

An Evaluation of the Spectral Properties of Nerve Agents for Laser Ionization Mass Spectrometry

Imasaka, Tomoko

Laboratory of Chemistry, Graduate School of Design, Kyushu University

Imasaka, Totaro

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

<https://hdl.handle.net/2324/7170841>

出版情報 : Analytical Sciences. 30, pp.1113-1120, 2014-12-10. The Japan Society for Analytical Chemistry

バージョン :

権利関係 : 2014 © The Japan Society for Analytical Chemistry



Supporting Information

An Evaluation of the Spectral Properties of Nerve Agents for Laser Ionization Mass Spectrometry

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 Motoooka, Nishi, Fukuoka 819-0395, Japan*

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

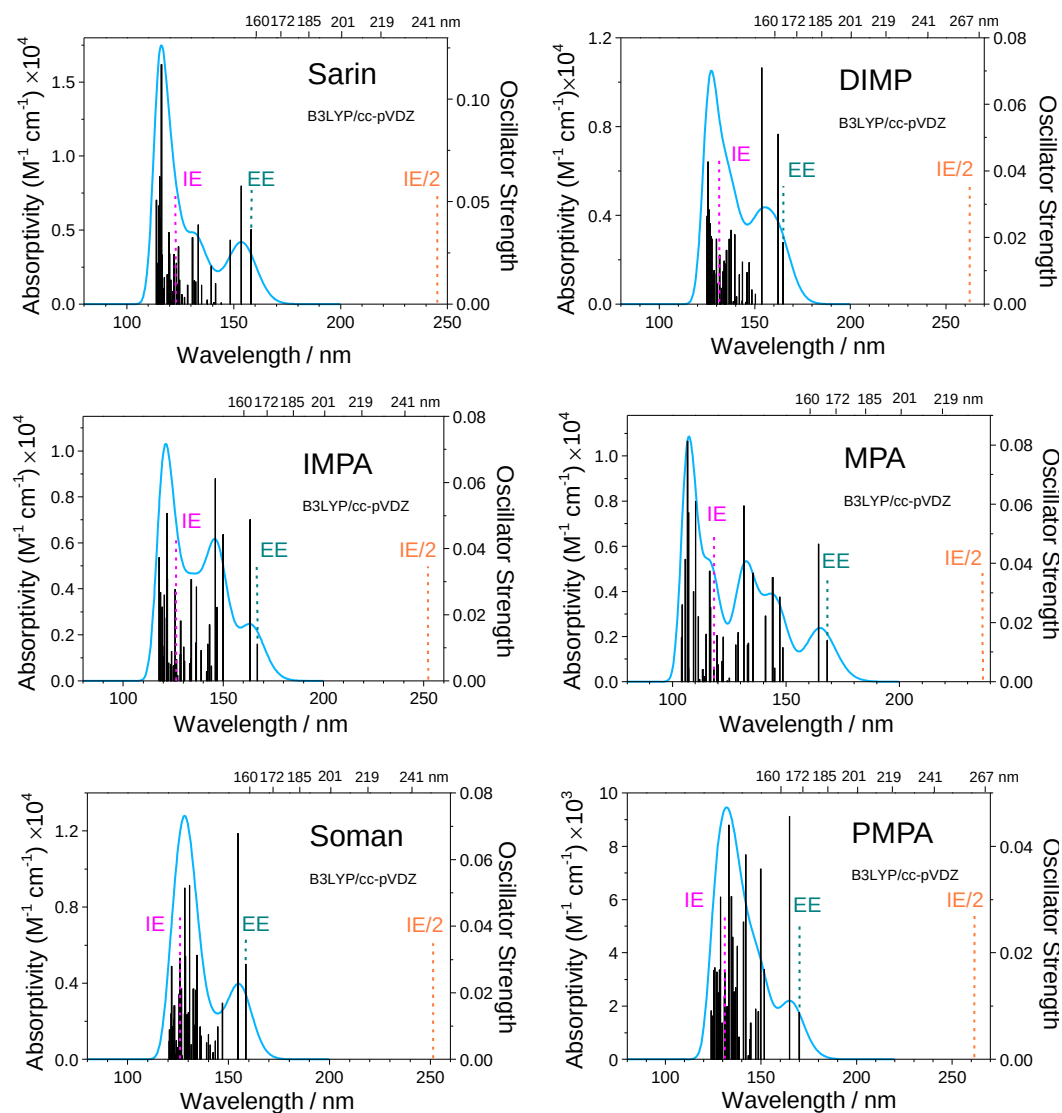


Fig. S1 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for sarin, DIMP, IMPA, MPA, soman, and PMPA calculated using B3LYP/cc-pVDZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

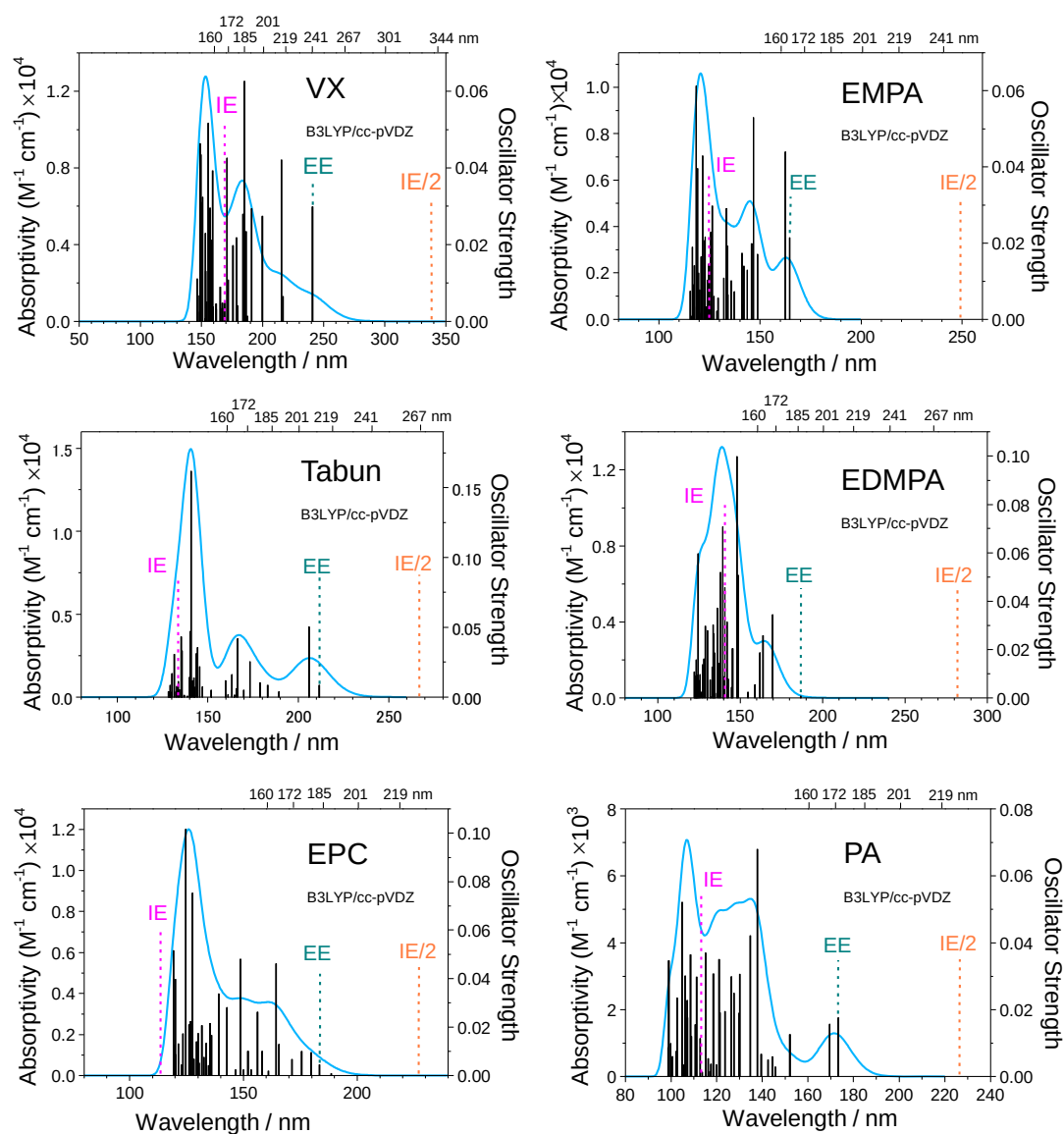


Fig. S2 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for VX, EMPA, tabun, EDMPA, EPC, and PA calculated using B3LYP/cc-pVDZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

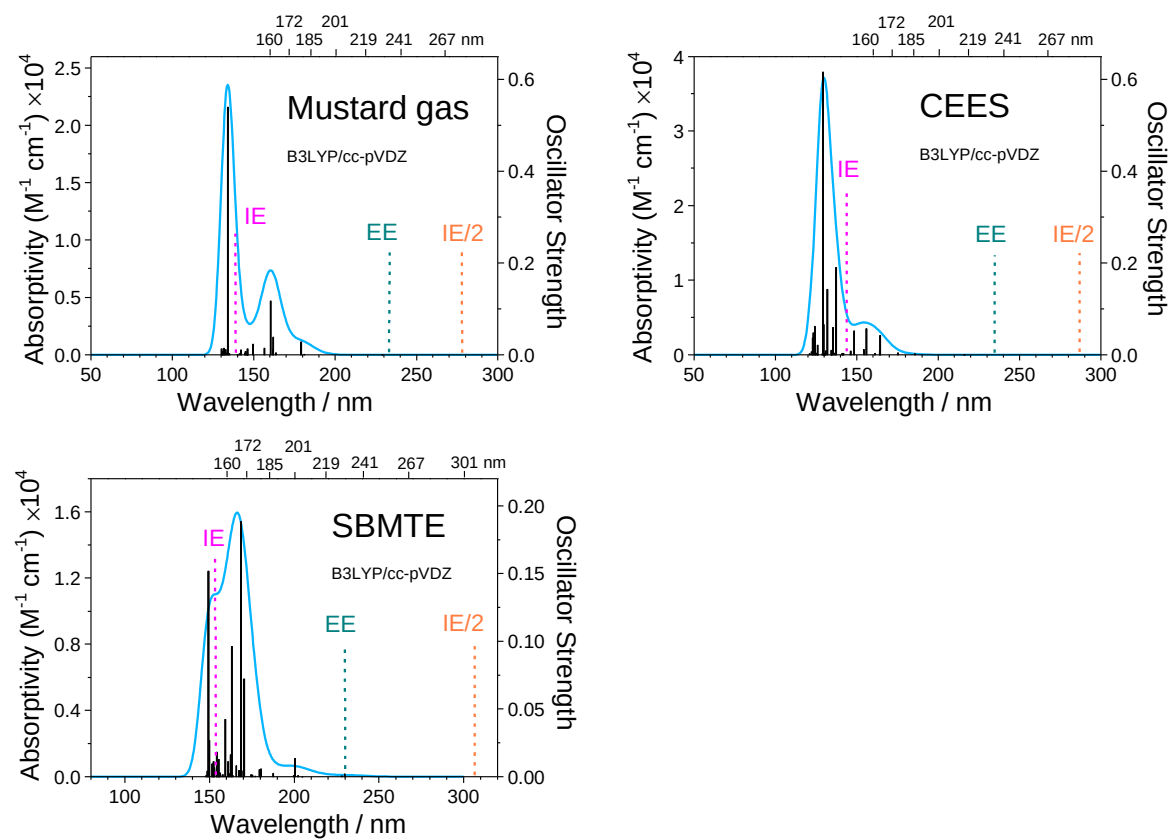


Fig. S3 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for mustard gas, CEES, and SBMTE calculated using B3LYP/cc-pVDZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

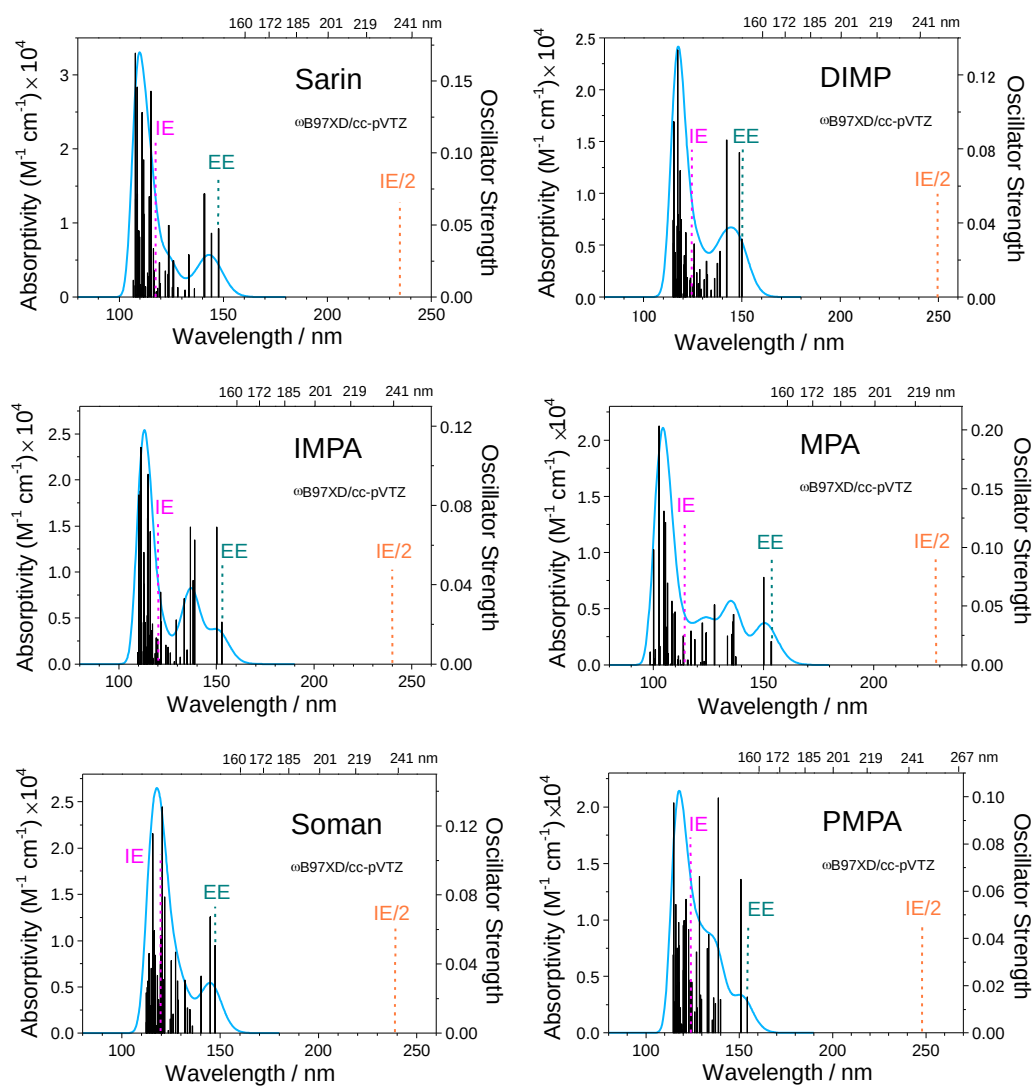


Fig. S4 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for Sarin, DIMP, IMPA, MPA, Soman, and PMPA calculated using $\omega\text{B97XD/cc-pVTZ}$. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

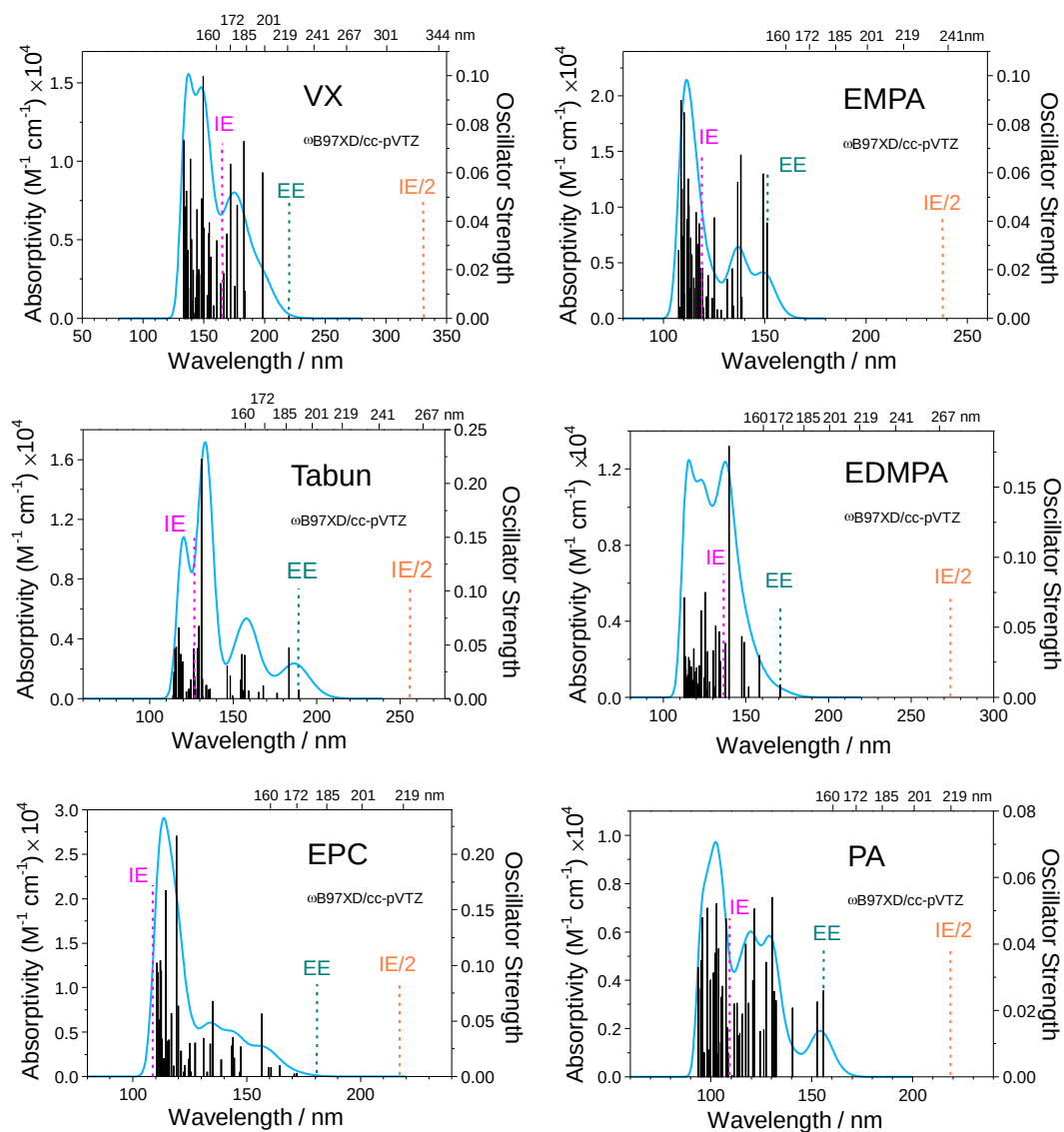


Fig. S5 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for VX, EMPA, Tabun, EDMPA, EPC, and PA calculated using ω B97XD/cc-pVTZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.

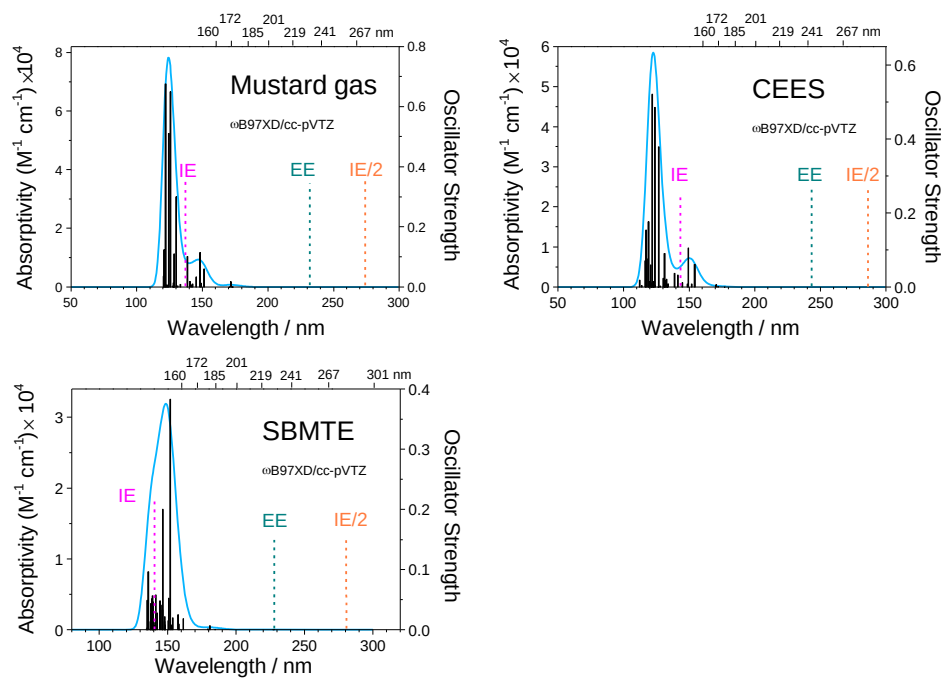


Fig. S6 Predicted VUV-UV absorption spectra and oscillator strengths (vertical lines) for Mustard gas, CEES, and SBMTE calculated using ω B97XD/cc-pVTZ. IE, ionization energy; IE/2, one half of the ionization energy; EE, transition energy for the first electronic excited state.