Resonant and non-resonant femtosecond ionization mass spectrometry of organochlorine pesticides

Siddihalu Lakshitha Madunil,a Totaro Imasaka,b and Tomoko Imasakaa*

aFaculty of Design, Kyushu University, 4-9-1, Shiobaru, Minami-ku, Fukuoka 815-8540: 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan.
bDivision of International Strategy, Center of Future Chemistry, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan.
cHikari Giken, Co., 2-10-30, Sakurazaka, Chuou-ku, Fukuoka 810-0024, Japan.

* Corresponding author.

E-mail address: imasaka@design.kyushu-u.ac.jp (Tomoko Imasaka).
Electronic Supplementary Information provides information regarding the spectral properties for thirteen pesticides and the relationship between signal intensity and laser pulse width.
Figure S-1 provides the chemical structures of the pesticides, the calculated absorption spectra for neutral (left) and ionic (right) species, and the mass spectra obtained by EI and MPI ($\Delta t = 35$ fs) as shown in the series below. The wavelengths corresponding to the first excited energy ($EE$), the ionization energy ($IE$), and the half value of the ionization energy ($IE/2$) are indicated in the figure.

1. HCB
2. DDT
3. dieldrin

![Chemical structure of dieldrin]

![Absorption spectra and oscillator strength graphs]

![Mass spectrum with m/z values]
4. heptachlor

The diagram shows the molecular structure of heptachlor, which is a chlorinated hydrocarbon. The molecule contains seven chlorine atoms. The absorbance and oscillator strength spectra are also depicted, indicating the absorption bands at different wavelengths. The mass spectra show the signal intensity at various m/z ratios, highlighting the molecular ion (M+) and other ions present in the sample.
5. aldrin
6. endrin
7. α-endosulfan
8. β-endosulfan

\[ \beta - \text{endosulfan} \]

![Diagram of β-endosulfan molecule]

![Graphs showing absorptivity and oscillator strength vs. wavelength]

![Mass spectrometry graph showing signal intensity vs. m/z]

![Another mass spectrometry graph showing signal intensity vs. m/z]
9. trans-chlordane
10. *cis*-chlordane
11. α-HCH

![α-HCH structure]

![Graphs showing absorbance and oscillator strength vs. wavelength]

![Mass spectra showing signal intensity vs. m/z]

![Mass spectra showing signal intensity vs. m/z]
12. β-HCH

![Chemical Structure]

![Absorbance vs Wavelength]

![Mass Spectrogram]

![Mass Spectrum]

\[ \text{Absorbance (M}^{-1} \text{cm}^{-1}) \times 10^4 \]

\[ \text{Oscillator Strength} \]

\[ \text{Signal Intensity (}\times 10^4\text{)} \]

\[ m/z \]

\[ \text{Signal Intensity} \]

\[ m/z \]
13. $\gamma$-HCH

\[
\begin{array}{c}
\text{Cl} \\
\text{C}_3 \text{H}_5 \\
\text{Cl} \\
\end{array}
\]

![Graph](image)

![Graph](image)

![Graph](image)

![Graph](image)
Figure S-2 provides information on dependence of laser pulse width on the signal intensity of the molecular ion for the pesticides examined in this study. (A) HCB (B) DDT (C) dieldrin (D) heptachlor (E) aldrin (F) endrin (G) β-endosulfan (H) trans-chlordane (I) cis-chlordane (J) γ-HCH.