efforts to develop sensors to allow discrete measurements of lead contents at-the-source for home-users. The existing detection mechanisms are based on colorimetry [22,23], biosensing [24], and electrochemical configurations [25], which, in addition to their low detection limits, have many other constraints. For instance, matrix interferences in the colorimetric method either disrupt the reaction between the reagent and the analyte or interfere the spectrometric light measurement [21]. In the biosensing method, more complex biological molecules, e.g., Daphnia magna, are needed with higher selectivity and less interference for reagents [26]. In the electrochemical sensing technique, lead-selective membranes are utilized on electrodes, where the response can be impacted by the interference from other ions presented in the water sample, effecting the solution ionic strength and potential drift [21]. Thus, an accessible, fast, sustainable, and efficient technology can fill this gap to detect Pb$^{2+}$ in aqueous resources at low ppm and ppb levels [27].

So far, there are increasing interests in recent years to take advantage of advanced materials to adsorb Pb$^{2+}$ nanoparticles at deficit concentrations from aqueous resources [28–33]. Metal-organic frameworks (MOFs) are highly porous 3D-materials made of metal ions linked with organic ligands. The size and shape of pores are affected by the coordination geometry of metals (e.g., tetrahedral, octahedral) that dictates the number of bounded ligands. Proper selection of metal ions and ligands can yield crystals with ultrahigh porosity as well as high thermal and chemical stability. Among MOFs, UiO-66(Zr) or Zr$_6$O$_4$(OH)$_4$ has a stable crystalline structure in water, introducing it as a promising candidate for sensing the aqueous contaminants and purification purposes [34]. Our recent studies have shown the favorable capability of UiO-66 for removing rhodamine-B [35], methyl viologen [36], and 4-aminopyridine [37] from water contents. The functionalization of UiO-66(Zr) with proper chemical groups is suggested to enhance its low affinity with Pb$^{2+}$ ions.

In this work, a new setup is introduced via functionalization of UiO-66(Zr) with SO$_3$H to capture Pb$^{2+}$ at low ppm levels in aqueous environments. Due to the strong coordination of Pb$^{2+}$ with SO$_3^-$ group, a small quantity of lead (<O.5 ppm) was left in the solution. To create a remote sensing setup for rapid detection within the range of a few milliseconds, the functionalized MOF was coated at the end-face of an optical fiber (single-mode fiber, SMF-28) and used as an in-fiber Fabry–Perot interferometer (FPI) [38]. The changes to the MOF optical properties due to adsorption of Pb$^{2+}$ were detected via wavelength shifts in the interference spectrum.

2. Methods

SO$_3$H-UiO-66(Zr) sensing element was synthesized through a growth solution proposed by Okoro et al. [24] with some modifications. Briefly, ZrCl$_4$ (1.93 g, 8.3 mmol) and monosodium 2-sulfoterephthalate (NaSO$_3$-BDC, 2.2 g, 8.2 mmol) were dissolved under stirring with N,N-dimethylformamide (DMF, 100 mL) and concentrated HCl (37%, 1.3 mL). Then, glacial acetic acid (100%, 16.6 mL; 35 equiv.) was added as a modulator. The mixture was continuously stirred for 2 h and left for 24 h at 120 °C in a pre-heated oven. After naturally cooling down to room temperature, the SO$_3$H-UiO-66(Zr) nanoparticles were centrifuged at 20,000 rpm for 10 min and washed with fresh DMF (at least three times), then with pure methanol (at least three times), and kept under constant
stirring with dichloromethane (DCM) overnight. They were dried for 5 h at 60 °C under reduced pressure.

The SMF-28 optical fiber was made of molten silica glass heated up to 2200 °C and drawn into tubes with varied diameters. In this work, fibers with a cladding diameter of 125 ± 0.7 µm and a core diameter of 8.2 µm were utilized. Before coating, the optical fiber made of SiO₂ glass was treated with hydroxyl (OH) functional groups. A piranha solution was prepared from a 3:1 mixture of sulfuric acid (98%) and hydrogen peroxide (30%), into which optical fibers were cleaved at a right angle and incubated for 30 min. To grow the MOF sensing element on the exposed surface of the optical fibers, the OH-functionalized optical fibers were placed in an untreated precursor solution of SO₃H-UiO-66(Zr), heated at 120 °C for 24 h. After this procedure, the fibers were gently washed with DMF, methanol and DCM, to remove unreacted reagents.

Fabry–Perot interferometry (FPI) was used as the optical detection method. When the light is propagated down to the core of fiber, it interacts with the sensing element. The element is in contact with lead-contaminated water, and by capturing the Pb²⁺, its optical thickness and refractive index change. The reflected light sends this information to the detector, where a custom-written software (MATLAB [39]) processes it [35–37]. The resultant FPI spectrum (interferograms) is obtained in correlation with the lead concentration in distilled (DI) water.

To test the lead uptake capacity of as-synthesized MOF, different amounts of SO₃H-UiO-66(Zr) (10, 15, 20 and 25 mg) were separately added to 5 mL diluted solution with 25.2 (0.12 mM), 43.5 (0.21 mM) and 64.0 (0.31 mM) ppm lead under constant stirring for 10, 30 and 60 min (impregnation). Before taking a sample (aliquot) from the middle of the vial, the solid was separated by centrifuging at 20,000 rpm for 5 min, then resting for 4 h at room temperature. The adsorption mechanism of Pb²⁺ onto SO₃H-UiO-66(Zr) was characterized by X-ray diffraction (XRD), N₂ gas porosimetry, and Fourier-transform infrared spectroscopy (FT-IR) methods (Appendix A).

3. Results and Discussion

3.1. Pb²⁺ Uptake by SO₃H-UiO-66(Zr) Powder

Figure 1a displays the XRD pattern of SO₃H-UiO-66(Zr) and SO₃Pb-UiO-66(Zr) powder. A change in the XRD pattern of the amorphous SO₃H-UiO-66(Zr) sample occurs by appearing the additional peaks in the SO₃Pb-UiO-66(Zr) sample (prescribed to PbSO₄ post-adsorption through peak matching in crystallographic database (Figure A1)). This suggests the formation of a material that matches with the crystallographic geometry of PbSO₄. The cleavage energy of the sulfonate group is prohibitively high under the adsorption conditions (pH = 5.6, room temperature/pressure, and in aqueous environment), and Pb(NO₃)₂ is soluble in water with different crystallographic geometries. The pH was achieved by atmospheric carbon dioxide dissolving into the DI water as a natural process. To avoid addition of interferent compounds to the water/Pb context, the pH was not regulated. Therefore, we conclude that Pb²⁺ cation is absorbed onto the sulfonate groups of SO₃H-UiO-66(Zr) structure where the tetrahedral R-SO₃ of the 2-sulfoterephthalate linker replaces the tetrahedral SO₄ of PbSO₄.

Standard N₂ gas porosimetry measurements confirm the uptake of lead within SO₃H-UiO-66(Zr), where the Brunauer-Emmett-Teller (BET) surface area decreases from 491 m²/g to 12 m²/g upon the lead uptake. Figure 1b shows the pore size distribution of SO₃H-UiO-66(Zr) before/after the lead uptake; this is associated with the additional mass of Pb²⁺ incorporated into the compound as well as the reduction of internal pore volume. The adsorption/desorption isotherms of SO₃H-UiO-66(Zr) before/after the lead uptake are shown in Figure 1c.
Figure 1. (a) XRD curves, (b) Pore size distribution, (c) N\textsubscript{2} adsorption/desorption isotherms, and (d) FT-IR spectra of SO\textsubscript{3}H-UiO-66(Zr) and SO\textsubscript{3}Pb-UiO-66(Zr) powder.

Upon the uptake of Pb\textsuperscript{2+}, significant changes in the observed transmittance reflect the change of dipole moment due to the adsorbed Pb\textsuperscript{2+}. Unchanged peak positions associated with the UiO-66(Zr) framework indicate that the structure does not undergo significant changes while the crystallinity increases (Figure 1d). For instance, the characteristic S=O stretching at 1375 cm\textsuperscript{-1} and 1167 cm\textsuperscript{-1} become weaker in the SO\textsubscript{3}Pb-UiO-66(Zr) sample, while C−H stretching peak at 1251 cm\textsuperscript{-1} has a very low intensity. Defects in SO\textsubscript{3}H-UiO-66(Zr) reduces the density of functional groups that interact with the laser. The reduced transmittance is seen in the figure in the gesture of smaller peaks.

3.2. Pb\textsuperscript{2+} Uptake of SO\textsubscript{3}H-UiO-66(Zr) Powder

Inductively coupled plasma-optical emission spectrometry (ICP-OES) was conducted to determine the trace level of lead in the aliquots after its impregnation. By nonlinear regression modelling, the equilibrium/optimized level of lead uptake capacity of as-synthesized MOF was determined as 33.7 mg with a maximum 94% uptake (r-squared fit of 99.7%).

Langmuir and Freundlich models are used to investigate the adsorbent/adsorbate interaction in MOFs. Langmuir isotherm assumes that in the uptake process, the adsorbent places itself as a monolayer on the surface of the material. This model can be linearly expressed in the form of Equation (1):

\[
\frac{C_e}{q_e} = \frac{K_L}{q_m} + \frac{C_e}{q_m}
\]

where \(C_e\) is the equilibrium solution concentration (mg/L or ppm), \(q_e\) is the amount of Pb\textsuperscript{2+} at the equilibrium (mg/g), \(K_L\) is the Langmuir adsorption constant related to the energy of adsorption, and \(q_m\) is the maximum adsorption capacity of the MOF (mg/g). A plot of \(C_e/q_e\) (y-axis) vs. \(C_e\) (x-axis) allows the calculation of \(q_m\) and \(K_L\) parameters (Figure 2a).
Another model, empirical Freundlich isotherm, assumes that the distribution of active sites in the MOF is homogeneous and is linearly expressed in the form of Equation (2):

\[
\ln q_e = \ln K_f + \ln C_e / n
\]  

(2)

here, \(C_e\) is the equilibrium solution concentration (mg/L or ppm), \(q_e\) is the amount of Pb\(^{2+}\) at the equilibrium (mg/g), \(K_f\) is the Freundlich adsorption constant, and \(n\) is an empirical value. A plot of \(\ln q_e\) (y-axis) vs. \(\ln C_e\) (x-axis) determines the magnitudes of \(K_f\) and \(n\) (Figure 2b).

Figure 2. Adsorption isotherms fitted by linearized form of (a) Langmuir and (b) Freundlich model for adsorbed Pb\(^{2+}\) by SO\(_3\)H-UiO-66(Zr).

Regression analysis of the data, the average values of \(K_f\), \(K_L\), \(q_m\) and \(n\) are shown in Table 1. In this study, the Freundlich model shows a better predictor than the Langmuir model with slightly higher \(R^2\), suggesting that the uptake of lead cations occurs mainly and homogeneously throughout the entire of MOF framework. Moreover, the calculated average \(n\) value for the adsorption of Pb\(^{2+}\) is 1.66, showing a good efficiency of SO\(_3\)Pb-UiO-66(Zr) for the lead adsorption [40,41].

Table 1. Langmuir and Freundlich isotherm constants for the uptake of lead (II) cation at room temperature.

| Langmuir Constants | Freundlich Constants |
|--------------------|----------------------|
| \(q_m\) (mg/g)     | \(K_L\) (mg/L) | \(R^2\) | \(K_f\) | \(n\) | \(R^2\) |
| 32.77              | 6.07               | 0.95    | 5.51    | 1.66    | 0.99 |

To determine whether a high degree of crystallinity affected the lead uptake, the untreated precursor solution of SO\(_3\)H-UiO-66(Zr) was heated at 120 °C for 48 h (rather 24 h); a highly crystallized as-synthesized MOF was achieved. As seen in the XRD patterns (Figure A2b), more defined Bragg peaks were observed for the MOF heated for 48 h in comparison to the one heated for 24 h. Based on the ICP-OES results, 10 mg of this highly formed MOF led to <0.5 ppm (2.4 µM) left-over lead in the initial 25.2 ppm-solution (99.99% uptake) for all impregnation ranges (10, 30 and 60 min). In contrast, non-functionalized UiO-66(Zr) MOF reduced the lead content from 25.2 ppm to 23.1 ppm after 60 min constant stirring.

3.3. Optical Fiber Sensing

After successfully validating the impregnation of lead within SO\(_3\)H-UiO-66(Zr), the coated element at the tip of optical fiber was utilized as a chemical sensor for the rapid (a few milliseconds) detection of lead in DI water. Figure 3a illustrates the SEM image of a deposited sensing element of sulfonated SO\(_3\)H-UiO-66(Zr) at the tip of optical fiber.
adjacent to a bare optical fiber in Figure 3b. The interference of two reflected beams was recorded using an optical spectrum analyzer (OSA, Ando Japan, AQ6317B, 600–1750 nm). An Agilent 83438A Erbium ASE (Agilent Technologies, Santa Rosa, CA, USA) was used as the light source with the wavelength range of 1500–1600 nm. The OSA was set on a continuous scan mode to record the interference signals every 5 s with a high sensitivity and 0.1 nm resolution.

Figure 3. SEM images of (a) SO$_3$H-UiO-66(Zr) optical fiber sensing element, and (b) bare optical fiber, (c) Interferograms in correlation with a lead concentration in DI water, and (d) EDX spectra of SO$_3$H-UiO-66(Zr) optical fiber sensing element after the lead uptake.

The average of all signals (100 trials) for each concentration was used as the final interference signal for a specific concentration. The fast response of the sensing element towards lead uptake was withdrawn by comparing the shape of signals at different sweeps. Figure 3c shows the spectral positions of the interferogram peak (normalized denoised interference intensity vs. wavelength) generated by SO$_3$H-UiO-66(Zr) sensing element at different lead concentrations. Briefly, the sensor was first placed in DI water for 5 min to
observe the pattern of sensing element upon the exposure to DI water. The same procedure was repeated after immersing the sensor in different lead solutions ("water 2" and "water 3" with 25.2 ppm and 43.5 ppm lead contents, respectively). Upon the introduction of lead nitrate solutions, the position of interferogram peak shifted to longer wavelengths. This indicated an increase in the lead adsorption by $\text{SO}_3\text{H-UiO-66(Zr)}$ sensing element and, thus, the optical thickness.

Energy-Dispersive X-ray (EDX) analysis was performed on the optical fiber sensing element after the lead uptake process, in order to confirm the attachment of lead with $\text{SO}_3\text{H-UiO-66(Zr)}$. As shown in Figure 3d, despite some detection difficulty due to the similarity of the energy of S-K$\alpha$ and Pb-M$\alpha$ (2.309 vs. 2.342 keV, respectively), zirconium (Zr) (as the main constituent of Zr-based MOF $\text{SO}_3\text{H-UiO-66}$) had 21.3% weight while Pb possessed 9.6% level in the samples with higher ppm. The presence of sulfur (S) confirmed the $\text{SO}_3\text{H-UiO-66(Zr)}$ structure.

As the reference for lead level in drinking water is 5 µg/L (5 ppb) [42], precision evaluation studies should be conducted to further overcome the detection limit. Nevertheless, optical fibers and $\text{SO}_3\text{H-UiO-66(Zr)}$ are stable within the range of pH 2–9 [43,44]. Yet, the remaining challenge is to consider the sensor in very harsh environments for prolonged periods of time where the wastewater might be extremely acidic or basic. Although the optical fiber sensors were not designed explicitly for this purpose, there is an opportunity to trigger the release of the guest species ($\text{Pb}^{2+}$) using light at a specific wavelength [45]. The pH change [46], ligand exchange [47], and ethanol regeneration solvent [48] have been proposed to recycle MOFs for further usages.

3.4. Mechanism of Pb$^{2+}$ Adsorption

Figure 4 shows the chemistry mechanism where the sensing material coordinates with Pb$^{2+}$ ions via $n$ sulfonate groups, $n \leq 6$.

![Diagram of adsorption of $[\text{Pb(OH}_2\text{)}]_{6}^{2+}$ on $\text{SO}_3\text{H-UiO-66(Zr)}$ in water](image)

As per our data, Pb adsorption occurs in a S-O-Pb$^+$ bonding manner. There are 10 lone pairs of electrons present in the oxygens of sulfonic acid group, where the tetrahedral R-SO$_3$ geometry would prohibit the direct S-Pb bonding. In fact, the presence of a crystalline phase identical to Pb(SO$_4$) is due to the coordination of Pb to SO$_3^-$ group with the O-carbon of 2-sulfonoterephthalic acid replacing one O in Pb(SO$_4$). The rapid uptake of Pb, shown from both the batch adsorption measurements and the optical fiber results, leads to both weak coordination and strong electrostatic attraction between Pb and R-O$^-$. The speciation of Pb(NO$_3$)$_2$ in aqueous solutions at the native pH of $\sim$5 is mainly Pb$^{2+}$, that exists within a solvation shell of approximately 6 H$_2$O molecules. The adsorptions would, therefore, have the following predominant reactions [49]:

\[
R - \text{SO}_2\text{OH}(s) + \text{Pb}^{2+}(aq) \rightarrow R - \text{SO}_3^- + \text{Pb}^{2+}(aq) + \text{H}_3\text{O}^+(aq) \rightarrow R - \text{SO}_2\text{O} - \text{Pb}^+ \quad (3)
\]

\[
R - \text{SO}_2\text{OH}(s) + \text{Pb}^{2+}(aq) \rightarrow R - \text{SO}_3^- + \text{Pb}^{2+}(aq) + \text{H}_3\text{O}^+(aq) \rightarrow R - \text{SO}_3^- ... \text{Pb}^{2+}_n \quad (4)
\]
Equation (3) demonstrates an electrostatic attraction to a singular sulfonate $O_-$, while Equation (4) presents the coordination between the delocalized sulfonate $e^-$ and $\text{Pb}^{2+}$. These are shown as a three-step process. The immersion of the MOF into water dissociates the sulfonic acid $\text{H}^+$ rapidly, after which lead is attracted to the sulfonate groups of $\text{SO}_3\text{H}^{-}\text{UiO-66(Zr)}$. Due to the rapid uptake, it is not expected that $\text{Pb(O.H.)}^{-}$ is adsorbed onto the sulfonates, as its fractional abundance at $\text{pH}$ 5–6 is low relative to the adsorption phenomenon [50].

4. Conclusions

The rapid detection of $\text{Pb}^{2+}$ by MOF-coated optical fibers was introduced for the first time. A solvothermal synthesized sulfonic acid functionalized MOF, $\text{SO}_3\text{H-UiO-66(Zr)}$, demonstrated the rapid uptake of lead from $\text{Pb(NO}_3)_2$ solution. The analysis of ICP-OES intensities showed the uptake capacity of $\text{SO}_3\text{H-UiO-66(Zr)}$ as 32.77 mg/g ($R^2 = 0.997$). This MOF was grown on an OH-functionalized SMF-28 conventional single-mode optical fiber that acted as a detector for $\text{Pb}^{2+}$ at the ppm-level concentrations. Spectral interferograms indicated the detection of $\text{Pb}^{2+}$ down to 25.2 ppm. Such a MOF optical fiber can be implemented as a device for simple/abrupt on-site detection of aqueous $\text{Pb}^{2+}$ or possibly other ions at ppm or sub-ppm levels. We envisage that this type of sensor would offer a novel and more effective composite to harvest heavy metals from contaminated water for clean water supply.

Further studies are currently undergoing to investigate the interference effects of a matrix containing more than one cation and anion in water, as other transition metal (II) ions may give a ‘false’ $\text{Pb}^{2+}$ detection reading.

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Conflicts of Interest: The authors declare no competing interests.

Appendix A

Appendix A.1. Sample Preparation and Analysis Conditions for X-ray Diffraction (XRD) Characterization

The sample was dry ground in a boron carbide mortar and pestle before being loaded into a low volume Si zero background sample holder. A “Bruker D8 Advance A25” X-ray Diffractometer operating under CuKα radiation (40 kV, 40 mA) and equipped with a Lynx Eye XE-T detector was employed to obtain the XRD patterns. The sample was scanned over the 2$\theta$ range of 5° to 85° at a step size of 0.02° and a count time of 1.6 s per step and spun at 15 RPM during the data collection.

Analyses were performed on the collected XRD data using the Bruker XRD search match program EVA™ v5. Crystalline phases were identified using the ICDD-JCPDS powder diffraction database. Pawley analyses were performed on the data using the Bruker TOPAS™ v6 program to determine lattice parameters and crystallite size (Table A1). Background signal was described using a combination of Chebyshev polynomial linear interpolation function and $1/x$ function. Cell parameters, vertical sample displacement,
full peak width at half maximum, and peak scale factor were all refined. Error ranges were calculated based on three estimated standard deviations as calculated by TOPAS. A diffractogram pattern of SO$_3$Pb-UiO-66(Zr) at 2$\theta$ region (5°–65°) superimposed over the simulated diffractograms of UiO-66 and PbSO$_4$ anglesite is shown in Figure A1.

Table A1. Phase summary of SO$_3$H-UiO-66(Zr).

| Lattice Parameter | Crystallite Size | Phase |
|-------------------|------------------|-------|
| 24 h              | NP (amorphous)   | NP (amorphous) UiO-66, except the (0 2 2) peak at $\sim$12° 2$\theta$ |
| 48 h              | 20.678 $\pm$ 0.001 Å | 170 $\pm$ 11 nm UiO-66, except the (0 2 2) peak at $\sim$12° 2$\theta$ |

Figure A1. Diffractogram pattern of SO$_3$Pb-UiO-66(Zr) at 2$\theta$ region (5°–65°), superimposed over the simulated diffractograms of UiO-66 and PbSO$_4$ anglesite.

Appendix A.2. N$_2$ Gas Porosimetry

Gas adsorption isotherms were measured for pressure within the range 0–120 kPa by a volumetric approach using a Micrometrics ASAP 2420 instrument. All samples were transferred to pre-dried and weighted analysis tubes and sealed with Transcal stoppers. They were evacuated and activated under a dynamic vacuum at $10^{-6}$ Torr at 140 °C for 8 h. Ultra-high purity N$_2$ was used for the experiments. N$_2$ adsorption and desorption measurements were conducted at 77 K. Surface area measurements were performed on N$_2$ isotherms at 77 K using the Brunauer-Emmer-Teller (BET) model with increasing adsorption values of 0.005 to 0.2.

Appendix A.3. Inductively Coupled Plasma-Optical Emission Spectrometry (Icp-Oes) Analysis Method

The samples were analyzed on an as-received basis by acidifying to 5(wt)% HNO$_3$. The solutions were then analyzed by using Varian 730-ES axial ICP-OES. Certified multi-element solutions were used to check the accuracy of the calibration standards and the method.
Appendix A.4. Characterization of SO$_3$H-UiO-66(Zr) (48 H Heating)

Figure A2. (a) N$_2$ adsorption/desorption isotherms and (b) XRD curves of SO$_3$H-Uio-66(Zr) [24 h] and SO$_3$H-Uio-66(Zr) [48 h] powder.

Appendix A.5. Optical Methodology

The interference signal was processed in MATLAB [39] using a special two-stage signal processing algorithm. The first part of the algorithm used Daubechies Wave Transform (DWT) to remove noise from the spectrum. Then, the second part of the algorithm performed frequency domain analysis (fast Fourier transform (FFT)) to determine the response of the SO$_3$H-Uio-66(Zr) to lead concentration in DI water. Table A2 shows the raw data (Normalized denoised interference intensity (NDII) vs. Wavelength) obtained from one sensor after signal processing.

Table A2. Normalized denoised interference intensity (NDII).

| Wavelength (nm) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| DI Water        | 25.2 ppm  | 43.5 ppm  | 64.0 ppm  |           |           |           |           |
| 1524.9          | 0.51753   | 0.49844   | 0.47935   | 0.47701   | 0.45939   | 0.49888   |
| 1525.02         | 0.50941   | 0.49544   | 0.48147   | 0.47317   | 0.46254   | 0.49268   |
| 1525.14         | 0.50486   | 0.49111   | 0.47736   | 0.47044   | 0.45853   | 0.49062   |
| 1525.26         | 0.51375   | 0.49504   | 0.47633   | 0.47243   | 0.46196   | 0.49004   |
| 1525.38         | 0.51785   | 0.49733   | 0.47681   | 0.47322   | 0.46254   | 0.49151   |
| 1525.5          | 0.52234   | 0.50184   | 0.48134   | 0.47885   | 0.4703    | 0.49534   |
| 1525.612        | 0.52747   | 0.50538   | 0.47969   | 0.47626   | 0.46483   | 0.49888   |
| 1525.739        | 0.52657   | 0.50136   | 0.47907   | 0.47243   | 0.46512   | 0.49652   |
| 1525.859        | 0.51843   | 0.50033   | 0.48223   | 0.47731   | 0.4654    | 0.49681   |
| 1525.979        | 0.52216   | 0.50271   | 0.48326   | 0.47507   | 0.46655   | 0.49859   |
| 1526.099        | 0.51376   | 0.5012    | 0.48864   | 0.48326   | 0.46943   | 0.49947   |
| 1526.219        | 0.5233    | 0.50652   | 0.48974   | 0.4814    | 0.4703    | 0.50036   |
Table A2. Cont.

| Wavelength (nm) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| DI Water 25.2 ppm | 0.52529 | 0.50493 | 0.48457 | 0.4814 | 0.46799 | 0.49918 |
| Water 2 43.5 ppm | 0.52852 | 0.50986 | 0.4912 | 0.48256 | 0.47001 | 0.50273 |
| Water 3 64.0 ppm | 0.52389 | 0.50668 | 0.48947 | 0.47955 | 0.46828 | 0.50066 |
| 1526.698 | 0.5253 | 0.50946 | 0.49362 | 0.48682 | 0.46943 | 0.5033 |
| 1526.818 | 0.52945 | 0.51289 | 0.49633 | 0.48466 | 0.47347 | 0.50749 |
| 1526.938 | 0.52949 | 0.51225 | 0.49501 | 0.48581 | 0.47376 | 0.506 |
| 1527.058 | 0.53234 | 0.51329 | 0.49424 | 0.48667 | 0.4755 | 0.50541 |
| 1527.178 | 0.53325 | 0.51465 | 0.49605 | 0.48657 | 0.4755 | 0.506 |
| 1527.298 | 0.53873 | 0.51937 | 0.50001 | 0.49241 | 0.47898 | 0.51137 |
| 1527.418 | 0.54171 | 0.52194 | 0.50217 | 0.49306 | 0.48218 | 0.51316 |
| 1527.537 | 0.53698 | 0.51937 | 0.50176 | 0.49316 | 0.48276 | 0.51047 |
| 1527.657 | 0.54221 | 0.52226 | 0.50231 | 0.49463 | 0.48247 | 0.51257 |
| 1527.777 | 0.5467 | 0.52468 | 0.50266 | 0.49412 | 0.48218 | 0.51346 |
| 1527.897 | 0.54672 | 0.52637 | 0.50602 | 0.49838 | 0.48334 | 0.51436 |
| 1528.017 | 0.54467 | 0.52685 | 0.50903 | 0.49883 | 0.48684 | 0.51766 |
| 1528.137 | 0.54123 | 0.52387 | 0.50651 | 0.49767 | 0.48633 | 0.51406 |
| 1528.257 | 0.5441 | 0.52492 | 0.50574 | 0.49726 | 0.48188 | 0.51496 |
| 1528.377 | 0.54442 | 0.52669 | 0.50896 | 0.49741 | 0.48392 | 0.51466 |
| 1528.496 | 0.54698 | 0.53057 | 0.51416 | 0.50437 | 0.48684 | 0.51856 |
| 1528.616 | 0.54976 | 0.53178 | 0.5138 | 0.50335 | 0.48889 | 0.52006 |
| 1528.736 | 0.55104 | 0.53137 | 0.5117 | 0.5031 | 0.48684 | 0.51856 |
| 1528.856 | 0.54944 | 0.53113 | 0.51282 | 0.50452 | 0.48772 | 0.52036 |
| 1528.976 | 0.55047 | 0.53235 | 0.51423 | 0.503 | 0.48801 | 0.52006 |
| 1529.216 | 0.55852 | 0.53884 | 0.51916 | 0.50962 | 0.49475 | 0.527 |
| 1529.336 | 0.555 | 0.53648 | 0.51796 | 0.50804 | 0.49182 | 0.52338 |
| 1529.456 | 0.5608 | 0.5403 | 0.5198 | 0.51024 | 0.49387 | 0.52579 |
| 1529.575 | 0.5663 | 0.54471 | 0.52312 | 0.51234 | 0.49681 | 0.52942 |
| 1529.695 | 0.56668 | 0.54405 | 0.52142 | 0.51275 | 0.49505 | 0.5273 |
| 1529.815 | 0.56786 | 0.5456 | 0.52334 | 0.51357 | 0.49888 | 0.53003 |
| 1529.935 | 0.56246 | 0.54226 | 0.52206 | 0.51285 | 0.49593 | 0.52821 |
| 1530.055 | 0.55992 | 0.54177 | 0.52362 | 0.51111 | 0.49593 | 0.5264 |
| 1530.175 | 0.56607 | 0.54683 | 0.52759 | 0.51613 | 0.50094 | 0.52851 |
| 1530.295 | 0.56429 | 0.5474 | 0.53051 | 0.51886 | 0.50153 | 0.53063 |
| 1530.415 | 0.56896 | 0.5497 | 0.53044 | 0.51819 | 0.5036 | 0.53154 |
| 1530.534 | 0.56563 | 0.54757 | 0.52951 | 0.51875 | 0.50094 | 0.53033 |
Table A2. Cont.

| Wavelength (nm) | NDII DI Water 25.2 ppm | NDII Water 2 43.5 ppm | NDII Water 3 64.0 ppm |
|-----------------|------------------------|-----------------------|-----------------------|
| 1529.096        | 0.55331                | 0.53405               | 0.51479               | 0.50575 | 0.49123 | 0.52277 |
| 1530.654        | 0.56891                | 0.54978               | 0.53065               | 0.51839 | 0.50272 | 0.53185 |
| 1530.774        | 0.5686                 | 0.55084               | 0.53308               | 0.52056 | 0.5042  | 0.53215 |
| 1530.894        | 0.57401                | 0.55429               | 0.53457               | 0.52432 | 0.50538 | 0.53549 |
| 1531.014        | 0.57661                | 0.5547                | 0.53279               | 0.52329 | 0.50509 | 0.53549 |
| 1531.134        | 0.57067                | 0.55273               | 0.53479               | 0.52247 | 0.50568 | 0.53428 |
| 1531.254        | 0.57597                | 0.5552                | 0.53443               | 0.52221 | 0.50686 | 0.5361  |
| 1531.374        | 0.58032                | 0.55866               | 0.537                  | 0.52443 | 0.50746 | 0.5361  |
| 1531.494        | 0.57778                | 0.5575                | 0.53722               | 0.52593 | 0.50746 | 0.53702 |
| 1531.613        | 0.58055                | 0.56064               | 0.54073               | 0.52784 | 0.51073 | 0.53885 |
| 1531.733        | 0.57708                | 0.55808               | 0.53908               | 0.52582 | 0.50835 | 0.53732 |
| 1531.853        | 0.58131                | 0.56113               | 0.54095               | 0.5265  | 0.51043 | 0.53732 |
| 1531.973        | 0.57906                | 0.56072               | 0.54238               | 0.52909 | 0.51132 | 0.53915 |
| 1532.093        | 0.58306                | 0.56477               | 0.54648               | 0.53356 | 0.51431 | 0.54129 |
| 1532.213        | 0.58573                | 0.56809               | 0.55045               | 0.53616 | 0.51849 | 0.54435 |
| 1532.333        | 0.58018                | 0.56477               | 0.54936               | 0.53512 | 0.51699 | 0.54129 |
| 1532.453        | 0.58271                | 0.56535               | 0.54799               | 0.53397 | 0.5164  | 0.54098 |
| 1532.572        | 0.58962                | 0.57                  | 0.55038               | 0.53679 | 0.51969 | 0.54496 |
| 1532.692        | 0.5882                | 0.57175               | 0.5553                | 0.54196 | 0.52239 | 0.54619 |
| 1532.812        | 0.59301                | 0.57575               | 0.55849               | 0.54468 | 0.5257  | 0.55141 |
| 1532.932        | 0.58986                | 0.572                | 0.55414               | 0.54076 | 0.52089 | 0.5465  |
| 1533.052        | 0.5902                | 0.57141               | 0.55262               | 0.53923 | 0.52239 | 0.54588 |
| 1533.172        | 0.59337                | 0.57575               | 0.55813               | 0.54311 | 0.5257  | 0.5468  |
| 1533.292        | 0.59498                | 0.57608               | 0.55718               | 0.54474 | 0.52449 | 0.5468  |
| 1533.412        | 0.59503                | 0.57658               | 0.55813               | 0.54364 | 0.5263  | 0.54926 |
| 1533.531        | 0.5945                | 0.57566               | 0.55682               | 0.54238 | 0.52359 | 0.54742 |
| 1533.651        | 0.59242                | 0.57433               | 0.55624               | 0.54269 | 0.52999 | 0.54496 |
| 1533.771        | 0.59648                | 0.57901               | 0.56154               | 0.54736 | 0.52901 | 0.54711 |
| 1533.891        | 0.59699                | 0.57934               | 0.56169               | 0.5482  | 0.52871 | 0.54803 |
| 1534.011        | 0.59912                | 0.58303               | 0.56694               | 0.55142 | 0.53204 | 0.55111 |
| 1534.131        | 0.60068                | 0.58286               | 0.56504               | 0.55179 | 0.53204 | 0.54895 |
| 1534.251        | 0.59938                | 0.58261               | 0.56584               | 0.553   | 0.53355 | 0.5508  |
| 1534.371        | 0.60338                | 0.58622               | 0.56906               | 0.55628 | 0.5398  | 0.55234 |
| 1534.49        | 0.604                  | 0.58697               | 0.56994               | 0.55553 | 0.53598 | 0.55234 |
| 1534.61        | 0.60676                | 0.58967               | 0.57258               | 0.55808 | 0.53962 | 0.5545  |
| 1534.73        | 0.60637                | 0.5879                | 0.56943               | 0.55866 | 0.53689 | 0.55326 |
| 1534.85        | 0.60773                | 0.58748               | 0.56723               | 0.55601 | 0.53719 | 0.55203 |
Table A2. Cont.

| Wavelength (nm) | NDII DI Water 25.2 ppm | NDII Water 2 43.5 ppm | NDII Water 3 64.0 ppm |
|-----------------|------------------------|----------------------|----------------------|
| 1534.97         | 0.60591 0.58807 0.57023 0.55749 | 0.53719 0.55234       |
| 1535.09         | 1535.21       | 1535.33       | 0.61246 0.59296 0.57346 0.55998 | 0.54145 0.55419 |
| 1535.45         | 0.61025 0.58874 0.56723 0.55575 | 0.53689 0.54772       |
| 1535.569        | 0.61255 0.59161 0.57067 0.55792 | 0.53932 0.54895       |
| 1535.689        | 0.61792 0.59668 0.57544 0.56376 | 0.54328 0.55357       |
| 1535.809        | 0.61768 0.59829 0.5789 0.56647 | 0.54756 0.5579        |
| 1535.929        | 0.61427 0.59541 0.57655 0.56429 | 0.5442 0.55296       |
| 1536.049        | 0.61592 0.59693 0.57794 0.56386 | 0.54603 0.55357       |
| 1536.169        | 0.62022 0.60015 0.58008 0.5693 | 0.54786 0.55419       |
| 1536.289        | 0.61962 0.60177 0.58392 0.57256 | 0.55247 0.5579        |
| 1536.409        | 0.61945 0.60202 0.58459 0.57267 | 0.55339 0.55914       |
| 1536.528        | 0.61952 0.59888 0.57824 0.56903 | 0.54878 0.55512       |
| 1536.648        | 0.61907 0.60024 0.58141 0.57058 | 0.5497 0.55512       |
| 1536.768        | 0.6239 0.60321 0.58252 0.57192 | 0.55124 0.55481       |
| 1536.888        | 0.62285 0.60372 0.58459 0.5708 | 0.55124 0.55419       |
| 1537.008        | 0.62361 0.60432 0.58503 0.57176 | 0.5537 0.55728       |
| 1537.128        | 0.62407 0.60355 0.58303 0.5701 | 0.55154 0.55419       |
| 1537.248        | 0.62814 0.60662 0.5851 0.57085 | 0.55216 0.55419       |
| 1537.368        | 0.62787 0.60704 0.58621 0.5754 | 0.55308 0.55542       |
| 1537.488        | 0.63204 0.60935 0.58666 0.57503 | 0.55647 0.55573       |
| 1537.607        | 0.63287 0.61106 0.58925 0.5804 | 0.5924 0.55883       |
| 1537.727        | 0.63163 0.61063 0.58963 0.58013 | 0.58832 0.55666      |
| 1537.847        | 0.63184 0.61088 0.58992 0.58078 | 0.55893 0.55635       |
| 1537.967        | 0.63351 0.61242 0.59133 0.58169 | 0.59955 0.5579       |
| 1538.087        | 0.63312 0.61491 0.5967 0.58282 | 0.56264 0.55914       |
| 1538.207        | 0.63598 0.61757 0.59916 0.58817 | 0.56481 0.56038       |
| 1538.327        | 0.63336 0.61697 0.60058 0.58477 | 0.56295 0.56255       |
| 1538.447        | 0.63753 0.61868 0.59983 0.58747 | 0.56481 0.56255       |
| 1538.566        | 0.63928 0.61765 0.59602 0.58758 | 0.56512 0.55914       |
| 1538.686        | 0.64145 0.62083 0.60021 0.59072 | 0.56792 0.56038       |
| 1538.806        | 0.64252 0.62402 0.60552 0.59305 | 0.56947 0.56348       |
| 1538.926        | 0.63883 0.61963 0.60043 0.58823 | 0.56699 0.56069       |
| 1539.046        | 0.64447 0.62144 0.59841 0.58925 | 0.56761 0.55976       |
| 1539.166        | 0.63852 0.62015 0.60178 0.58925 | 0.56885 0.55945       |
| 1539.286        | 0.64516 0.62583 0.6065 0.59273 | 0.5729 0.561         |
Table A2. Cont.

| Wavelength (nm) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) | NDII (mW) |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| DI Water 25.2 ppm | 0.6517 | 0.62929 | 0.60688 | 0.59735 | 0.5729 | 0.56193 |
| Water 2 43.5 ppm | 0.65148 | 0.62903 | 0.60658 | 0.59506 | 0.57509 | 0.56131 |
| Water 3 64.0 ppm | 0.64663 | 0.62773 | 0.60883 | 0.59588 | 0.57352 | 0.55976 |
| 1539.406 | 0.64923 | 0.62903 | 0.60883 | 0.59833 | 0.57477 | 0.56224 |
| 1539.526 | 0.65419 | 0.63328 | 0.61237 | 0.60139 | 0.57696 | 0.56441 |
| 1539.645 | 0.6544 | 0.63553 | 0.61562 | 0.60434 | 0.57947 | 0.56784 |
| 1539.765 | 0.65757 | 0.63701 | 0.61645 | 0.60478 | 0.58072 | 0.56628 |
| 1539.885 | 0.66163 | 0.64093 | 0.62023 | 0.60642 | 0.58607 | 0.56784 |
| 1540.005 | 0.66687 | 0.64146 | 0.62145 | 0.60878 | 0.59885 | 0.56784 |
| 1540.125 | 0.66888 | 0.64714 | 0.6254 | 0.61049 | 0.59017 | 0.57033 |
| 1540.245 | 0.66733 | 0.64635 | 0.626 | 0.61401 | 0.59207 | 0.5719 |
| 1540.365 | 0.6667 | 0.63919 | 0.61758 | 0.60533 | 0.58418 | 0.56753 |
| 1540.484 | 0.6656 | 0.64504 | 0.62448 | 0.61208 | 0.59143 | 0.5719 |
| 1540.604 | 0.67077 | 0.64968 | 0.62859 | 0.61467 | 0.59397 | 0.57252 |
| 1540.724 | 0.67384 | 0.65152 | 0.6292 | 0.6171 | 0.59492 | 0.57534 |
| 1540.844 | 0.6695 | 0.64924 | 0.62898 | 0.6155 | 0.59555 | 0.57503 |
| 1540.964 | 0.66931 | 0.65082 | 0.63233 | 0.61809 | 0.59428 | 0.57377 |
| 1541.084 | 0.67271 | 0.65275 | 0.63279 | 0.61688 | 0.59618 | 0.57534 |
| 1541.204 | 0.68003 | 0.65645 | 0.63287 | 0.62009 | 0.59936 | 0.57691 |
| 1541.324 | 0.68196 | 0.65768 | 0.6334 | 0.62347 | 0.60159 | 0.57754 |
| 1541.444 | 0.67908 | 0.65609 | 0.6331 | 0.61809 | 0.60127 | 0.57817 |
| 1541.563 | 0.67796 | 0.65733 | 0.6367 | 0.62286 | 0.60478 | 0.57879 |
| 1541.683 | 0.68338 | 0.66165 | 0.63992 | 0.62485 | 0.6051 | 0.58037 |
| 1541.803 | 0.6828 | 0.66263 | 0.64246 | 0.62674 | 0.60702 | 0.58194 |
| 1542.043 | 0.68196 | 0.65768 | 0.6334 | 0.62347 | 0.60159 | 0.57754 |
| 1542.163 | 0.67908 | 0.65609 | 0.6331 | 0.61809 | 0.60127 | 0.57817 |
| 1542.283 | 0.67796 | 0.65733 | 0.6367 | 0.62286 | 0.60478 | 0.57879 |
| 1542.403 | 0.68338 | 0.66165 | 0.63992 | 0.62485 | 0.6051 | 0.58037 |
| 1542.522 | 0.6828 | 0.66263 | 0.64246 | 0.62674 | 0.60702 | 0.58194 |
| 1542.642 | 0.68196 | 0.65768 | 0.6334 | 0.62347 | 0.60159 | 0.57754 |
| 1542.762 | 0.67908 | 0.65609 | 0.6331 | 0.61809 | 0.60127 | 0.57817 |
| 1542.882 | 0.67796 | 0.65733 | 0.6367 | 0.62286 | 0.60478 | 0.57879 |
| 1543.002 | 0.68338 | 0.66165 | 0.63992 | 0.62485 | 0.6051 | 0.58037 |
| 1543.122 | 0.6828 | 0.66263 | 0.64246 | 0.62674 | 0.60702 | 0.58194 |
| 1543.242 | 0.69194 | 0.66785 | 0.64376 | 0.6307 | 0.6099 | 0.58383 |
| 1543.362 | 0.68645 | 0.66484 | 0.64323 | 0.62814 | 0.60894 | 0.58509 |
| 1543.482 | 0.68584 | 0.66519 | 0.64454 | 0.63181 | 0.6099 | 0.58636 |
| 1543.601 | 0.69129 | 0.6683 | 0.64531 | 0.63209 | 0.61214 | 0.58794 |
| 1543.721 | 0.69079 | 0.66847 | 0.64615 | 0.63394 | 0.61086 | 0.58762 |
| Wavelength | NDII   | NDII   | NDII   | NDII   | NDII   | NDII   |
|------------|--------|--------|--------|--------|--------|--------|
| nm         | mW     | mW     | mW     | mW     | mW     | mW     |
| DI Water   | 25.2 ppm | Water 2 | 43.5 ppm | Water 3 | 64.0 ppm |
| 1543.841   | 0.6961 | 0.67248 | 0.64886 | 0.63617 | 0.61632 | 0.59238 |
| 1543.961   | 0.69443 | 0.67141 | 0.64839 | 0.63545 | 0.61407 | 0.59016 |
| 1544.081   | 0.6941 | 0.67256 | 0.65102 | 0.6364 | 0.61471 | 0.59269 |
| 1544.201   | 0.69518 | 0.67337 | 0.65156 | 0.63645 | 0.616 | 0.59142 |
| 1544.321   | 0.69867 | 0.67783 | 0.65699 | 0.64178 | 0.6189 | 0.59651 |
| 1544.441   | 0.70701 | 0.68266 | 0.65831 | 0.64296 | 0.62407 | 0.59874 |
| 1544.56    | 0.70144 | 0.67836 | 0.65528 | 0.64257 | 0.62245 | 0.5981 |
| 1544.68    | 0.70117 | 0.67881 | 0.65645 | 0.64313 | 0.62213 | 0.59683 |
| 1544.8     | 0.70591 | 0.6832 | 0.66049 | 0.646 | 0.62569 | 0.5997 |
| 1544.92    | 0.70794 | 0.68562 | 0.6633 | 0.65182 | 0.62991 | 0.60385 |
| 1545.04    | 0.70924 | 0.68732 | 0.6654 | 0.65103 | 0.63024 | 0.60706 |
| 1545.16    | 0.70735 | 0.68661 | 0.66587 | 0.65091 | 0.62991 | 0.60673 |
| 1545.28    | 0.71117 | 0.68993 | 0.66869 | 0.65391 | 0.63056 | 0.6093 |
| 1545.4     | 0.71107 | 0.69074 | 0.67041 | 0.65482 | 0.63284 | 0.61123 |
| 1545.52    | 0.71115 | 0.69192 | 0.67269 | 0.65862 | 0.63317 | 0.61252 |
| 1545.639   | 0.71684 | 0.6948 | 0.67276 | 0.65879 | 0.6348 | 0.61413 |
| 1545.759   | 0.71638 | 0.69426 | 0.67214 | 0.658 | 0.63317 | 0.61252 |
| 1545.879   | 0.71627 | 0.69444 | 0.67261 | 0.65788 | 0.63414 | 0.61316 |
| 1545.999   | 0.71613 | 0.69598 | 0.67583 | 0.65976 | 0.63643 | 0.61478 |
| 1546.119   | 0.71838 | 0.69742 | 0.67646 | 0.66084 | 0.63741 | 0.6151 |
| 1546.239   | 0.72598 | 0.70177 | 0.67756 | 0.66409 | 0.64068 | 0.61898 |
| 1546.359   | 0.72277 | 0.70123 | 0.67969 | 0.66329 | 0.64166 | 0.61962 |
| 1546.479   | 0.7235 | 0.70195 | 0.6804 | 0.66569 | 0.64396 | 0.62092 |
| 1546.598   | 0.725 | 0.70404 | 0.68308 | 0.66723 | 0.64659 | 0.62222 |
| 1546.718   | 0.72222 | 0.70277 | 0.68332 | 0.6686 | 0.64462 | 0.62124 |
| 1546.838   | 0.73196 | 0.7095 | 0.68704 | 0.67038 | 0.64955 | 0.62709 |
| 1546.958   | 0.72775 | 0.70668 | 0.68561 | 0.67043 | 0.64922 | 0.62774 |
| 1547.078   | 0.73353 | 0.71151 | 0.68949 | 0.67313 | 0.65318 | 0.63067 |
| 1547.198   | 0.73033 | 0.71023 | 0.69013 | 0.67336 | 0.65186 | 0.631 |
| 1547.318   | 0.73222 | 0.71169 | 0.69116 | 0.67502 | 0.65252 | 0.63035 |
| 1547.438   | 0.73384 | 0.71489 | 0.69594 | 0.67761 | 0.65649 | 0.63525 |
| 1547.557   | 0.7323 | 0.71352 | 0.69474 | 0.67876 | 0.65285 | 0.63394 |
| 1547.677   | 0.73636 | 0.71599 | 0.69562 | 0.67836 | 0.65517 | 0.63557 |
| 1547.797   | 0.7328 | 0.71397 | 0.69514 | 0.67761 | 0.65616 | 0.63361 |
| 1547.917   | 0.73969 | 0.71901 | 0.69833 | 0.68078 | 0.65948 | 0.63885 |
| 1548.037   | 0.7416 | 0.72112 | 0.70064 | 0.68436 | 0.66147 | 0.64115 |
| 1548.157   | 0.74294 | 0.72287 | 0.7028 | 0.68587 | 0.66413 | 0.64181 |
Table A2. Cont.

| Wavelength (nm) | DI Water 25.2 ppm | Water 2 43.5 ppm | Water 3 64.0 ppm |
|-----------------|--------------------|------------------|------------------|
| 1548.277        | 0.74673            | 0.72645          |                  |
| 1548.397        | 0.7439             | 0.72323          |                  |
| 1548.516        | 0.74703            | 0.72728          |                  |
| 1548.636        | 0.75317            | 0.73236          |                  |
| 1548.756        | 0.75597            | 0.73505          |                  |
| 1548.876        | 0.75013            | 0.73338          |                  |
| 1548.996        | 0.75196            | 0.73236          |                  |
| 1549.116        | 0.7561             | 0.73681          |                  |
| 1549.236        | 0.75338            | 0.73662          |                  |
| 1549.356        | 0.75768            | 0.73885          |                  |
| 1549.475        | 0.75861            | 0.74191          |                  |
| 1549.595        | 0.76076            | 0.74043          |                  |
| 1549.715        | 0.75874            | 0.74108          |                  |
| 1549.835        | 0.76532            | 0.74685          |                  |
| 1549.955        | 0.77077            | 0.75059          |                  |
| 1550.075        | 0.76692            | 0.74891          |                  |
| 1550.195        | 0.76662            | 0.74807          |                  |
| 1550.315        | 0.76931            | 0.75227          |                  |
| 1550.435        | 0.77103            | 0.75415          |                  |
| 1550.554        | 0.77644            | 0.75997          |                  |
| 1550.674        | 0.77855            | 0.76053          |                  |
| 1550.794        | 0.77572            | 0.75846          |                  |
| 1550.914        | 0.77438            | 0.75865          |                  |
| 1551.034        | 0.77538            | 0.761             |                  |
| 1551.154        | 0.78577            | 0.76751          |                  |
| 1551.274        | 0.77862            | 0.76373          |                  |
| 1551.394        | 0.78722            | 0.76647          |                  |
| 1551.513        | 0.78558            | 0.76779          |                  |
| 1551.633        | 0.78389            | 0.76789          |                  |
| 1551.753        | 0.79135            | 0.77319          |                  |
| 1551.873        | 0.79585            | 0.77594          |                  |
| 1551.993        | 0.79432            | 0.77509          |                  |
| 1552.113        | 0.7939             | 0.77575          |                  |
| 1552.233        | 0.7995             | 0.77946          |                  |
| 1552.353        | 0.80633            | 0.78795          |                  |
Table A2. Cont.

| Wavelength (nm) | NDII DI Water 25.2 ppm | NDII Water 2 43.5 ppm | NDII Water 3 64.0 ppm |
|----------------|------------------------|----------------------|----------------------|
| 1552.473       | 0.80423                | 0.78661              | 0.76899              |
| 1552.592       | 0.80431                | 0.78853              | 0.77275              |
| 1552.712       | 0.80448                | 0.78757              | 0.77066              |
| 1552.832       | 0.80695                | 0.78968              | 0.77241              |
| 1552.952       | 0.81271                | 0.79591              | 0.77911              |
| 1553.072       | 0.81535                | 0.79639              | 0.77743              |
| 1553.192       | 0.81192                | 0.79514              | 0.77836              |
| 1553.312       | 0.81002                | 0.79553              | 0.78104              |
| 1553.432       | 0.80936                | 0.79659              | 0.78382              |
| 1553.551       | 0.81399                | 0.80063              | 0.78727              |
| 1553.671       | 0.82159                | 0.80536              | 0.78913              |
| 1553.791       | 0.82201                | 0.80671              | 0.79141              |
| 1553.911       | 0.82297                | 0.80584              | 0.78871              |
| 1554.031       | 0.82577                | 0.80952              | 0.79327              |
| 1554.151       | 0.82942                | 0.81457              | 0.79972              |
| 1554.271       | 0.83184                | 0.81612              | 0.8004               |
| 1554.391       | 0.83197                | 0.81661              | 0.80125              |
| 1554.51        | 0.82876                | 0.81428              | 0.7998               |
| 1554.63        | 0.83265                | 0.81895              | 0.80525              |
| 1554.75        | 0.83875                | 0.82217              | 0.80559              |
| 1554.87        | 0.84071                | 0.82525              | 0.80969              |
| 1554.99        | 0.83796                | 0.82344              | 0.80892              |
| 1555.11        | 0.83917                | 0.82498              | 0.81063              |
| 1555.23        | 0.84242                | 0.82794              | 0.81346              |
| 1555.35        | 0.8488                 | 0.83216              | 0.81552              |
| 1555.469       | 0.84929                | 0.83481              | 0.82033              |
| 1555.589       | 0.85237                | 0.83609              | 0.81981              |
| 1555.709       | 0.85114                | 0.83668              | 0.82222              |
| 1555.829       | 0.85743                | 0.84112              | 0.82481              |
| 1555.949       | 0.86059                | 0.84369              | 0.82679              |
| 1556.069       | 0.85977                | 0.84497              | 0.83017              |
| 1556.189       | 0.85971                | 0.84507              | 0.83043              |
| 1556.309       | 0.86231                | 0.84784              | 0.83337              |
| 1556.429       | 0.86566                | 0.84943              | 0.8332               |
| 1556.548       | 0.86356                | 0.85003              | 0.8365               |
| 1556.668       | 0.86858                | 0.8538               | 0.83902              |
| 1556.788       | 0.87084                | 0.8551               | 0.83936              |

mW = milliwatt
Table A2. Cont.

| Wavelength (nm) | NDII 0.25 ppm | NDII 25.2 ppm | NDII 43.5 ppm | NDII 64.0 ppm |
|-----------------|---------------|---------------|---------------|---------------|
| DI Water        | 0.87313       | 0.85838       | 0.84363       | 0.82758       | 0.79964       | 0.81126       |
| 1556.908        | 0.87394       | 0.85918       | 0.84442       | 0.82929       | 0.8          | 0.81163       |
| 1557.148        | 0.87538       | 0.86108       | 0.84678       | 0.82998       | 0.8011       | 0.81568       |
| 1557.268        | 0.88238       | 0.86668       | 0.85098       | 0.83373       | 0.80438      | 0.81863       |
| 1557.388        | 0.88802       | 0.87099       | 0.85396       | 0.83683       | 0.80914      | 0.82159       |
| 1557.507        | 0.89148       | 0.8725        | 0.85352       | 0.8415        | 0.81134      | 0.82345       |
| 1557.627        | 0.88677       | 0.87019       | 0.85361       | 0.83787       | 0.81134      | 0.82345       |
| 1557.747        | 0.89029       | 0.873         | 0.85571       | 0.84182       | 0.81317      | 0.82419       |
| 1557.867        | 0.89629       | 0.87895       | 0.86161       | 0.84412       | 0.81795      | 0.8279        |
| 1558.087        | 0.89623       | 0.87976       | 0.86329       | 0.84489       | 0.82164      | 0.83013       |
| 1558.107        | 0.89502       | 0.88238       | 0.86974       | 0.85156       | 0.82423      | 0.83684       |
| 1558.227        | 0.89439       | 0.88127       | 0.86815       | 0.84969       | 0.82312      | 0.83684       |
| 1558.347        | 0.90021       | 0.88471       | 0.86921       | 0.85233       | 0.8246       | 0.83684       |
| 1558.467        | 0.90288       | 0.88755       | 0.87222       | 0.85246       | 0.82682      | 0.83984       |
| 1558.586        | 0.90357       | 0.88927       | 0.87497       | 0.85877       | 0.82979      | 0.84246       |
| 1558.706        | 0.91208       | 0.89344       | 0.8748        | 0.85677       | 0.8309       | 0.84246       |
| 1558.826        | 0.90884       | 0.89364       | 0.87844       | 0.86245       | 0.83462      | 0.84509       |
| 1558.946        | 0.91572       | 0.89904       | 0.88236       | 0.86484       | 0.83909      | 0.8496        |
| 1559.066        | 0.92115       | 0.9018        | 0.88245       | 0.86504       | 0.83947      | 0.8496        |
| 1559.186        | 0.92187       | 0.90426       | 0.88665       | 0.87029       | 0.84021      | 0.85413       |
| 1559.306        | 0.92322       | 0.90641       | 0.8896        | 0.8725        | 0.8462       | 0.85602       |
| 1559.426        | 0.92339       | 0.90753       | 0.89167       | 0.87699       | 0.8492       | 0.85753       |
| 1559.545        | 0.92797       | 0.91031       | 0.89265       | 0.87915       | 0.85409      | 0.8636        |
| 1559.665        | 0.92835       | 0.91041       | 0.89247       | 0.87908       | 0.85259      | 0.86246       |
| 1559.785        | 0.93072       | 0.9138        | 0.89688       | 0.8815        | 0.85711      | 0.8655        |
| 1559.905        | 0.93318       | 0.9171        | 0.90102       | 0.88333       | 0.85975      | 0.8693        |
| 1560.025        | 0.93376       | 0.91906       | 0.90436       | 0.88602       | 0.85975      | 0.86969       |
| 1560.145        | 0.9364        | 0.92133       | 0.90626       | 0.88818       | 0.86429      | 0.87274       |
| 1560.265        | 0.93608       | 0.9204        | 0.90472       | 0.8868        | 0.8624       | 0.87121       |
| 1560.385        | 0.93648       | 0.92123       | 0.9058        | 0.89022       | 0.86392      | 0.87159       |
| 1560.505        | 0.94176       | 0.9265        | 0.91124       | 0.89213       | 0.86505      | 0.87503       |
| 1560.624        | 0.94274       | 0.92785       | 0.91296       | 0.89555       | 0.86847      | 0.87809       |
| 1560.744        | 0.94275       | 0.92858       | 0.91441       | 0.89773       | 0.87075      | 0.88193       |
| 1560.864        | 0.94308       | 0.92879       | 0.9145        | 0.89991       | 0.87227      | 0.87809       |
| 1560.984        | 0.94631       | 0.93159       | 0.91687       | 0.90308       | 0.87266      | 0.8827        |
| 1561.104        | 0.94526       | 0.93325       | 0.92124       | 0.90302       | 0.87647      | 0.88385       |
| Wavelength nm | NDII mW | NDII mW | NDII mW | NDII mW | NDII mW | NDII mW | NDII mW |
|--------------|--------|--------|--------|--------|--------|--------|--------|
| 1561.224     | 0.95679 | 0.93888 | 0.92097 | 0.90806 | 0.88259 | 0.88847 |
| 1561.344     | 0.95615 | 0.94066 | 0.92517 | 0.90892 | 0.88489 | 0.88963 |
| 1561.464     | 0.95451 | 0.9361 | 0.92471 | 0.90925 | 0.88297 | 0.89002 |
| 1561.583     | 0.95615 | 0.94139 | 0.92663 | 0.91211 | 0.88604 | 0.89388 |
| 1561.703     | 0.95373 | 0.9416 | 0.92947 | 0.91264 | 0.88835 | 0.89272 |
| 1561.823     | 0.95509 | 0.94379 | 0.93249 | 0.91591 | 0.8922 | 0.89775 |
| 1561.943     | 0.95365 | 0.94243 | 0.93121 | 0.91711 | 0.8895 | 0.89775 |
| 1562.063     | 0.95803 | 0.94421 | 0.93039 | 0.91598 | 0.88874 | 0.8962 |
| 1562.183     | 0.95876 | 0.94526 | 0.93176 | 0.91564 | 0.89105 | 0.89737 |
| 1562.303     | 0.96019 | 0.94662 | 0.93305 | 0.92045 | 0.89452 | 0.89853 |
| 1562.423     | 0.96544 | 0.95145 | 0.93746 | 0.92139 | 0.89683 | 0.9028 |
| 1562.542     | 0.96202 | 0.95029 | 0.93856 | 0.92279 | 0.89722 | 0.90164 |
| 1562.662     | 0.96345 | 0.95239 | 0.94133 | 0.92514 | 0.90303 | 0.90436 |
| 1562.782     | 0.96405 | 0.95292 | 0.94179 | 0.92682 | 0.90303 | 0.90475 |
| 1562.902     | 0.96694 | 0.95418 | 0.94142 | 0.92803 | 0.90381 | 0.9067 |
| 1563.022     | 0.97088 | 0.95892 | 0.94696 | 0.93139 | 0.90964 | 0.91177 |
| 1563.142     | 0.97729 | 0.96125 | 0.9452 | 0.93327 | 0.91042 | 0.91099 |
| 1563.262     | 0.98311 | 0.96601 | 0.94891 | 0.93698 | 0.91588 | 0.91412 |
| 1563.382     | 0.97743 | 0.96326 | 0.94909 | 0.93638 | 0.91471 | 0.91334 |
| 1563.501     | 0.98363 | 0.96738 | 0.95113 | 0.93881 | 0.9198 | 0.91568 |
| 1563.621     | 0.97304 | 0.96283 | 0.95262 | 0.93969 | 0.91549 | 0.91647 |
| 1563.741     | 0.97548 | 0.96558 | 0.95568 | 0.94097 | 0.91862 | 0.91725 |
| 1563.861     | 0.97912 | 0.96791 | 0.9567 | 0.93982 | 0.92176 | 0.91961 |
| 1563.981     | 0.97801 | 0.96601 | 0.95401 | 0.93901 | 0.9194 | 0.91647 |
| 1564.101     | 0.98781 | 0.97407 | 0.96033 | 0.94436 | 0.92529 | 0.92 |
| 1564.221     | 0.98063 | 0.97067 | 0.96071 | 0.94619 | 0.92529 | 0.92157 |
| 1564.341     | 0.97838 | 0.97057 | 0.96276 | 0.94762 | 0.92765 | 0.92393 |
| 1564.461     | 0.98368 | 0.97322 | 0.96276 | 0.94898 | 0.92883 | 0.92354 |
| 1564.58      | 0.9874 | 0.97695 | 0.9665 | 0.9534 | 0.93278 | 0.92472 |
| 1564.7       | 0.99038 | 0.98036 | 0.97034 | 0.9577 | 0.93831 | 0.93104 |
| 1564.82      | 0.9892 | 0.97855 | 0.9679 | 0.95681 | 0.93633 | 0.93064 |
| 1564.94      | 0.98566 | 0.97823 | 0.9708 | 0.95872 | 0.9399 | 0.93183 |
| 1565.06      | 0.98168 | 0.97493 | 0.96818 | 0.95879 | 0.93792 | 0.92867 |
| 1565.18      | 0.9932 | 0.98261 | 0.97202 | 0.96242 | 0.94347 | 0.93301 |
| 1565.3       | 0.99244 | 0.98303 | 0.97362 | 0.9618 | 0.94506 | 0.9346 |
| 1565.42      | 0.98877 | 0.98143 | 0.97409 | 0.96214 | 0.94625 | 0.93618 |
Table A2. Cont.

| Wavelength (nm) | NDII 25.2 ppm mW | NDII 43.5 ppm mW | NDII 64.0 ppm mW |
|-----------------|------------------|------------------|------------------|
| DI Water        |                  |                  |                  |
| 1565.539        | 0.99264          | 0.98421          | 0.97578          |
| 1565.659        | 0.99326          | 0.98325          | 0.97324          |
| 1565.779        | 0.99524          | 0.98678          | 0.97832          |
| 1565.899        | 0.99464          | 0.98549          | 0.97634          |
| 1566.019        | 0.99779          | 0.98796          | 0.97813          |
| 1566.139        | 0.9967           | 0.98817          | 0.97964          |
| 1566.259        | 1.001            | 0.99107          | 0.98114          |
| 1566.379        | 0.99199          | 0.98817          | 0.98435          |
| 1566.499        | 0.99769          | 0.99107          | 0.98445          |
| 1566.618        | 0.99921          | 0.99386          | 0.98851          |
| 1566.738        | 1.00015          | 0.99386          | 0.98757          |
| 1566.858        | 0.99771          | 0.99472          | 0.99173          |
| 1566.978        | 0.99288          | 0.99117          | 0.98946          |
| 1567.098        | 0.99197          | 0.99408          | 0.99619          |
| 1567.218        | 0.99499          | 0.99526          | 0.99553          |
| 1567.338        | 0.99414          | 0.99289          | 0.99164          |
| 1567.458        | 0.99635          | 0.99537          | 0.99439          |
| 1567.577        | 0.99623          | 0.99332          | 0.99041          |
| 1567.697        | 0.99897          | 0.99644          | 0.99391          |
| 1567.817        | 0.99721          | 0.99547          | 0.99373          |
| 1567.937        | 0.99596          | 0.99451          | 0.99306          |
| 1568.057        | 0.99614          | 0.99569          | 0.99524          |
| 1568.177        | 0.99668          | 0.99634          | 0.996         |
| 1568.297        | 0.99786          | 0.99817          | 0.99848          |
| 1568.417        | 1.00069          | 0.99892          | 0.99715          |
| 1568.536        | 0.99799          | 0.99795          | 0.99791          |
| 1568.656        | 0.99838          | 0.99881          | 0.99924          |
| 1568.776        | 1.00095          | 1                | 0.99905          |
| 1568.896        | 0.99784          | 0.99892          | 1                |
| 1569.016        | 0.99719          | 0.99774          | 0.99829          |
| 1569.136        | 0.99194          | 0.99483          | 0.99772          |
| 1569.256        | 0.99605          | 0.99655          | 0.99705          |
| 1569.376        | 0.9924           | 0.99558          | 0.99876          |
| 1569.495        | 0.98929          | 0.99236          | 0.99543          |
| 1569.615        | 0.9903           | 0.99225          | 0.9942           |
| 1569.735        | 0.99004          | 0.99193          | 0.99382          |
| 1569.855        | 0.9858           | 0.98967          | 0.99354          |
| Wavelength (nm) | NDII Water 25.2 ppm | NDII Water 43.5 ppm | NDII Water 64.0 ppm |
|----------------|----------------------|---------------------|---------------------|
| 1569.975       | 0.98847              | 0.99214             | 0.99581             |
| 1570.095       | 0.98734              | 0.99096             | 0.99458             |
| 1570.215       | 0.98598              | 0.99085             | 0.99572             |
| 1570.335       | 0.98584              | 0.98817             | 0.9905              |
| 1570.455       | 0.98741              | 0.99085             | 0.99429             |
| 1570.574       | 0.98662              | 0.98989             | 0.99316             |
| 1570.694       | 0.98788              | 0.99085             | 0.99382             |
| 1570.814       | 0.98669              | 0.98978             | 0.99287             |
| 1570.934       | 0.99066              | 0.99096             | 0.99126             |
| 1571.054       | 0.98401              | 0.98806             | 0.99211             |
| 1571.174       | 0.98135              | 0.98635             | 0.99135             |
| 1571.294       | 0.98314              | 0.98796             | 0.99278             |
| 1571.414       | 0.98806              | 0.98914             | 0.99022             |
| 1571.533       | 0.97941              | 0.98207             | 0.98473             |
| 1571.653       | 0.97832              | 0.98228             | 0.98624             |
| 1571.773       | 0.97741              | 0.98154             | 0.98567             |
| 1571.893       | 0.97334              | 0.97908             | 0.98482             |
| 1572.013       | 0.97069              | 0.97738             | 0.98407             |
| 1572.133       | 0.97226              | 0.97642             | 0.98058             |
| 1572.253       | 0.97158              | 0.97674             | 0.9819              |
| 1572.373       | 0.97191              | 0.97695             | 0.98199             |
| 1572.493       | 0.97258              | 0.97738             | 0.98218             |
| 1572.612       | 0.96465              | 0.97078             | 0.97691             |
| 1572.732       | 0.96542              | 0.97248             | 0.97954             |
| 1572.852       | 0.96262              | 0.96887             | 0.97512             |
| 1572.972       | 0.96064              | 0.9676              | 0.97456             |
| 1573.092       | 0.95602              | 0.96463             | 0.97324             |
| 1573.212       | 0.95367              | 0.96177             | 0.96987             |
| 1573.332       | 0.95202              | 0.95935             | 0.96668             |
| 1573.452       | 0.9468               | 0.9566              | 0.9664              |
| 1573.571       | 0.94577              | 0.95534             | 0.96491             |
| 1573.691       | 0.95032              | 0.95766             | 0.965               |
| 1573.811       | 0.95038              | 0.95755             | 0.96472             |
| 1573.931       | 0.94029              | 0.95092             | 0.96155             |
| 1574.051       | 0.93684              | 0.9484              | 0.95996             |
| 1574.171       | 0.94019              | 0.9504              | 0.96061             |
| 1574.291       | 0.93787              | 0.94966             | 0.96145             |
Table A2. Cont.

| Wavelength (nm) | NDII 25.2 ppm mW | NDII 43.5 ppm mW | NDII 64.0 ppm mW |
|----------------|------------------|------------------|------------------|
| DI Water       | 0.94057          | 0.9505           | 0.96043          |
|                | 0.94442          | 0.95587          | 0.96969          |
|                | 0.94212          | 0.95159          | 0.96639          |
|                | 0.94306          | 0.95317          | 0.96887          |
|                | 0.94107          | 0.95252          | 0.96777          |
|                | 0.93846          | 0.95252          | 0.96708          |
|                | 0.93607          | 0.94706          | 0.96112          |
|                | 0.92962          | 0.94105          | 0.95565          |
|                | 0.9244           | 0.94307          | 0.95544          |
|                | 0.9219           | 0.94327          | 0.95555          |
|                | 0.92879          | 0.94105          | 0.95565          |
|                | 0.92443          | 0.93912          | 0.95272          |
|                | 0.92278          | 0.93516          | 0.95142          |
|                | 0.91926          | 0.93268          | 0.9466           |
|                | 0.91864          | 0.93103          | 0.947             |
|                | 0.9136           | 0.92809          | 0.94355          |
|                | 0.90969          | 0.9259           | 0.94409          |
|                | 0.90866          | 0.9259           | 0.93867          |
|                | 0.90877          | 0.92161          | 0.94131          |
|                | 0.90661          | 0.92133          | 0.93766          |
|                | 0.89853          | 0.9166           | 0.93152          |
|                | 0.89619          | 0.91351          | 0.93307          |
|                | 0.89344          | 0.90888          | 0.92581          |
|                | 0.89323          | 0.90924          | 0.9293           |
|                | 0.89029          | 0.90499          | 0.92554          |
|                | 0.87996          | 0.89814          | 0.91965          |
|                | 0.87895          | 0.89364          | 0.91431          |
|                | 0.87522          | 0.88535          | 0.91145          |
|                | 0.87804          | 0.89616          | 0.91524          |
|                | 0.87059          | 0.89149          | 0.91052          |
|                | 0.88532          | 0.9054           | 0.9308           |
|                | 0.85992          | 0.87804          | 0.89616          |
|                | 0.85749          | 0.87915          | 0.89932          |
|                | 0.8583           | 0.87889          | 0.89971          |
|                | 0.85838          | 0.88532          | 0.9054           |
|                | 0.85589          | 0.87266          | 0.89806          |
|                | 0.85052          | 0.87071          | 0.89305          |
|                | 0.84547          | 0.86558          | 0.88818          |
|                | 0.84388          | 0.86311          | 0.88792          |
|                | 0.84057          | 0.86043          | 0.90018          |
| Wavelength nm | DI Water 25.2 ppm mW | Water 2 43.5 ppm mW | Water 3 64.0 ppm mW |
|---------------|----------------------|----------------------|----------------------|
| 1578.726      | 0.81845              | 0.84003              |                      |
| 1578.846      | 0.81583              | 0.83806              |                      |
| 1578.966      | 0.81443              | 0.8356               |                      |
| 1579.086      | 0.80873              | 0.82784              |                      |
| 1579.206      | 0.80486              | 0.82451              |                      |
| 1579.326      | 0.80134              | 0.82266              |                      |
| 1579.446      | 0.79802              | 0.82109              |                      |
| 1579.565      | 0.78503              | 0.8102               |                      |
| 1579.685      | 0.78422              | 0.80633              |                      |
| 1579.805      | 0.78272              | 0.80536              |                      |
| 1579.925      | 0.77712              | 0.80092              |                      |
| 1580.045      | 0.77461              | 0.79764              |                      |
| 1580.165      | 0.77084              | 0.79438              |                      |
| 1580.285      | 0.76761              | 0.78968              |                      |
| 1580.405      | 0.75576              | 0.78136              |                      |
| 1580.525      | 0.75866              | 0.78089              |                      |
| 1580.644      | 0.75028              | 0.77632              |                      |
| 1580.764      | 0.74705              | 0.773                |                      |
| 1580.884      | 0.74328              | 0.76921              |                      |
| 1581.004      | 0.74383              | 0.76534              |                      |
| 1581.124      | 0.73345              | 0.75771              |                      |
| 1581.244      | 0.72756              | 0.75405              |                      |
| 1581.364      | 0.72969              | 0.75583              |                      |
| 1581.484      | 0.71835              | 0.74555              |                      |
| 1581.603      | 0.71562              | 0.74043              |                      |
| 1581.723      | 0.71143              | 0.73746              |                      |
| 1581.843      | 0.70927              | 0.73273              |                      |
| 1581.963      | 0.7058               | 0.73116              |                      |
| 1582.083      | 0.69731              | 0.72489              |                      |
| 1582.203      | 0.69655              | 0.72241              |                      |
| 1582.323      | 0.68691              | 0.71434              |                      |
| 1582.443      | 0.69047              | 0.71571              |                      |
| 1582.562      | 0.68405              | 0.71078              |                      |
| 1582.682      | 0.68787              | 0.71114              |                      |
| 1582.802      | 0.67707              | 0.70431              |                      |
| 1582.922      | 0.68058              | 0.70395              |                      |
Table A2. Cont.

| Wavelength nm | NDII mW | NDII mW | NDII mW | NDII mW | NDII mW | NDII mW |
|---------------|---------|---------|---------|---------|---------|---------|
| 1583.042      | 0.66695 | 0.69543 | 0.72391 | 0.75247 | 0.79346 | 0.80942 |
| 1583.162      | 0.66529 | 0.69318 | 0.72107 | 0.74915 | 0.7902  | 0.80722 |
| 1583.282      | 0.65903 | 0.68993 | 0.72083 | 0.7474  | 0.7902  | 0.80649 |
| 1583.402      | 0.65319 | 0.68382 | 0.71445 | 0.74397 | 0.78767 | 0.80282 |
| 1583.521      | 0.6524  | 0.68149 | 0.71058 | 0.74073 | 0.78262 | 0.80026 |
| 1583.641      | 0.64782 | 0.67595 | 0.70408 | 0.73456 | 0.77579 | 0.79625 |
| 1583.761      | 0.64309 | 0.67123 | 0.69937 | 0.72878 | 0.77399 | 0.7908  |
| 1583.881      | 0.63588 | 0.66555 | 0.69522 | 0.72337 | 0.76756 | 0.78319 |
| 1584.001      | 0.63381 | 0.66165 | 0.68949 | 0.71975 | 0.76399 | 0.7803  |
| 1584.121      | 0.62773 | 0.65671 | 0.68569 | 0.71568 | 0.76186 | 0.77814 |
| 1584.241      | 0.61853 | 0.64836 | 0.67819 | 0.71037 | 0.7537  | 0.76916 |
| 1584.361      | 0.60992 | 0.64154 | 0.67316 | 0.70439 | 0.74735 | 0.76415 |
| 1584.48       | 0.60254 | 0.63362 | 0.6647  | 0.69597 | 0.73962 | 0.75845 |
| 1584.6        | 0.6022  | 0.63189 | 0.66158 | 0.69422 | 0.73682 | 0.75596 |
| 1584.72       | 0.59431 | 0.62592 | 0.65753 | 0.69039 | 0.73333 | 0.75135 |
| 1584.84       | 0.59387 | 0.62376 | 0.65365 | 0.68749 | 0.72845 | 0.74711 |
| 1584.96       | 0.58845 | 0.61765 | 0.64685 | 0.6809  | 0.72533 | 0.73972 |
| 1585.08       | 0.57725 | 0.60943 | 0.64161 | 0.6729  | 0.71771 | 0.73445 |
| 1585.2        | 0.57635 | 0.60687 | 0.63739 | 0.67233 | 0.71668 | 0.72921 |
| 1585.32       | 0.56972 | 0.60321 | 0.6367  | 0.66935 | 0.71461 | 0.72851 |
| 1585.44       | 0.56321 | 0.59888 | 0.63455 | 0.66997 | 0.71288 | 0.72607 |
| 1585.559      | 0.55866 | 0.59237 | 0.62608 | 0.65811 | 0.70533 | 0.71913 |
| 1585.679      | 0.55165 | 0.58613 | 0.62061 | 0.65182 | 0.69952 | 0.71255 |
| 1585.799      | 0.54801 | 0.57951 | 0.61101 | 0.64668 | 0.69441 | 0.70636 |
| 1585.919      | 0.54668 | 0.57817 | 0.60966 | 0.64392 | 0.69339 | 0.70567 |
| 1586.039      | 0.53969 | 0.57366 | 0.60763 | 0.6433  | 0.69237 | 0.70361 |
| 1586.159      | 0.53413 | 0.56668 | 0.59923 | 0.6326  | 0.68324 | 0.69642 |
| 1586.279      | 0.52738 | 0.55932 | 0.59126 | 0.62641 | 0.6755  | 0.68791 |
| 1586.399      | 0.52211 | 0.5515  | 0.58089 | 0.61809 | 0.6678  | 0.6781  |
| 1586.518      | 0.51973 | 0.55068 | 0.58163 | 0.61975 | 0.6678  | 0.67911 |
| 1586.638      | 0.50932 | 0.54503 | 0.58074 | 0.61749 | 0.66513 | 0.67844 |
| 1586.758      | 0.50863 | 0.54185 | 0.57507 | 0.60999 | 0.65881 | 0.67339 |
| 1586.878      | 0.49881 | 0.53291 | 0.56701 | 0.60341 | 0.65186 | 0.66401 |
| 1586.998      | 0.49703 | 0.52976 | 0.56249 | 0.59789 | 0.64922 | 0.65901 |
| 1587.118      | 0.4939  | 0.52645 | 0.559   | 0.59659 | 0.64363 | 0.65735 |
| 1587.238      | 0.48947 | 0.52242 | 0.55537 | 0.59169 | 0.6397  | 0.65138 |
| 1587.358      | 0.48467 | 0.51897 | 0.55327 | 0.58996 | 0.64035 | 0.65138 |
| Wavelength (nm) | NDII 25.2 ppm mW | NDII 43.5 ppm mW | NDII 64.0 ppm mW |
|----------------|------------------|------------------|------------------|
| 1587.478       | 0.47755          | 0.51425          | 0.55095          |
| 1587.597       | 0.47758          | 0.51113          | 0.54468          |
| 1587.717       | 0.47239          | 0.50477          | 0.53715          |
| 1587.837       | 0.47051          | 0.5039           | 0.53729          |
| 1587.957       | 0.47251          | 0.50358          | 0.53465          |
| 1588.077       | 0.46462          | 0.49607          | 0.52752          |
| 1588.197       | 0.45914          | 0.48922          | 0.5193           |
| 1588.317       | 0.45084          | 0.48148          | 0.51212          |
| 1588.437       | 0.45141          | 0.48015          | 0.50889          |
| 1588.556       | 0.44547          | 0.47564          | 0.50581          |
| 1588.676       | 0.43471          | 0.46712          | 0.49953          |
| 1588.796       | 0.4273           | 0.45842          | 0.48954          |
| 1588.916       | 0.42047          | 0.45245          | 0.48443          |
| 1589.036       | 0.41625          | 0.44773          | 0.47921          |
| 1589.156       | 0.41291          | 0.4437           | 0.47449          |
| 1589.276       | 0.4109           | 0.44075          | 0.4706           |
| 1589.396       | 0.40296          | 0.43365          | 0.46434          |
| 1589.516       | 0.39574          | 0.42757          | 0.4594           |
| 1589.635       | 0.39227          | 0.42196          | 0.45165          |
| 1589.755       | 0.38384          | 0.4163           | 0.44876          |
| 1589.875       | 0.38351          | 0.41296          | 0.44241          |
| 1589.995       | 0.38148          | 0.41015          | 0.43882          |
| 1590.115       | 0.37601          | 0.4033           | 0.43059          |
| 1590.235       | 0.36726          | 0.39458          | 0.4219           |
| 1590.355       | 0.36501          | 0.3926           | 0.42019          |
| 1590.474       | 0.36299          | 0.3894           | 0.41581          |
| 1590.594       | 0.35732          | 0.38679          | 0.41626          |
| 1590.714       | 0.34983          | 0.3807           | 0.41157          |
| 1590.834       | 0.34006          | 0.37156          | 0.40306          |
| 1590.954       | 0.33374          | 0.36498          | 0.39622          |
| 1591.074       | 0.33253          | 0.36306          | 0.39359          |
| 1591.194       | 0.33218          | 0.36128          | 0.39038          |
| 1591.314       | 0.33136          | 0.35972          | 0.38808          |
| 1591.434       | 0.31875          | 0.35045          | 0.38215          |
| 1591.553       | 0.31471          | 0.34314          | 0.37157          |
| 1591.673       | 0.31183          | 0.34006          | 0.36829          |
| 1591.793       | 0.30852          | 0.33671          | 0.3649           |
Table A2. Cont.

| Wavelength (nm) | NDII 25.2 ppm | NDII 43.5 ppm | NDII 64.0 ppm |
|-----------------|----------------|----------------|----------------|
| 1591.913        | 0.30491        | 0.33337        | 0.36183        |
| 1592.033        | 0.29943        | 0.32782        | 0.35621        |
| 1592.153        | 0.29143        | 0.31886        | 0.34629        |
| 1592.273        | 0.29393        | 0.31749        | 0.34105        |
| 1592.393        | 0.29109        | 0.31585        | 0.34061        |
| 1592.512        | 0.2936         | 0.31797        | 0.34234        |
| 1592.632        | 0.28931        | 0.31352        | 0.33773        |
| 1592.752        | 0.28369        | 0.30704        | 0.33039        |
| 1592.872        | 0.27234        | 0.29884        | 0.32534        |
| 1592.992        | 0.2732         | 0.29851        | 0.32382        |
| 1593.112        | 0.26826        | 0.29601        | 0.32376        |
| 1593.232        | 0.26865        | 0.2946         | 0.32055        |
| 1593.352        | 0.26116        | 0.28802        | 0.31488        |
| 1593.472        | 0.25245        | 0.27863        | 0.30481        |
| 1593.591        | 0.24561        | 0.27393        | 0.30225        |
| 1593.711        | 0.24993        | 0.27327        | 0.29661        |
| 1593.831        | 0.24602        | 0.26951        | 0.293          |
| 1593.951        | 0.23659        | 0.26144        | 0.28629        |
| 1594.071        | 0.23407        | 0.25492        | 0.27577        |
| 1594.191        | 0.22427        | 0.24683        | 0.26939        |
| 1594.311        | 0.22383        | 0.2458         | 0.26777        |
| 1594.431        | 0.21726        | 0.23943        | 0.2616         |
| 1594.55         | 0.21433        | 0.23413        | 0.25393        |
| 1594.67         | 0.21065        | 0.22993        | 0.24921        |
| 1594.79         | 0.20236        | 0.22258        | 0.2428         |
| 1594.91         | 0.20005        | 0.21892        | 0.23779        |
| 1595.03         | 0.19201        | 0.21428        | 0.23655        |
| 1595.15         | 0.18687        | 0.21115        | 0.23543        |
| 1595.27         | 0.18641        | 0.20815        | 0.22989        |
| 1595.39         | 0.17714        | 0.19984        | 0.22254        |
| 1595.51         | 0.17003        | 0.19374        | 0.21745        |
| 1595.629        | 0.16737        | 0.18963        | 0.21189        |
| 1595.749        | 0.17025        | 0.18981        | 0.20937        |
| 1595.869        | 0.16465        | 0.18559        | 0.20653        |
| 1595.989        | 0.15777        | 0.17975        | 0.20173        |
| 1596.109        | 0.15917        | 0.17733        | 0.19549        |
| 1596.229        | 0.15205        | 0.17075        | 0.18945        |
Table A2. Cont.

| Wavelength (nm) | DI Water 25.2 ppm | Water 2 43.5 ppm | Water 3 64.0 ppm |
|-----------------|-------------------|------------------|------------------|
| 1596.349        | 0.1483            | 0.16799          | 0.18768          |
| 1596.469        | 0.15143           | 0.17009          | 0.18876          |
| 1596.588        | 0.14725           | 0.16559          | 0.18393          |
| 1596.708        | 0.1398            | 0.15856          | 0.17732          |
| 1596.828        | 0.13635           | 0.15387          | 0.17139          |
| 1596.948        | 0.13061           | 0.15068          | 0.17075          |
| 1597.068        | 0.13024           | 0.14968          | 0.16912          |
| 1597.188        | 0.13361           | 0.15015          | 0.16669          |
| 1597.308        | 0.12101           | 0.14322          | 0.16543          |
| 1597.428        | 0.123             | 0.14029          | 0.15758          |
| 1597.547        | 0.11168           | 0.13325          | 0.15482          |
| 1597.667        | 0.11353           | 0.13169          | 0.14985          |
| 1597.787        | 0.10959           | 0.12799          | 0.14639          |
| 1597.907        | 0.11296           | 0.12759          | 0.14222          |
| 1598.027        | 0.10872           | 0.12511          | 0.1415           |
| 1598.147        | 0.10307           | 0.11835          | 0.13363          |
| 1598.267        | 0.09768           | 0.1139           | 0.13012          |
| 1598.387        | 0.09588           | 0.11242          | 0.12896          |
| 1598.506        | 0.09783           | 0.11447          | 0.13114          |
| 1598.626        | 0.09874           | 0.11418          | 0.12962          |
| 1598.746        | 0.09054           | 0.10727          | 0.124            |
| 1598.866        | 0.09031           | 0.10349          | 0.11667          |
| 1598.986        | 0.08617           | 0.10107          | 0.11597          |
| 1599.106        | 0.08495           | 0.10214          | 0.11933          |
| 1599.226        | 0.08423           | 0.0999           | 0.11557          |
| 1599.346        | 0.08195           | 0.09659          | 0.11123          |
| 1599.466        | 0.07659           | 0.09163          | 0.10667          |
| 1599.585        | 0.07036           | 0.08698          | 0.1036           |
| 1599.705        | 0.07307           | 0.08698          | 0.10089          |
| 1599.825        | 0.07467           | 0.08864          | 0.10261          |
| 1599.945        | 0.07456           | 0.0862           | 0.09784          |
| 1600.065        | 0.06658           | 0.08091          | 0.09524          |
| 1600.185        | 0.06177           | 0.07609          | 0.09041          |
| 1600.305        | 0.06521           | 0.07565          | 0.08609          |
| 1600.425        | 0.06803           | 0.0791           | 0.09017          |
| 1600.544        | 0.06521           | 0.07713          | 0.08905          |
| 1600.664        | 0.0621            | 0.07412          | 0.08614          |
| Wavelength (nm) | NDII 25.2 ppm (mW) | NDII 43.5 ppm (mW) | NDII 64.0 ppm (mW) |
|---------------|------------------|------------------|------------------|
| 1600.784      | 0.06797          | 0.07139          | 0.07481          |
| 1600.904      | 0.0595           | 0.06857          | 0.07764          |
| 1601.024      | 0.05365          | 0.06397          | 0.07429          |
| 1601.144      | 0.06275          | 0.06797          | 0.07319          |
| 1601.264      | 0.05572          | 0.06407          | 0.07242          |
| 1601.384      | 0.05036          | 0.05735          | 0.06434          |
| 1601.504      | 0.03907          | 0.05078          | 0.06249          |
| 1601.623      | 0.03699          | 0.04642          | 0.05585          |
| 1601.743      | 0.04603          | 0.05094          | 0.05585          |
| 1601.863      | 0.03358          | 0.04483          | 0.05608          |
| 1601.983      | 0.03574          | 0.04404          | 0.05234          |
| 1602.103      | 0.03452          | 0.03982          | 0.04512          |
| 1602.223      | 0.03154          | 0.0362           | 0.04086          |
| 1602.343      | 0.01942          | 0.03176          | 0.0441           |
| 1602.463      | 0.03481          | 0.03756          | 0.04031          |
| 1602.582      | 0.02745          | 0.03395          | 0.04045          |
| 1602.702      | 0.02854          | 0.03155          | 0.03456          |
| 1602.822      | 0.0235           | 0.02832          | 0.03314          |
| 1602.942      | 0.0235           | 0.02832          | 0.03314          |
| 1603.062      | 0.02442          | 0.03009          | 0.03576          |
| 1603.182      | 0.02383          | 0.0278           | 0.03177          |
| 1603.302      | 0.02276          | 0.02485          | 0.02694          |
| 1603.422      | 0.01307          | 0.01799          | 0.02291          |
| 1603.542      | 0.0225           | 0.0202           | 0.0179           |
| 1603.661      | 0.01551          | 0.01702          | 0.01853          |
| 1603.781      | 0.01964          | 0.0201           | 0.02056          |
| 1603.901      | 0.00754          | 0.01328          | 0.01902          |
| 1604.021      | 0.01217          | 0.01344          | 0.01471          |
| 1604.141      | 0.00703          | 0.01022          | 0.01341          |
| 1604.261      | 5.9 × 10⁻⁴        | 0.00738          | 0.01417          |
| 1604.381      | 0.00491          | 0.01109          | 0.01727          |
| 1604.5        | 0.00188          | 0.00814          | 0.0144           |
| 1604.62       | 0.00543          | 0.00819          | 0.01095          |
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