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Imasaka, Tomoko

Laboratory of Chemistry, Graduate School of Design, Kyushu University

Imasaka, Totaro

Department of Applied Chemistry, Graduate School of Engineering, Kyushu University

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Supporting Information

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Tomoko IMASAKA^{*†} and Totaro IMASAKA^{***, ***}

** Laboratory of Chemistry, Graduate School of Design, Kyushu University, 4-9-1 Shiobaru, Minami, Fukuoka 815-8540, Japan*

*** Department of Applied Chemistry, Graduate School of Engineering, Kyushu University, 744 Motooka, Nishi, Fukuoka 819-0395, Japan*

**** Division of Optoelectronics and Photonics, Center for Future Chemistry, Kyushu University, 744 Motooka, Nishi, Fukuoka 819-0395, Japan*

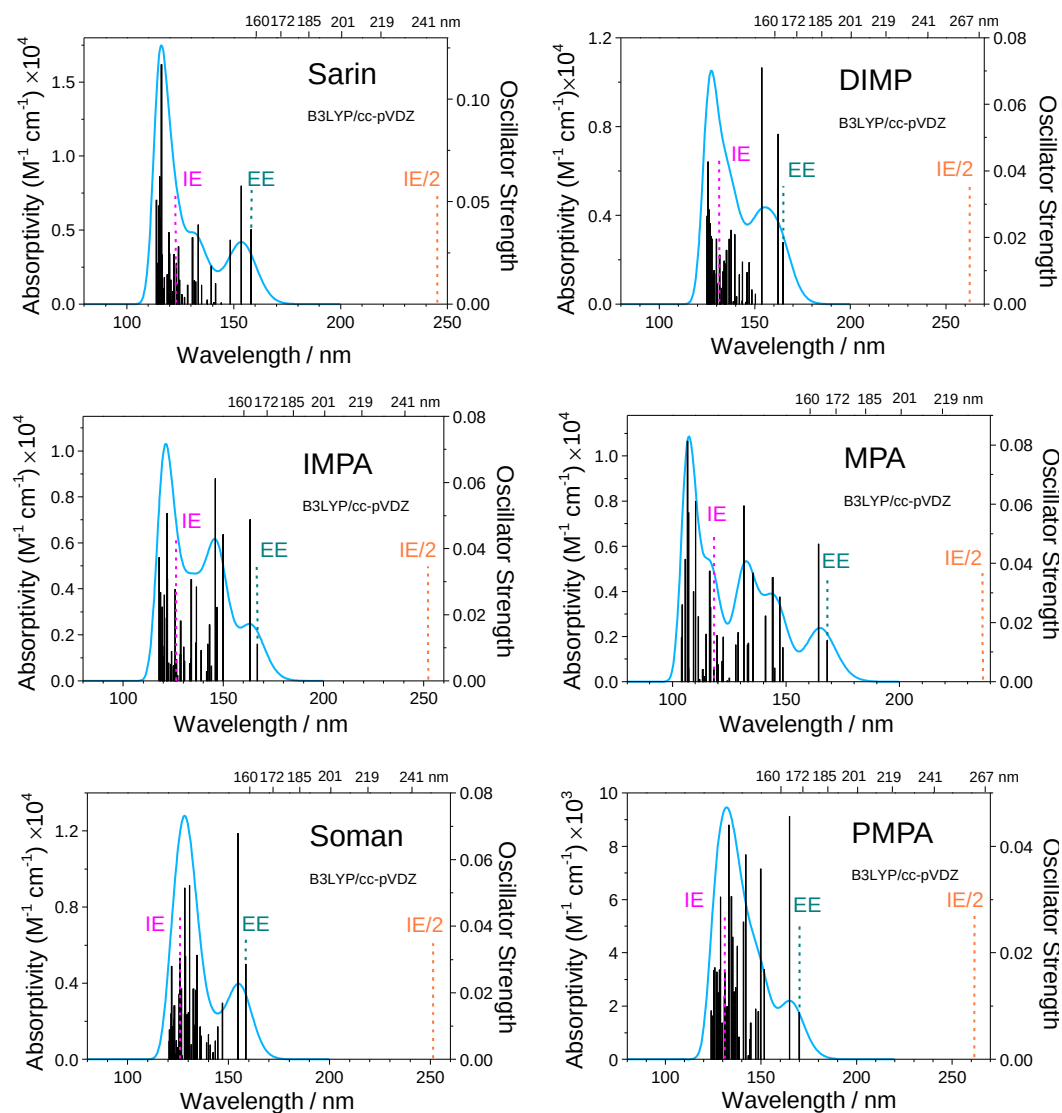


Fig. S1 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for sarin, DIMP, IMPA, MPA, soman, and PMPA calculated using B3LYP/cc-pVDZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

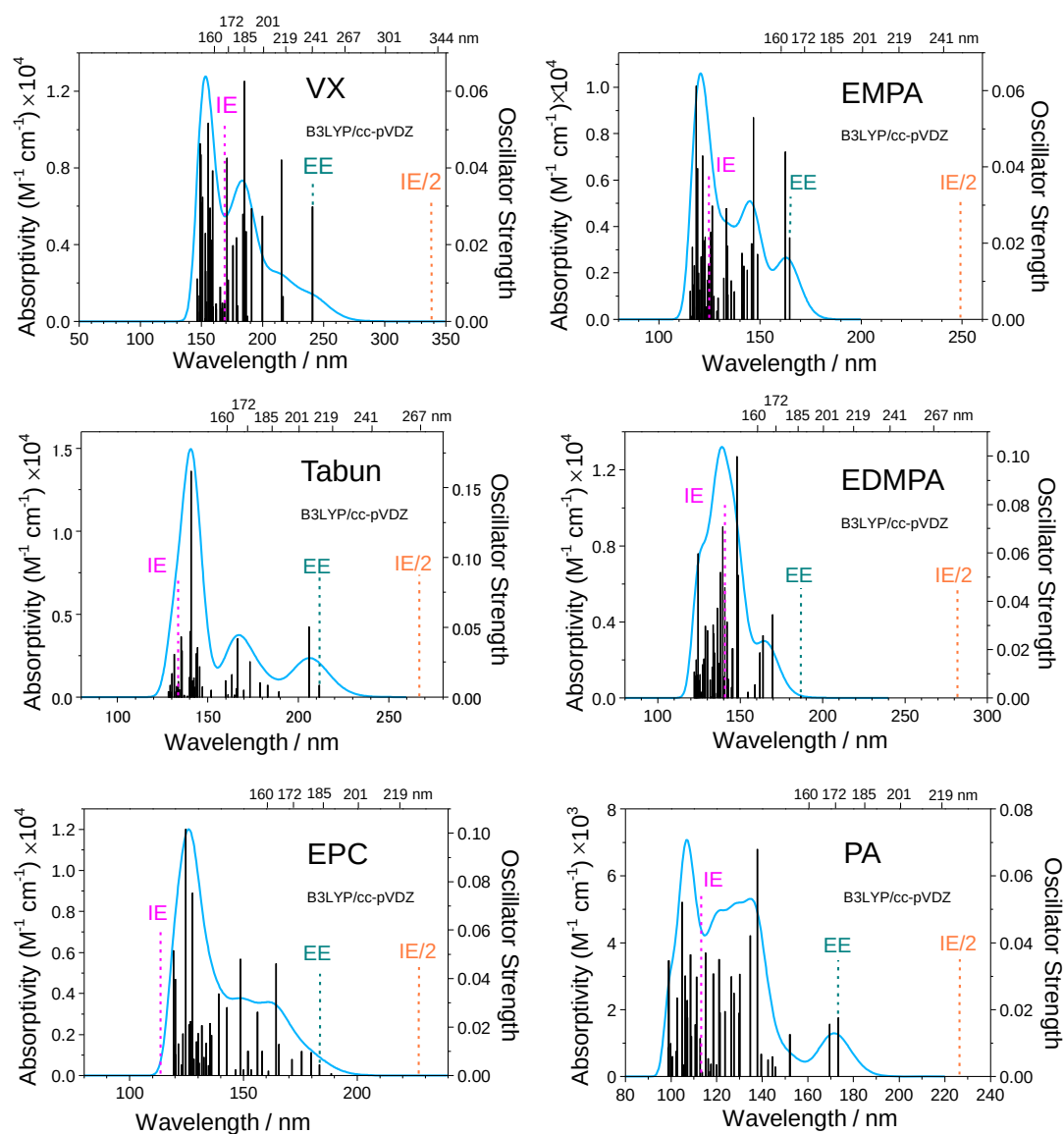


Fig. S2 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for VX, EMPA, tabun, EDMPA, EPC, and PA calculated using B3LYP/cc-pVDZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

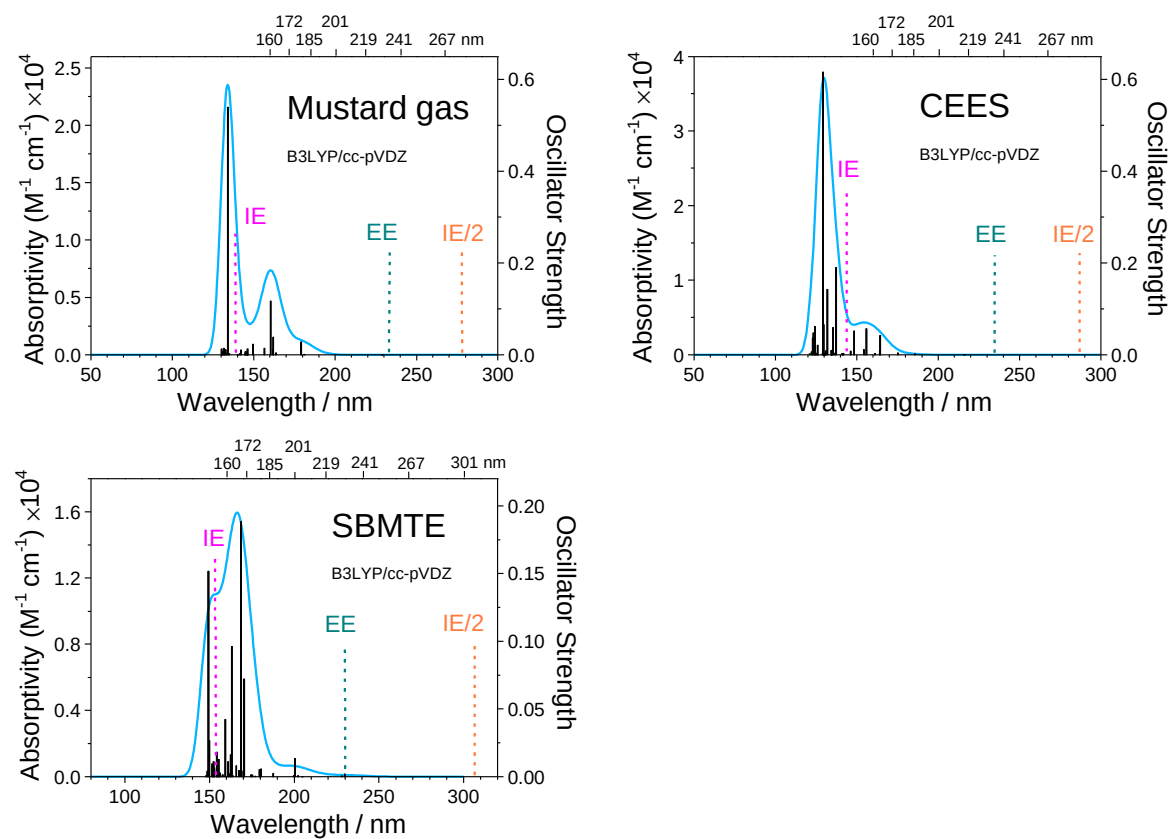


Fig. S3 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for mustard gas, CEES, and SBMTE calculated using B3LYP/cc-pVDZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

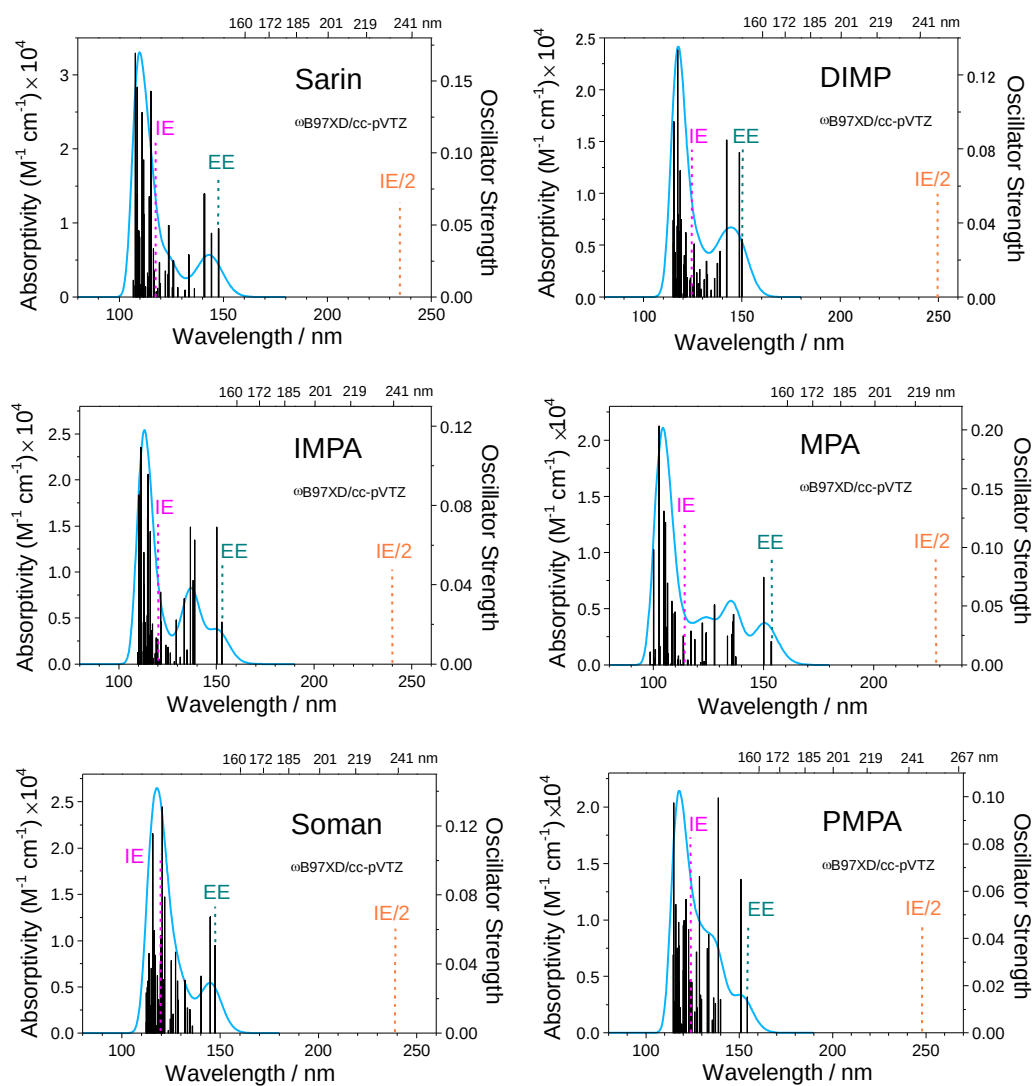


Fig. S4 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for Sarin, DIMP, IMPA, MPA, Soman, and PMPA calculated using $\omega\text{B97XD/cc-pVTZ}$. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

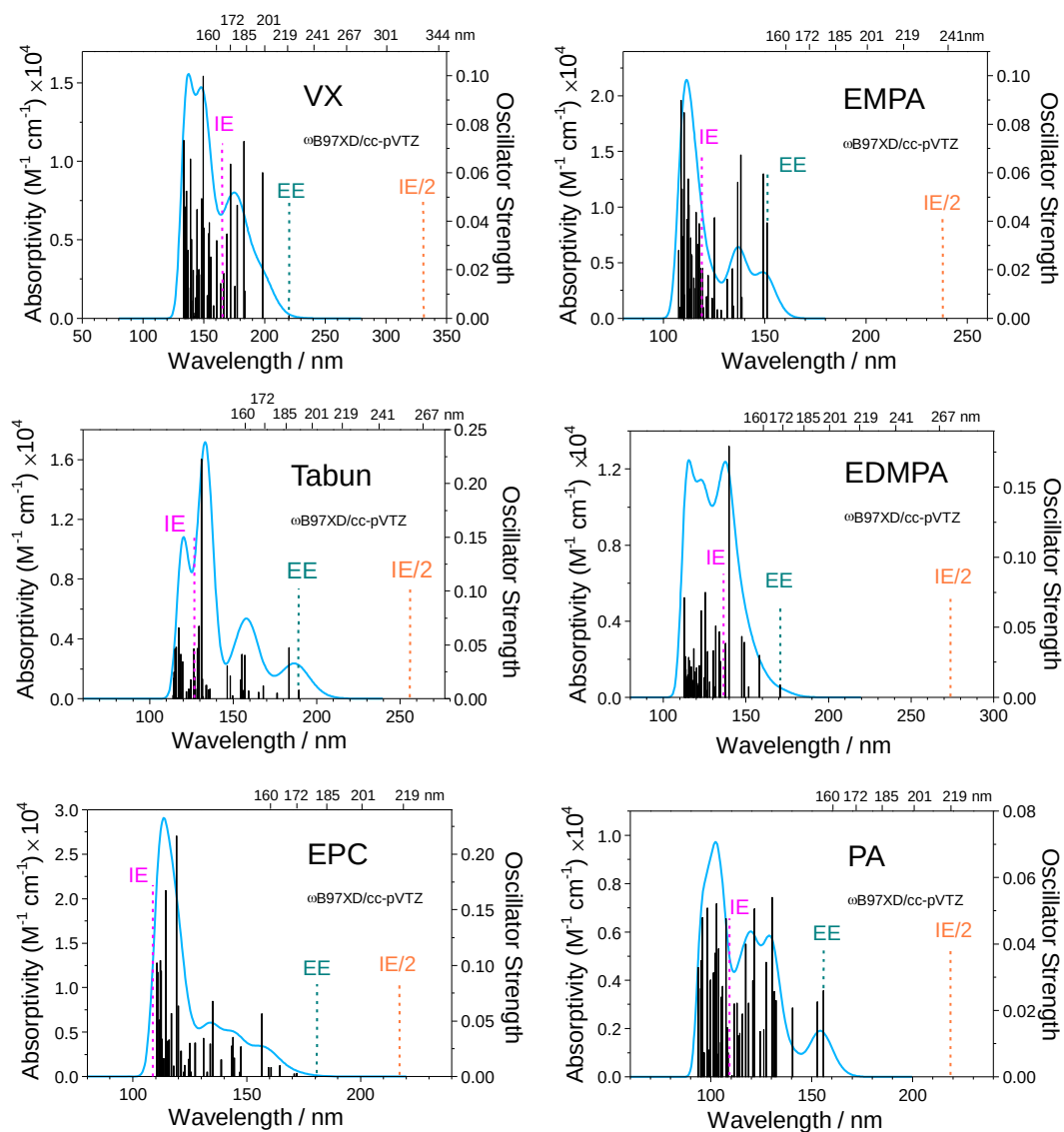


Fig. S5 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for VX, EMPA, Tabun, EDMPA, EPC, and PA calculated using ω B97XD/cc-pVTZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

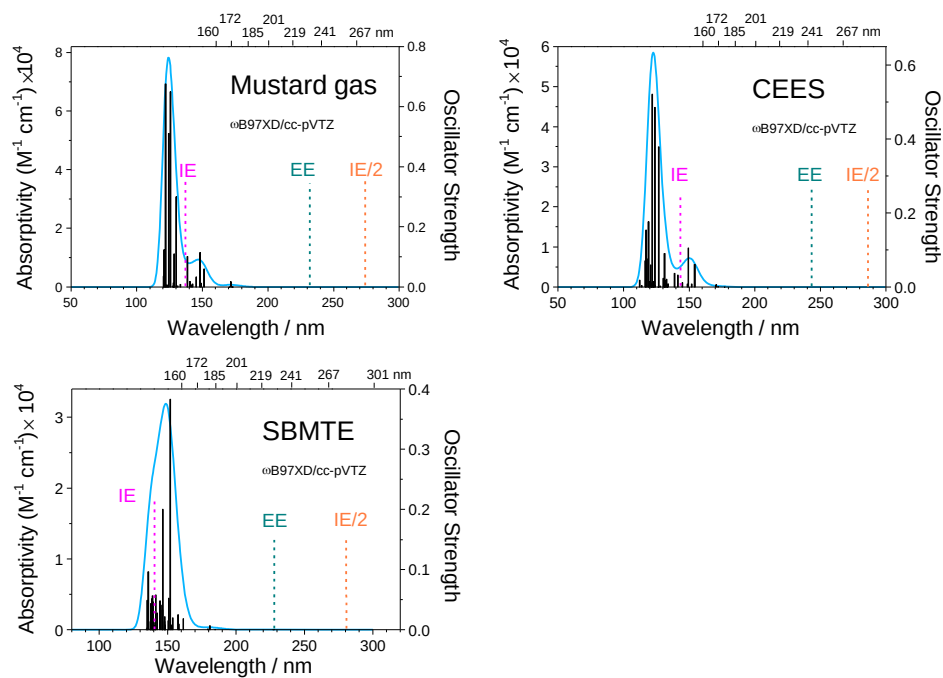


Fig. S6 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for Mustard gas, CEES, and SBMTE calculated using ω B97XD/cc-pVTZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.