Researchers reveal new competition mechanism in vacuum ultraviolet photoionization of dichloromethane

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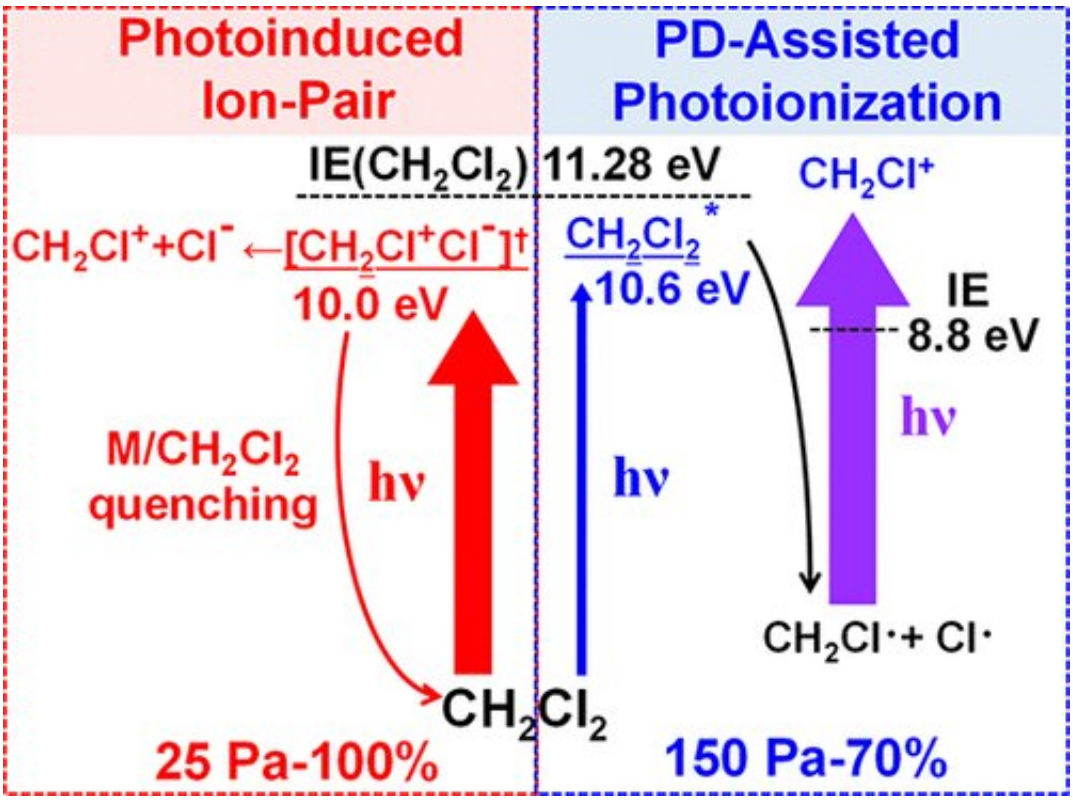

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A research group led by Prof. Li Haiyang from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS)

has revealed a new competition mechanism in vacuum ultraviolet photoionization of dichloromethane using a home-built time-of-flight mass spectrometer (TOFMS).

The study was published in The *Journal of Physical Chemistry Letters* on Jan. 31.

Dichloromethane (CH_2Cl_2) is widely used as industrial solvent, reaction medium in pharmaceutical industry and feedstock for producing other chemicals. CH_2Cl_2 can cause environmental harm and health hazards due to its low boiling point and high volatility.

Strong presence of vacuum ultraviolet (VUV) light in the solar emission spectrum can induce the production of ozone-depleting Cl atom; therefore, the photochemistry of CH_2Cl_2 is crucial to stratospheric ozone chemistry.

In this study, the researchers have revealed the photoionization mechanism of CH_2Cl_2 under the irradiation of 10.0 and 10.6 eV light from a VUV krypton (Kr) lamp.

They demonstrated that CH_2Cl^+ was produced by two competitive channels: photoinduced ion-pair and photodissociation-assisted photoionization (PD-PI). The ion-pair channel was quenched efficiently at high number density of CH_2Cl_2, which reduced its contribution.

Moreover, they indicated that the dominant photodissociation channel of CH_2Cl_2 was $CH_2Cl_2 + h\nu \rightarrow CH_2Cl\cdot + Cl\cdot$, and the formed $Cl\cdot$ radical could further react with the CH_2Cl_2 molecule to form $CHCl_2\cdot$ radical. Then CH_2Cl^+ was generated by the photoionization of $CHCl_2\cdot$. Finally, they derived kinetic equations for the quantitative description of the production efficiencies of CH_2Cl^+ and CH_2Cl^+.

"Our study enhances the overall understanding of the complicated photoexcitation behaviors of CH_2Cl_2 in the VUV regime, which helps to study the atmospheric photochemical process of haloalkanes and provides guidance for the photodegradation of hazardous haloalkanes," said Prof. Li.

More information: Yi Yu et al, Ionization of Dichloromethane by a Vacuum Ultraviolet Krypton Lamp: Competition Between Photoinduced Ion-Pair and Photodissociation-Assisted Photoionization, *The Journal of Physical Chemistry Letters* (2023). DOI: 10.1021/acs.jpclett.2c03572

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