SUPPLEMENTARY DATA

Photodegradation Routes of the Herbicide Bromoxynilin Solution and Sorbed on Silica Nanoparticles.

1.- Characterization of the nanoparticles:

1.1 Fourier transform infrared spectroscopy (FTIR)

Fourier transform infrared spectra in the range from 4000 to 400 cm\(^{-1}\) were recorded on a Bruker EQUINOX 55 apparatus with a resolution of 2 cm\(^{-1}\), using a KBr disk. To obtain a high signal-to-noise ratio 128 scans were accumulated for each sample.

The FTIR spectra of BXN and NP-BXN are compared in Table S1.

Table S1: Bands observed in FTIR spectra of BXN and NP-BXN.

<table>
<thead>
<tr>
<th></th>
<th>BXN</th>
<th>NP-BXN</th>
</tr>
</thead>
<tbody>
<tr>
<td>2928.7</td>
<td>2928.8</td>
<td></td>
</tr>
<tr>
<td>2868.1</td>
<td>2860.1 / 2872.9</td>
<td></td>
</tr>
<tr>
<td>2229.7</td>
<td>2233.7</td>
<td></td>
</tr>
<tr>
<td>1465.2</td>
<td>1468.6</td>
<td></td>
</tr>
<tr>
<td>1548.5</td>
<td>1545.1</td>
<td></td>
</tr>
<tr>
<td>717.6</td>
<td>704.2</td>
<td></td>
</tr>
</tbody>
</table>
**Figure S1:** FTIR spectra of BXN (red) and NP-BXN (black).

1.2 Brunauer-Emmett-Teller (BET) analysis

The specific surface area (SSA) was determined via nitrogen (N\textsubscript{2}) adsorption isothems at 77 K in the reduced pressure range from 0.04 to 0.12 using the Brunauer-Emmett-Teller (BET) method \(^{(1)}\). For this purpose, a gas adsorption apparatus (Micromeritics ASAP 2020 V1.04 E) was employed.

1.3 Thermogravimetry (TG)

The thermogravimetric curve was performed with a Shimadzu TA-50 thermogravimeter analyzer, under He atmosphere with heating rate of 0.17 Ks\(^{-1}\). The instrument was calibrated with CaC\textsubscript{2}O\textsubscript{4}.3H\textsubscript{2}O.

1.4 UV-Visible Spectroscopy

The absorption spectra were taken with a computer-controlled Hewlett Packard 8453 spectrophotometer.
**Figure S2:** Absorption component of the UV-visible spectrum of NP-BXN.

1.5 Dynamic light scattering

The hydrodynamic diameter and size distribution of particles was measured by dynamic light scattering using a Malvern 4700 goniometer and 7132 correlator with an argon-ion laser operating at 488 nm. All measurements were made at a scattering angle of 90° at temperature of 25 °C. The measurements were analyzed by triplicate and the results were analyzed with Zetasizer software (provided by the manufacturer).

2.- Kinetics of Bromide Ion Formation

From Scheme 1:

\[-\frac{d[BXN]}{dt} = k_4 \times [BXN]\]  \hspace{1cm} (S1)

\[\frac{d[DHBN]}{dt} = k_4 \times [BXN] - k_5 \times [DHBN]\]  \hspace{1cm} (S2)

\[\frac{d[Br^-]}{dt} = k_4 \times [BXN] + k_5 \times [DHBN]\]  \hspace{1cm} (S3)

Integration of eq. (S1) yields eq. (S4).

\[[BXN] = [BXN]_0 \times e^{-k_4 t}\]  \hspace{1cm} (S4)

From eqs. (S2) and (S4), eq. (S5) is obtained.

\[-\frac{d[DHBN]}{dt} = k_4 \times [BXN]_0 \times e^{-k_4 t} - k_5 \times [DHBN]\]  \hspace{1cm} (S5)

Integration of eq. (S5) leads to eq. (S6).

\[[DHBN] = \frac{k_4 \times [BXN]_0}{(k_5 - k_4)} \times (e^{-k_4 t} - e^{-k_5 t})\]  \hspace{1cm} (S6)
From eqs. (S3), (S4), and (S6), we can write eq. (S7).

\[
\frac{d[Br^-]}{dt} = k_4 \times [BXN]_0 \times e^{-k_4 t} + \frac{k_4 \times k_5 \times [BXN]_0}{(k_5 - k_4)} \times \left( e^{-k_5 t} - e^{-k_4 t} \right)
\]  

(S7)

Rearrangement and integration of eq. (S7) leads to eq. (S8).

\[
[Br^-] = \frac{(2k_5 - k_4) \times [BXN]_0}{(k_5 - k_4)} \times \left( 1 - e^{-k_5 t} \right) - \frac{k_4 \times [BXN]_0}{(k_5 - k_4)} \times \left( 1 - e^{-k_4 t} \right)
\]  

(S8)

If k5 >> k4, eq. (S9) is obtained from eq. (S8).

\[
[Br^-] \approx 2 \times [BXN]_0 \times \left( 1 - e^{-k_4 t} \right)
\]  

(S9)

3.- Calculation of \( k_a \).

The photolysis rate of aqueous BXN can be expressed as:

\[
-\frac{d[BXN]}{dt} = k_a \Phi[BXN] \quad \text{eq. (S10)}
\]

Where \( \Phi \) is the photolysis quantum yield and \( k_a \) is the specific rate of light absorption.

The rate constant \( k_a \) was calculated from equation (S11) as recommended by Zepp (3).

\[
k_a = \frac{2.303}{6.02 \times 10^{20}} \times \sum \tilde{\varepsilon}_\lambda Z_\lambda \quad \text{eq. (S11)}
\]

Where \( \tilde{\varepsilon}_\lambda \) is the average absorption coefficient at a wavelength interval centered at \( \lambda \) and \( Z_\lambda \) is the underwater solar irradiance in this wavelength interval. Table S2 lists the values of \( \tilde{\varepsilon}_\lambda \) and \( Z_\lambda \) employed in the calculations.

From the data shown in Table S2 and eq. (S2) the calculated value of \( k_a \) is \( 7.92 \times 10^{-3} \) s\(^{-1}\) and the photolysis rate \( k_a \times \Phi \) yields \( 5.07 \times 10^{-4} \) s\(^{-1}\) for BXN and \( 1.66 \times 10^{-5} \) s\(^{-1}\) for NP-BXN.
Table S2: The values of $\bar{\varepsilon}_\lambda$ from this work and $Z_\lambda$ in water midday, midsummer, latitude 40°N from ref. (2).

<table>
<thead>
<tr>
<th>$\lambda$(nm)</th>
<th>$\bar{\varepsilon}_\lambda$(M$^{-1}$cm$^{-1}$)</th>
<th>$Z_\lambda$(photons/cm$^2$s) ×10$^{-14}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>297.5</td>
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<td>300.0</td>
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<tr>
<td>330.0</td>
<td>210.0</td>
<td>8.4600</td>
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References