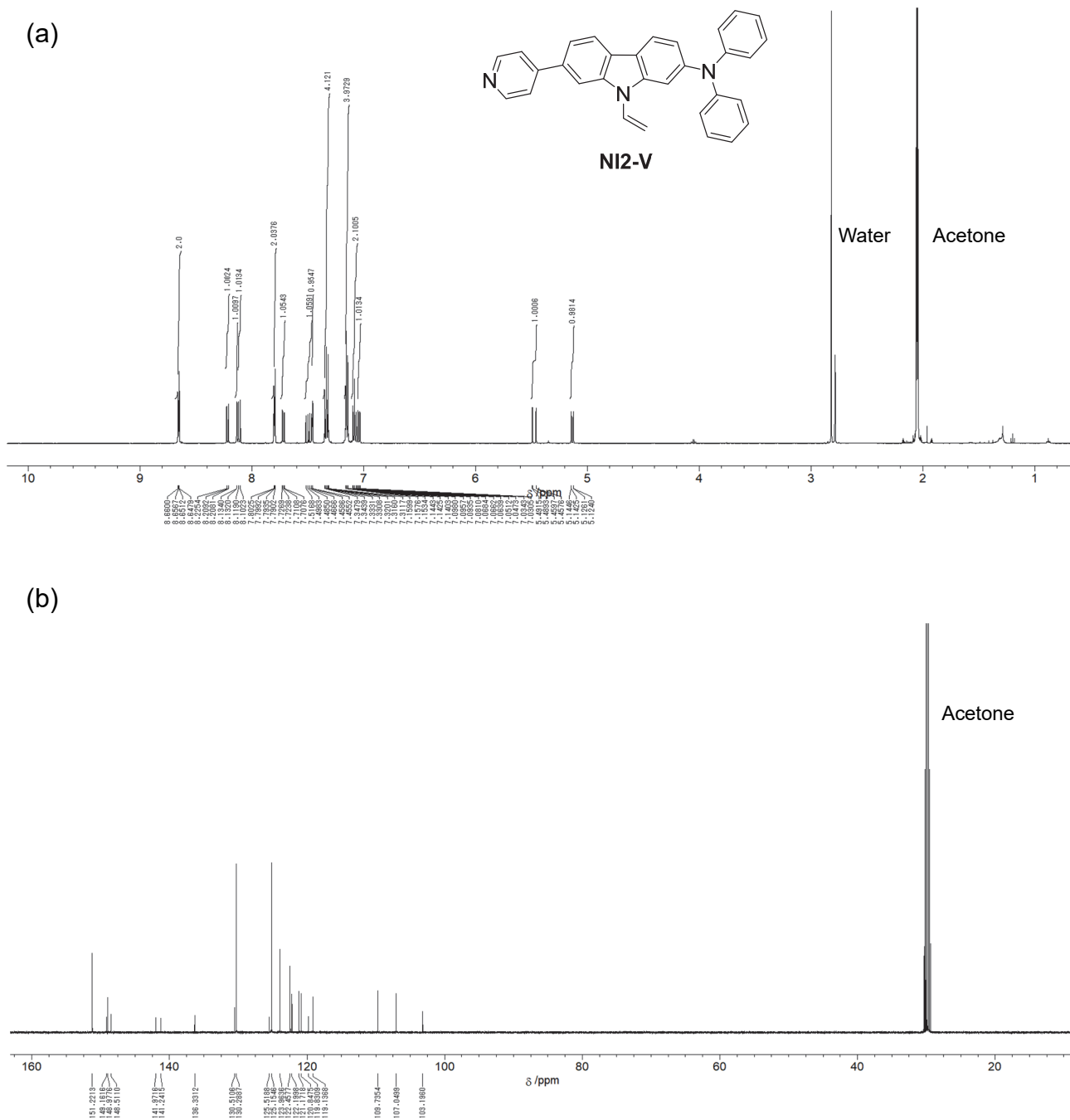


**Electronic Supplementary Information**

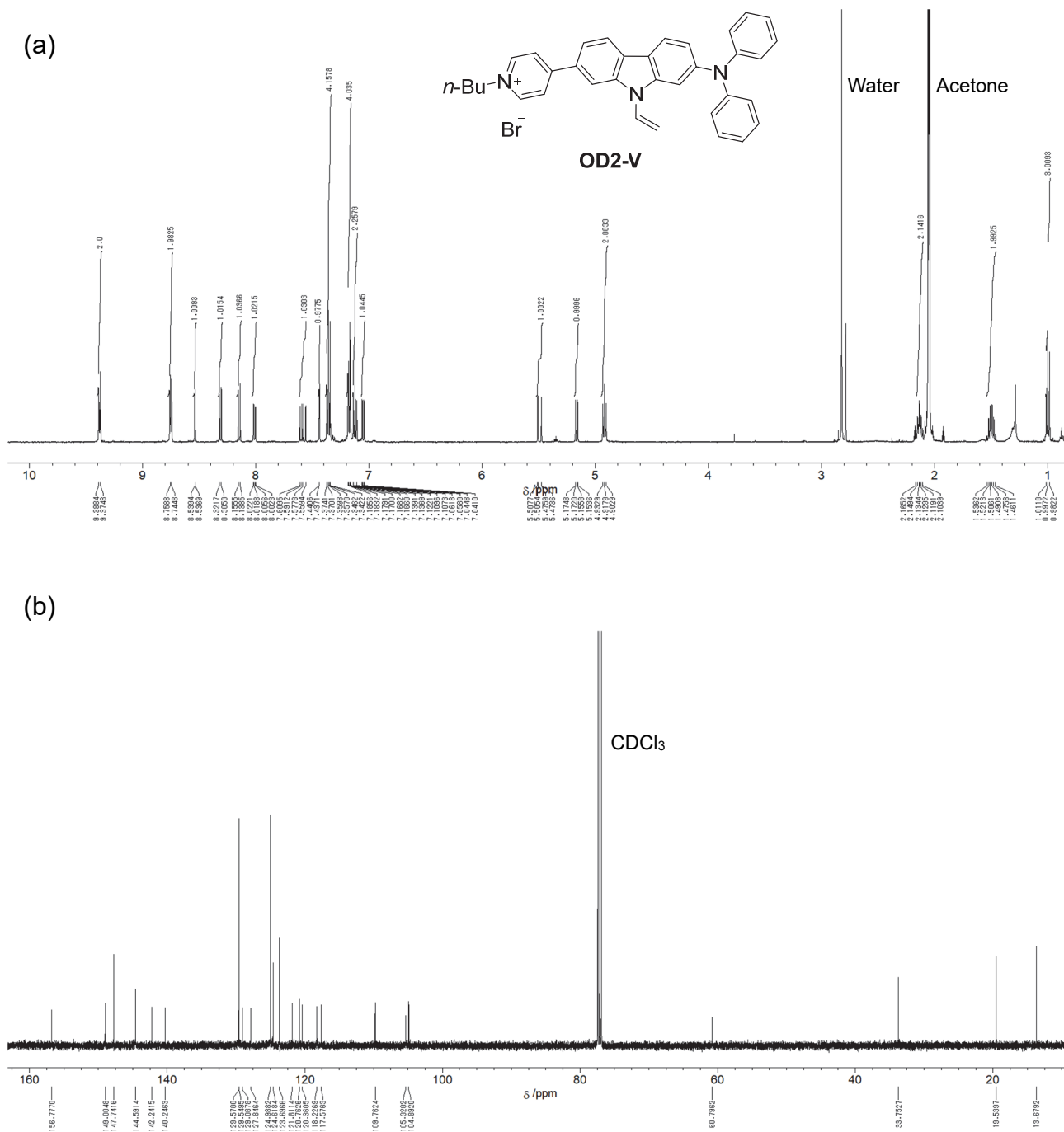
**Organohalogenochromism (OHC) of D- $\pi$ -A pyridinium dye polymer  
films and colorimetric detection of volatile organic halogen  
compounds**

Kumpei Kozuka, Keiichi Imato and Yousuke Ooyama\*

*Applied Chemistry Program, Graduate School of Advanced Science and Engineering, Hiroshima University, 1-4-1 Kagamiyama, Higashi-Hiroshima 739-8527, Japan. E-mail: yooyama@hiroshima-u.ac.jp*

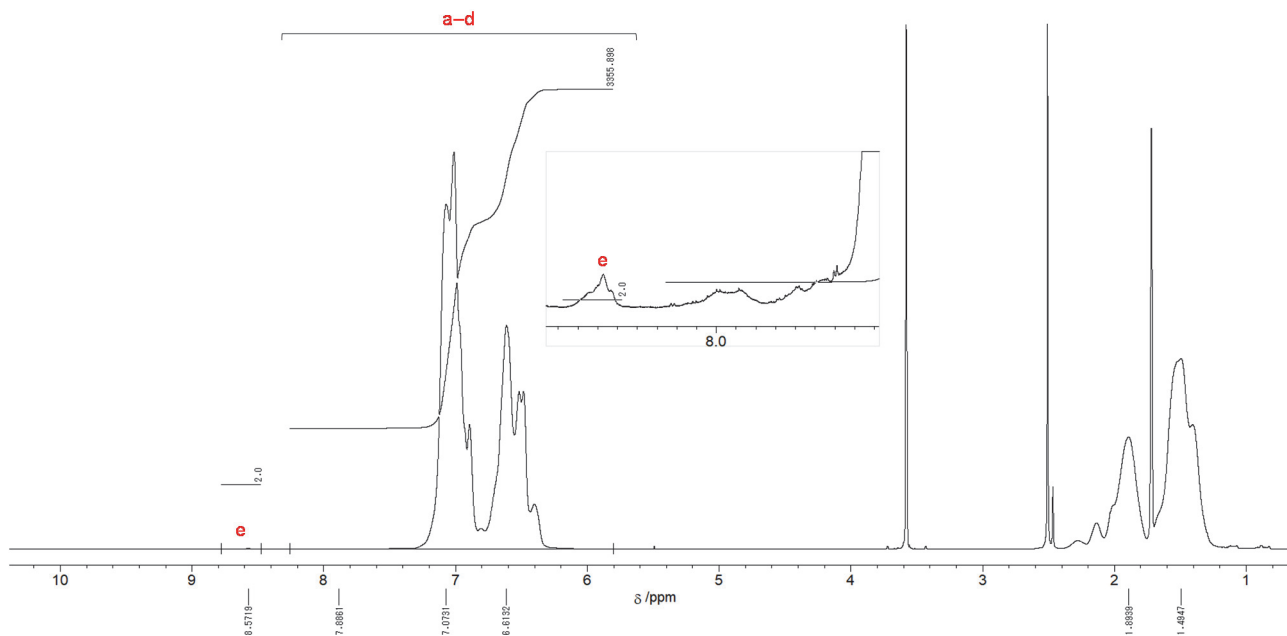
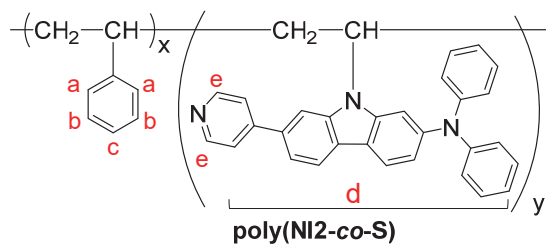


**Fig. S1** (a) <sup>1</sup>H NMR (500 MHz) and (b) <sup>13</sup>C NMR (125 MHz) spectra of NI2-V in acetone-*d*<sub>6</sub>.



**Fig. S2** (a)  $^1\text{H}$  NMR (500 MHz) spectrum of **OD2-V** in acetone- $d_6$  and (b)  $^{13}\text{C}$  NMR (125 MHz) spectrum of **OD2-V** in  $\text{CDCl}_3$ .

(a)



(b)

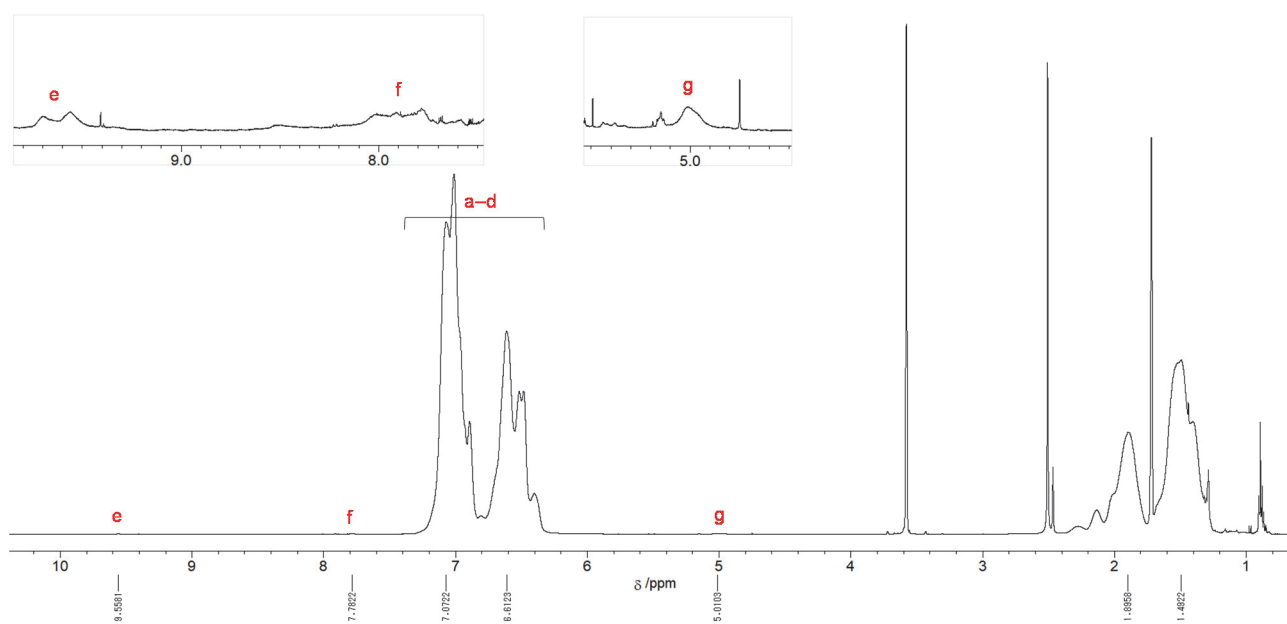
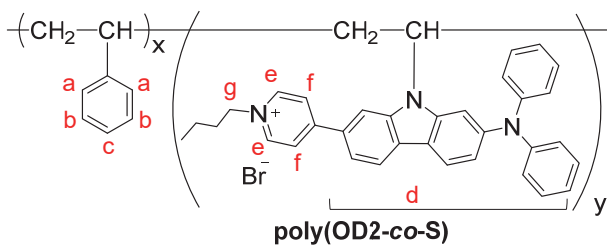
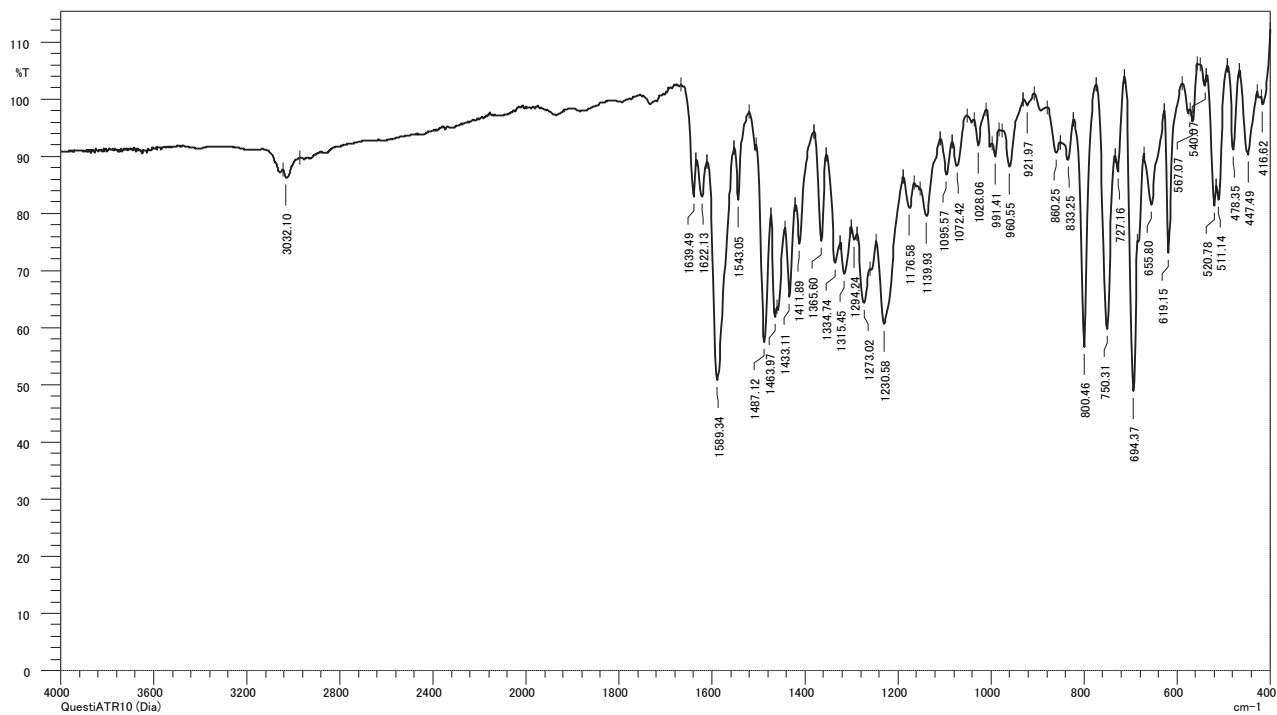


Fig. S3  $^1\text{H}$  NMR (500 MHz) spectra of (a) poly(NI2-co-S) and (b) poly(OD2-co-S) in THF- $d_8$ .

(a)



(b)

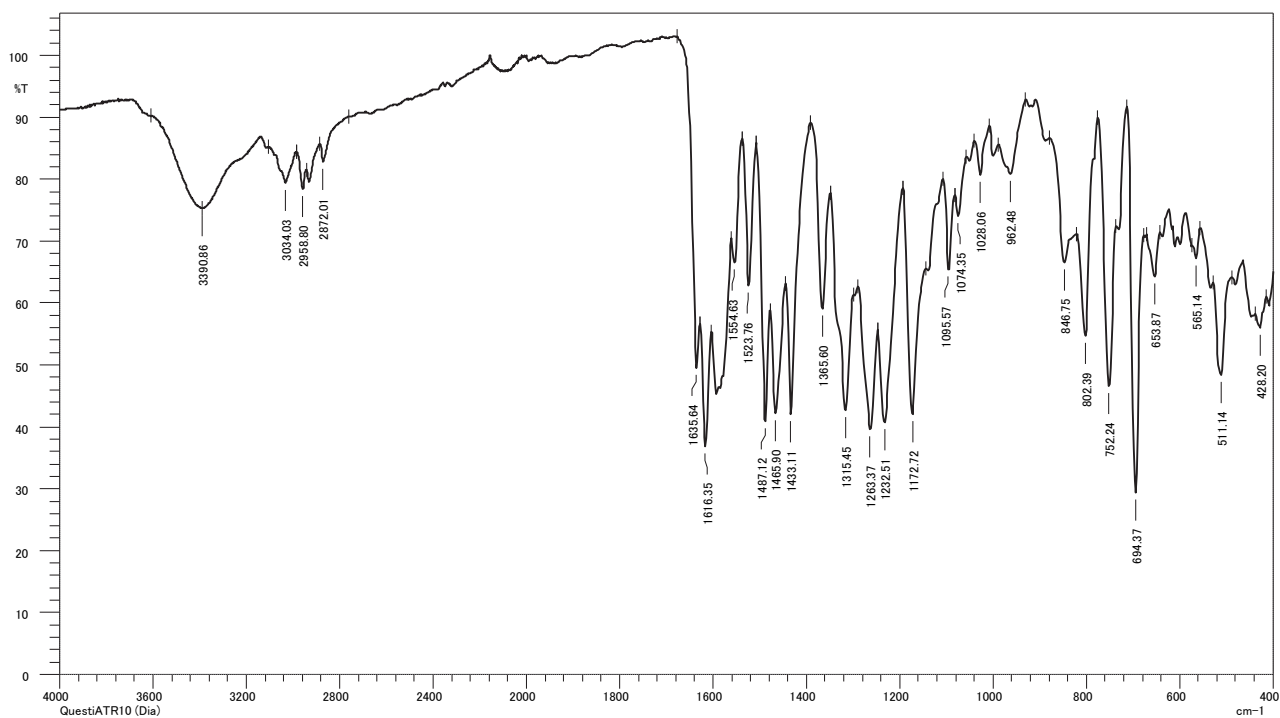
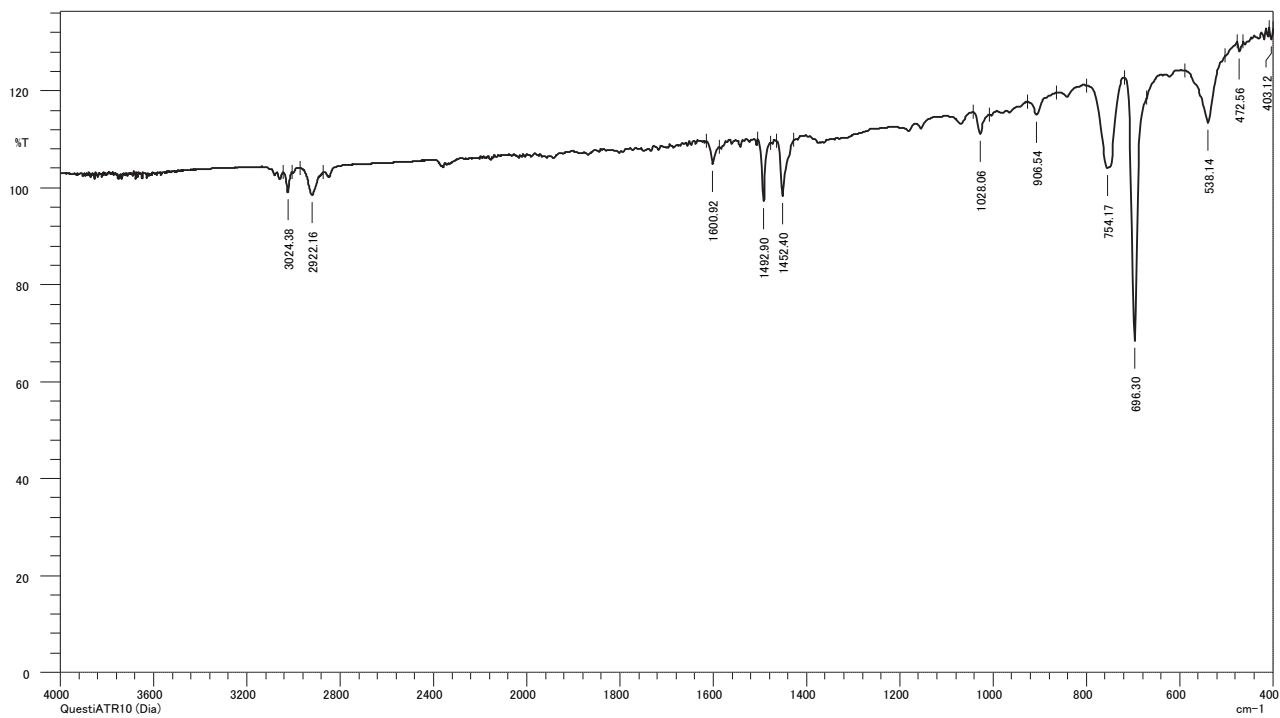
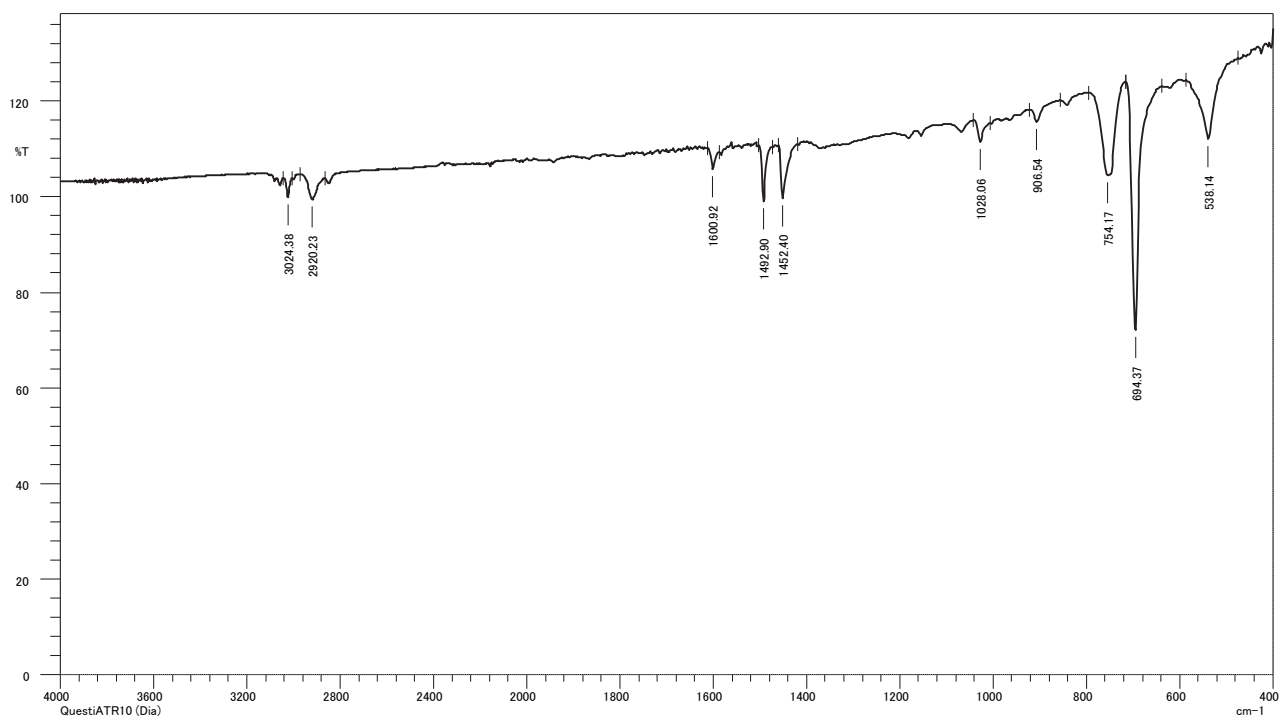


Fig. S4 FT-IR (ATR) spectra of (a) NI2-V and (b) OD2-V.

(a)

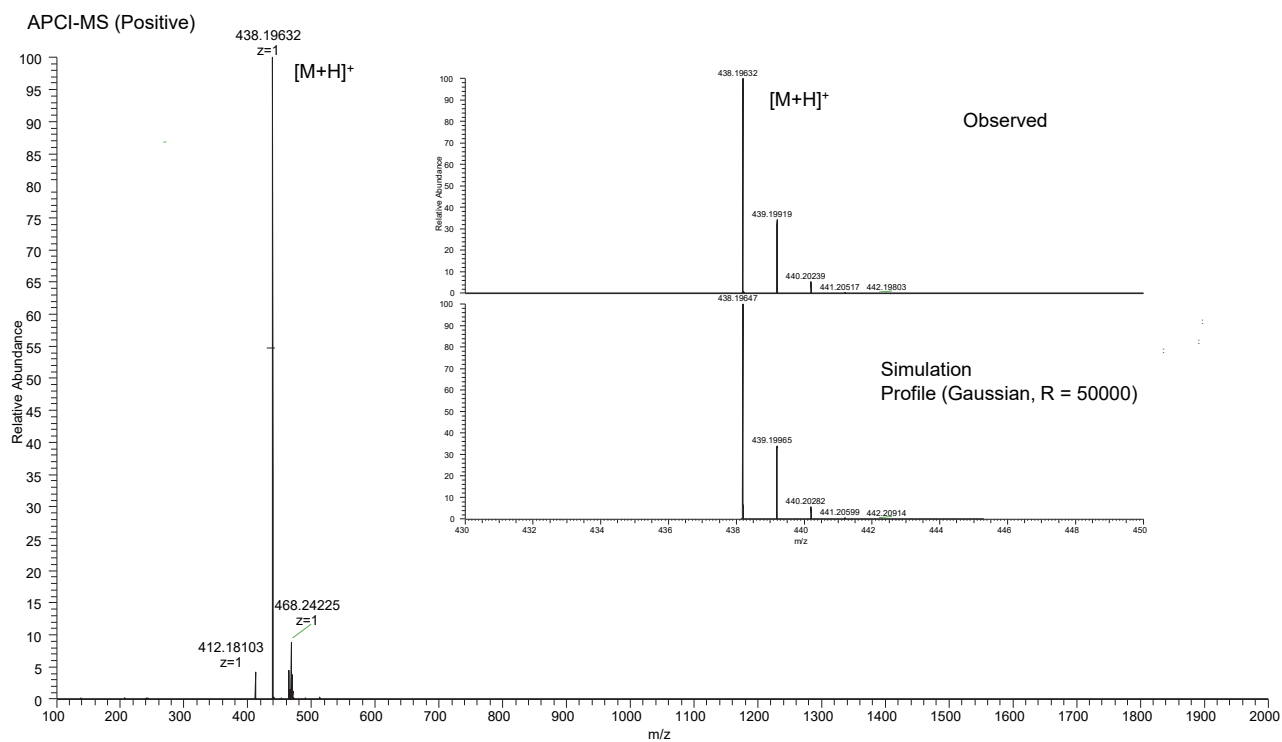


(b)



**Fig. S5** FT-IR (ATR) spectra of (a) **poly(NI2-co-S)** and (b) **poly(OD2-co-S)**.

(a)



(b)

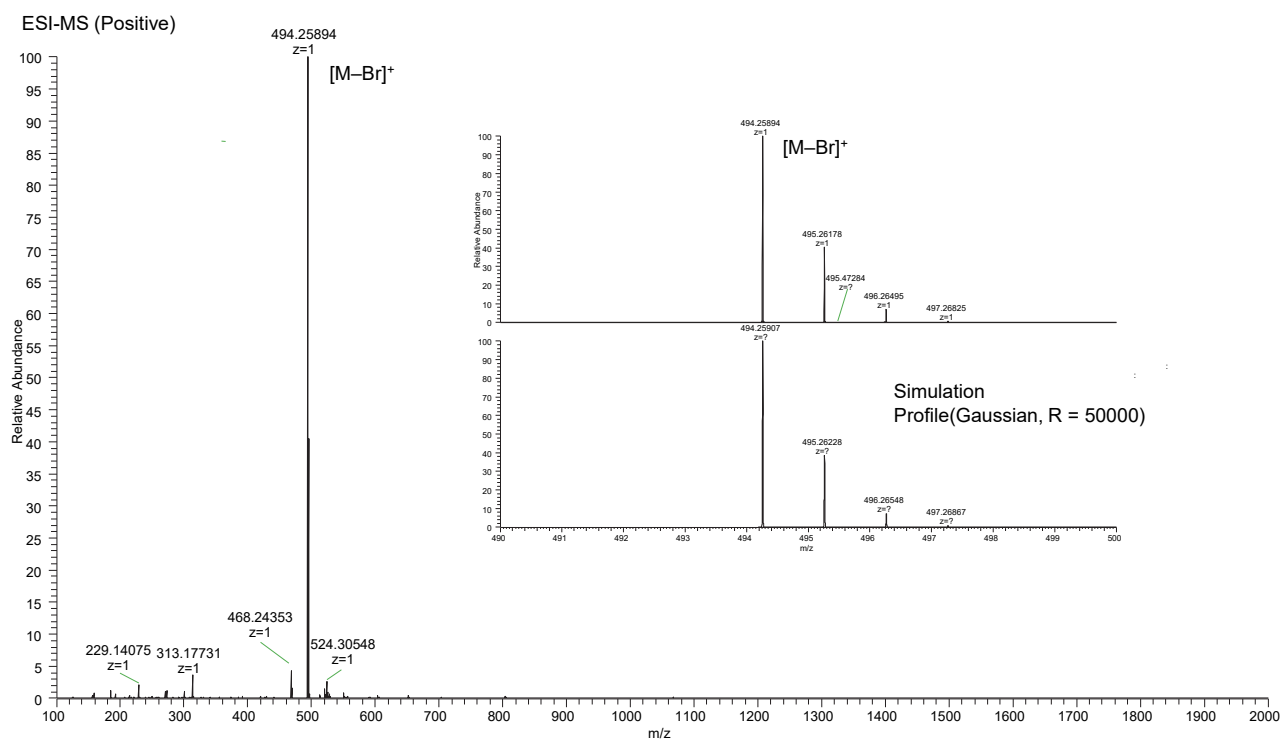
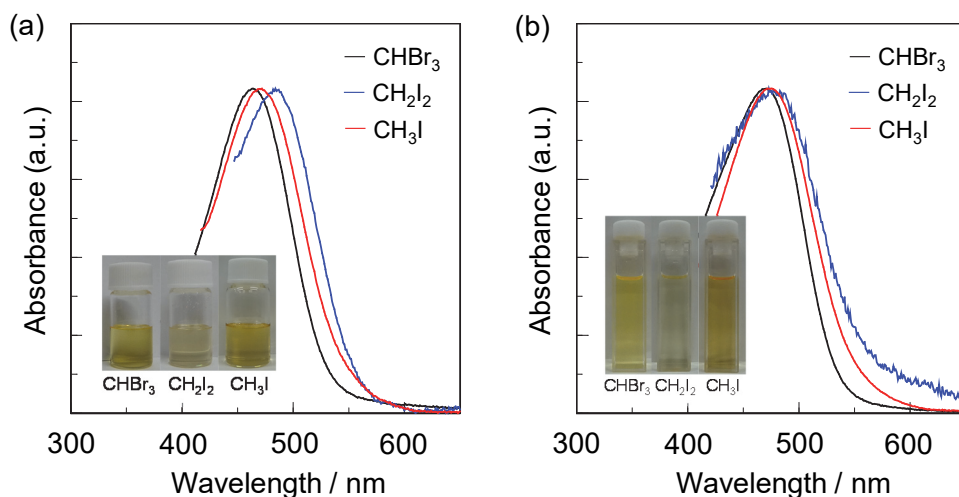
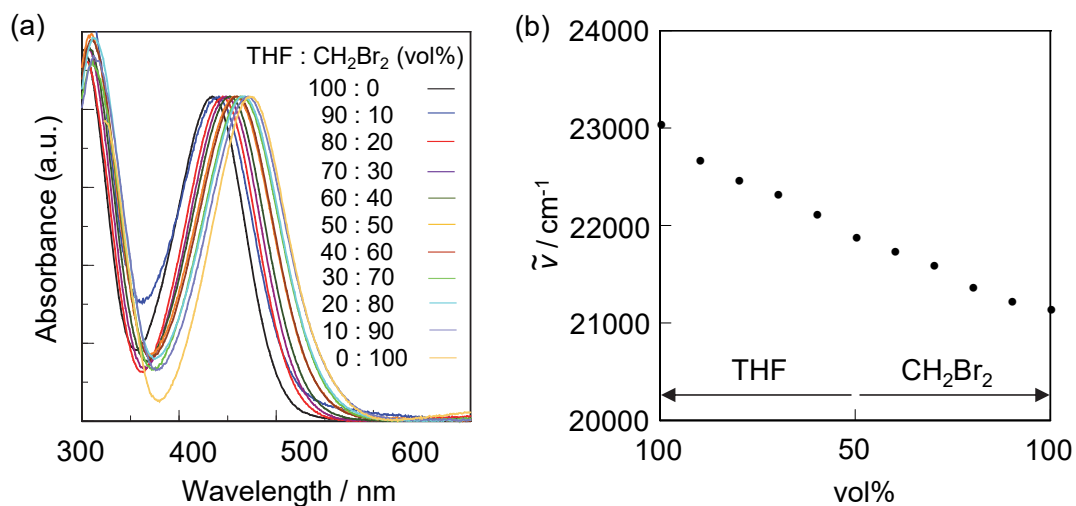


Fig. S6 HRMS spectra of (a) NI2-V and (b) OD2-V.

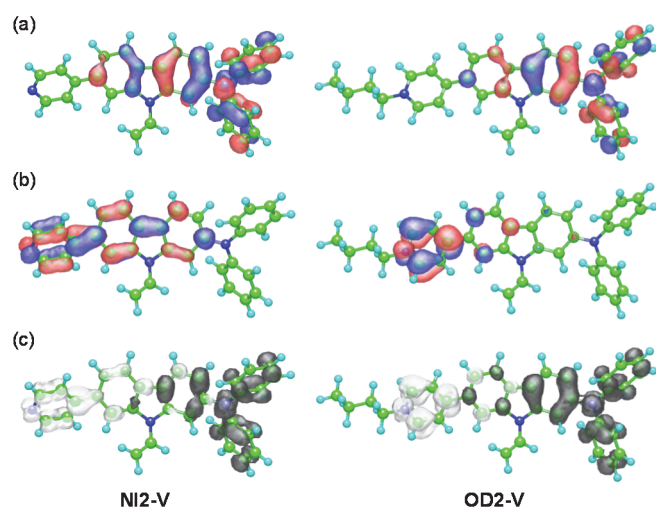


**Fig. S7** Photoabsorption spectra of (a) **NI2-V** and (b) **poly(NI2-co-S)** in  $\text{CHBr}_3$ ,  $\text{CH}_2\text{I}_2$ , and  $\text{CH}_3\text{I}$ . **NI2-V** and **poly(NI2-co-S)** react with  $\text{CHBr}_3$ ,  $\text{CH}_2\text{I}_2$ , and  $\text{CH}_3\text{I}$  solvents to form the pyridinium salts with the ICT-based  $\lambda_{\text{max}(\text{exp})}^{\text{abs-solution}}$  at 460–480 nm. Insets in (a) and (b): color images of **NI2-V** and **poly(NI2-co-S)** in  $\text{CHBr}_3$ ,  $\text{CH}_2\text{I}_2$ , and  $\text{CH}_3\text{I}$ .

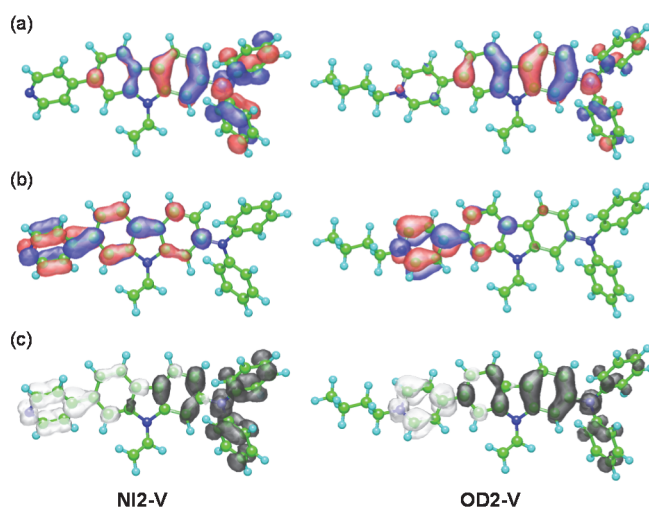


**Fig. S8** (a) Photoabsorption spectra of **OD2-V** in a THF/ $\text{CH}_2\text{Br}_2$  mixture and (b) the plot of the photoabsorption maximum wavenumbers ( $\tilde{\nu}$ ) against the mixture composition.





**Fig. S9** (a) HOMO and (b) LUMO of NI2-V and the dye cation (OD2-V<sup>+</sup>) for OD2-V. The red and blue lobes denote the positive and negative phases of the coefficients of the molecular orbitals. The size of each lobe is proportional to the MO coefficient. (c) Calculated electron density changes accompanying the first electronic excitation of NI2-V and OD2-V<sup>+</sup> (by the SCRF Onsager Model (solvent = 1,4-dioxane)). The black and white lobes signify decrease and increase in electron density accompanying the electronic transition, respectively. Their areas indicate the magnitude of the electron density change.



**Fig. S10** (a) HOMO and (b) LUMO of NI2-V and the dye cation (OD2-V<sup>+</sup>) for OD2-V. The red and blue lobes denote the positive and negative phases of the coefficients of the molecular orbitals. The size of each lobe is proportional to the MO coefficient. (c) Calculated electron density changes accompanying the first electronic excitation of NI2-V and OD2-V<sup>+</sup> (by the SCRF Onsager Model (solvent = DMSO)). The black and white lobes signify decrease and increase in electron density accompanying the electronic transition, respectively. Their areas indicate the magnitude of the electron density change.