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Raman investigation of hydration structure of iodide and iodate*

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In the troposphere, the destruction of ozone and the formation of new particles are closely related to the iodine content, which mainly comes from iodide (I^-) and iodate (IO_3^-) in the seawater. Therefore, understanding the interactions between I^-, IO_3^- and water molecules plays a certain role in alleviating the destruction of the ozone layer. Raman spectroscopy is commonly used to obtain the information of the interaction between I^-, IO_3^- and water molecules quickly and accurately. Herein, the effect of I^- and IO_3^- on the change in Raman band characteristics of water is investigated to reflect the associated intermolecular interactions change. With the addition of the two ions, the Raman band corresponding to OH stretching vibration moves towards the high wavenumber, indicating the formation of hydration structure. The narrowing of the Raman band from OH stretching vibration under weak hydrogen bond agrees well with the hydrogen bond variation, while the abnormal broadening of the Raman band from OH stretching vibration under strong hydrogen bond indicates the formation of H-down structure. With the increase of ions concentration, the frequency shift of the Raman band from OH stretching vibration under both weak and strong hydrogen bonds becomes more apparent. Meanwhile, the frequency shift of I^- is more obvious than that of IO_3^-, which indicates that I^- is more likely to form the hydration structure with water than IO_3^-. These results contribute to analyzing the different interactions between I^-–water and IO_3^-–water, then helping to prevent ozone depletion.

Keywords: Raman spectroscopy, hydrogen bond, hydration structure

PACS: 33.20.Fb, 34.20.Gj, 36.40.Mr **DOI:** 10.1088/1674-1056/abe2fa

1. Introduction

In the atmosphere, the ozone layer of the stratosphere is the natural protective barrier of the earth, which can absorb ultraviolet rays effectively and warm the atmosphere.[1–3] In recent years, with the emission of harmful gases such as nitrous oxide (N_2O), carbon tetrachloride (CCl_4), methane (CH_4) and the most important chlorofluorocarbons (CFC), the ozone layer has been damaged and partially thinned.[4] Researchers have also found that iodine in the atmosphere has a destructive effect on the ozone layer besides the harmful gases mentioned above.[5–7] Iodine in the atmosphere mainly comes from seawater, and it is transferred from seawater at the boundary layer of the ocean atmosphere.[8] The conversion process mainly includes the oxidation of I^- into volatile iodine element (I_2) and the atomization of iodide together with other ions or organic substances.[9] Through these chemical reactions, the distribution and concentration of I^- and IO_3^- in sea aerosols change greatly while new iodine-containing substances are generated, which causes different degrees of damage to the ozone layer. Since iodine mainly comes from seawater, the interactions between I^-, IO_3^- and water molecules in the seawater directly affect the transfer of iodine into the atmosphere. Therefore, the study of the interactions between I^-–water and IO_3^-–water at different concentrations is constructive for understanding the mechanism of the transformation process, thus contributing to the exploration of different degrees of atmospheric damage caused by concentration and spatial distribution of iodine, which is of great significance for the corresponding environmental governance.

In the liquid state, water molecules are connected with each other through complex hydrogen bonds (H bonds), forming clusters of varying sizes. These H bonds usually have a lifetime of only picoseconds and undergo dynamic breaking and re-bonding. At the same time, water molecules also rotate rapidly at a picosecond time scale, and hydrogen atoms also exhibit quantum effects, where the liquid water presents a dynamic equilibrium state. When ions are dissolved in water, they disturb the water environment and hydration by forming a hydration layer outside the ions with surrounding water molecules. Then, both anions and cations will affect the structure of the hydration layer with the increase of ion concentration. Cations may lead to the aggregation of ions, and the increase of anions affects the number of water molecules in the hydration layer. It is generally believed that the influ-

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ence of anions on the H bond structure in the hydration layer is more obvious than that of cations, and anions mainly affect the water molecules in the first hydration layer.[10–13] The number of water molecules in the hydration layer varies from 5 to 50 due to the difference in ionic electronegativity, size, polarity, etc. The signal-to-noise ratio and accuracy of experimental methods are stringent due to the complex structure of the H bond network in liquid water and the uncertainties of the interaction between anions and water molecules. The theoretical and experimental methods that can be used to investigate the structure of water molecules in liquid water mainly include ab initio molecular dynamics simulations,[14] neutron scattering,[15,16] vibration spectroscopy,[17] etc. The Raman spectroscopy of water has high accuracy, making it suitable for studying the interactions between halogen ions and water molecules. Moreover, there are also notable differences between infrared spectroscopy and Raman spectroscopy in the field of local structure research of water,[18,19] From the mechanism, the infrared spectroscopy shows dipole moment transition of the molecule, while Raman spectroscopy shows the change of molecular polarizability. From the experimental perspective, as the Raman spectroscopy is more sensitive to the movement of free OH groups,[20] it can be used to study the local H bond structure of water directly. However, the infrared absorption coefficient[21] should be introduced when using infrared spectroscopy, which not only makes the relevant research complicated, but it also introduces errors. Moreover, Raman spectroscopy has the characteristics of low cost, convenient operation, and high signal-to-noise ratio. Therefore, Raman spectroscopy measurement has great advantages in studying the local H bond structure of water compared with other research methods.

As is known to all, the change of the H bond of water affects the OH vibration of water directly. Raman spectroscopy can accurately detect the information of OH vibration of water molecules.[22,23] The double peak distribution of water is detected, and the change of H bond can be analyzed accurately through the change of spectral peak position, so as to predicting the interactions between halogen ions and water molecules. In addition, although IO_3^- has low solubility in seawater, the strong H bonds and weak H bonds in the hydration cluster structure increase the chance of staying at the water-air interface, thus promoting its transfer from the ocean boundary layer to the atmosphere. Studies on the interaction between halogen ions and water molecules have been widely reported,[24–26] but the Raman spectroscopy studies on aqueous solutions with different concentrations of I^- and IO_3^- are relatively rare reported.

In this paper, Raman spectroscopy is used to study the interactions between I^-/IO_3^- and water molecules. The influence of I^- and IO_3^- can be inferred by studying the change of double peaks position of Raman spectra of water at different concentrations. The OH stretching vibration peaks of the water all move towards the high wavenumber after the addition of I^- and IO_3^-, but the abnormal broadening of the P_{sh} indicates the formation of the H-down structure. As the concentration increases, the hydration is becoming increasingly obvious. The result is of great importance to analyze the interaction between iodine and water molecules in seawater and understand the mechanism of iodide's transformation from seawater to the atmosphere, so as to alleviate the damage of I^- and IO_3^- to the atmosphere.

2. Experimental setup

The Raman spectra of the aqueous solution of potassium iodate and potassium iodide were measured using a Renishaw InVia micro-confocal Raman spectrometer at room temperature(20 °C) and ambient pressure (1.0×10^5 Pa). The 514.5 nm Ar^+ laser source with an output power of 4 mW was focused on the sample. The 1200 lines/mm grating was used in the experiment, which produced a spectral resolution of 4 cm^{-1}. Then the spectrum was obtained using a 20×magnification objective lens (LEICA DMLM 0.12 NA).

The samples of potassium iodate and potassium iodide, analytically pure (> 99.5% v/v%), provided by Beijing Chemical Works, were used without further purification. The potassium iodide-water and potassium iodate-water binary solution were prepared with different concentrations 0.05, 0.5, 1, 1.5, 2 mol/L and 0.01, 0.05, 0.1, 0.3, 0.5 mol/L respectively by adding certain amount (0.415, 4.15, 8.3, 12.45, 16.6 g potassium iodide and 0.107, 0.535, 1.07, 3.21, 5.35 g potassium iodate) of solute into 50 mL water. The binary solution was pipetted into a glass capillary (inner diameter is 0.9–1.1 mm, wall thickness is 0.10–0.15 mm), which was tested by placing it on the stage.

3. Results and discussion

The Raman spectrum of pure water is shown in Fig. 1. The deconvoluted peak positions are located at 3213 cm^{-1} for the left peak and 3436 cm^{-1} for the right peak. These two peaks belong to the OH stretching vibration mode under the H bond. Generally, the two Raman bands could be attributed to the OH stretching vibration under strong (around 3200 cm^{-1}) and weak (around 3400 cm^{-1}) H bonds.[27,28] The left peak corresponds to the OH peak under the action of the strong H bond, while the right peak corresponds to the OH peak under the action of the weak H bond. The left peak (3213 cm^{-1}) and the right peak (3436 cm^{-1}) are referred to as P_{sh} (OH vibration under strong H bond) and P_{wh} (OH vibration under weak H bond), respectively. According to the relationship between H bond energy and OH stretching vibration frequency given in Fig. 2,[29] the H bond strengths corresponding to the two peaks of P_{sh} and P_{wh} in pure water are 19.48 kJ/mol and 10.56 kJ/mol, respectively. 0.05 mol/L I^- and IO_3^- were added to the water separately to analyze the hydration of the two ions

at the same concentration. The spectra were deconvoluted, as shown in Fig. 3. The full width half maximum (FWHM) and Raman shift of peaks were read out, and the data are listed in Table 1.

Table 1. The FWHM and Raman shift after deconvolution of I^- and IO_3^- at the concentration of 0.05 mol/L (unit: cm^{-1}).

	P_{sh}		P_{wh}	
	Raman shift	FWHM	Raman shift	FWHM
H_2O	3213	154	3436	263
I^- aqueous solution	3229	181	3451	233
IO_3^- aqueous solution	3227	174	3447	235

Compared with pure water, the OH stretching vibration peak generally shows the same change trend after adding I^- and IO_3^- ions. By comparing I^- and IO_3^- at the concentration of 0.05 mol/L, both peaks of P_{sh} and P_{wh} move towards high wavenumber, the FWHM of P_{sh} peak is widened while the FWHM of P_{wh} peak is narrowed.

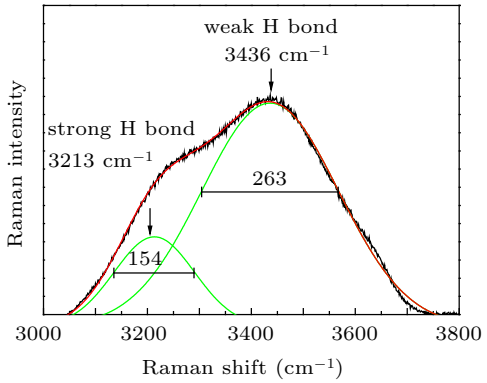


Fig. 1. Raman spectrum of pure water with the deconvolution results being curved in the green line.

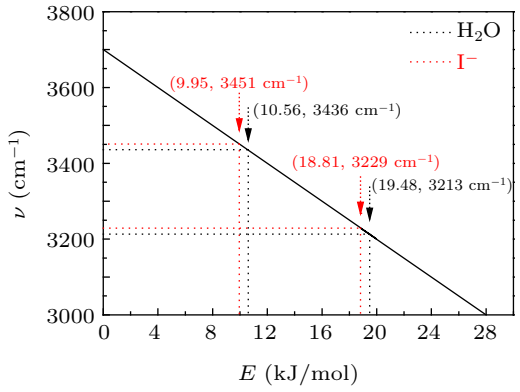


Fig. 2. The relationship between hydrogen bond energy and OH stretching vibration frequency in liquid water.

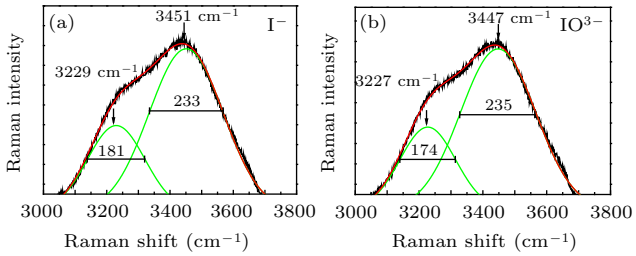


Fig. 3. Deconvoluted Raman spectra of 0.05 mol/L I^- (a) and IO_3^- (b) aqueous solution.

To gain insights into the relationship between solution concentration and H bond structure, the frequency shift of the P_{wh} and P_{sh} of I^- aqueous solution was analyzed. Compared with pure water, both P_{wh} and P_{sh} move towards high wavenumber, indicating that the OH stretching vibration under the strong H bond is enhanced, corresponding to the weakening of the H bond. The change of H bond strength is mainly caused by the addition of I^- ions, which destroys the original H bond structure by forming a new interaction between anionic water molecules, namely the hydration layer. Therefore, the interaction force between anions and water molecules is smaller than the original interaction between water molecules, thus weakening the H bond.[30,31] According to the previous theoretical calculation, at this concentration, the number of water molecules in iodide's first hydration layer is 5–6,[13,32] as shown in Fig. 4. Using the corresponding relationship between OH vibration frequency and H bond strength as shown in Fig. 2, it can be concluded that the H bond strengths corresponding to the two peaks in I^-aqueous solution at 0.05 are 18.81 kJ/mol and 9.95 kJ/mol, respectively, which are weaker than that of pure water.

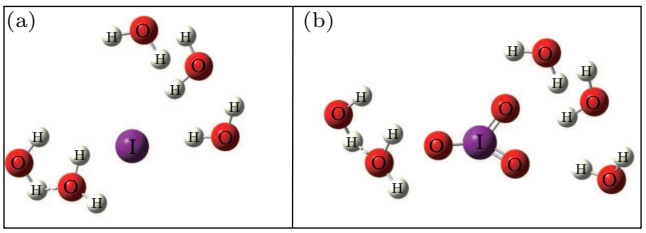


Fig. 4. Schematic first hydration layer of I^- at 0.05 mol/L.

Then, the variation of FWHM of I^- ions aqueous is studied. The narrowing of the P_{wh} is mainly caused by the weakening of the H bond, which agrees well with the inference above.[33,34] The frequency shift of P_{sh}, shifting to the right, is consistent with the trend of the P_{wh}, indicating that the H bond is weakened. However, the widening of the P_{sh} indicates that the H bond is strengthened, which does not conform to the inference of the H bond weakening above. The main reason could be the existence of the H-down structure of the H bond in the hydration layer,[35] as shown in Fig. 5. The H-down structure comes from the bilayer structure of water, which is composed of an H-up structure and an H-down structure.[36] The orientation of the H-up structure is upwards, while the orientation of the H-down structure is towards bulk water. Generally speaking, the OH stretching band depends not only on the influence of the H bond on OH stretching vibration, but also on the molecular coupling, which is mainly the intramolecular, intermolecular vibration coupling, and Fermi resonance. Both intramolecular and intermolecular coupling can enhance OH stretching vibration on water molecule surface, and intermolecular coupling is stronger than intramolecular coupling.

The intramolecular coupling results in a bimodal structure of water, while the intermolecular coupling causes a red shift in OH stretching.[37–39] After the formation of the hydration bilayer, the central ion acts on the orientation of H bonds, resulting in the enhancement of vibration coupling and the formation of H-down structure, which widens the P_{sh}.[40] This unique structure causes anions to tend to stay in the interfacial region. According to the actual situation of the ocean, the H-down structure makes the I^- tend to stay in the boundary layer of the ocean. Since the H-down structure in the water corresponds to the H-down structure formed at the interface, the result is helpful to analyze the iodine transfer process in the marine interfacial layer.

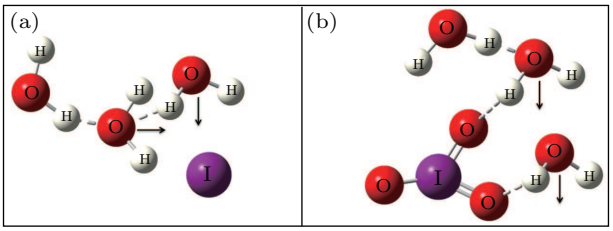


Fig. 5. The H-down structure of (a) I^- and (b) IO_3^-.

Finally, the difference between I^- and IO_3^- is analyzed. Ions at different concentrations were added to further investigate the difference in the interaction between I^-–water and IO_3^-–water. For I^-, five concentrations of 0.05, 0.5, 1, 1.5, and 2 mol/L were selected. The spectra and corresponding frequency shift trend chart are listed below, as shown in Fig. 6. With the increase of I^- concentration, the spectra continue to move towards high wavenumber, which indicates that the number of hydration layers decreases gradually, leading to the weakening of the H bond and the strengthening of OH stretching vibration. At the same time, the FWHM also presents a similar trend; the P_{wh} continues to narrow, the P_{sh} continues to widen, which also confirms the gradual decrease of the hydration layer. The main reason is that the hydration number decrease in the process of concentration increase, which weakens the interaction between ions and water molecules, resulting in the weakening of the H bond and the increasing of OH stretching vibration intensity, and the corresponding spectra shift to high wavenumber. The main reasons for the decrease of the hydration number are as follows: firstly, the H bond will be weakened with the introduction of anions; the higher the anionic concentration is, the weaker the H bond will be; secondly, in order to increase the number of anions, the concentration of the solute will increase accordingly, so the corresponding cations will increase gradually. The resulting ion polymerization will eliminate the water molecules in the hydration layer, thus reducing the hydration layer; thirdly, hydrated anions and cations form solvent-shared electron pairs and clusters. The water molecules on the first hydration layer of anions are replaced by cations, which may weaken hydration by affecting their polarizability. The weakening effect becomes more serious with the concentration increases. The number of hydration layers is reduced instantaneously due to the aggregation of a large number of ions. The decrease of the hydration number also influences the charge transfer (CT) process from anion to water. Based on previous reports,[41,42] the excitation source might cause the CT transition from the anion to the water in I^- aqueous solution, known as photon-driven charge transfer (PDCT).[43,44] PDCT leads to the pre-resonance enhancement of the Raman signal of OH stretching vibration.[42] When the wavelength of the excitation laser is fixed at 514.5 nm, the decrease of the hydration number reduces the PDCT between I^- and the water molecule, thus leading to the decrease of the energy gap between the virtual excited state and the CT−excited state. Then the Raman band move towards high wavenumber with the increase of I^- concentration.

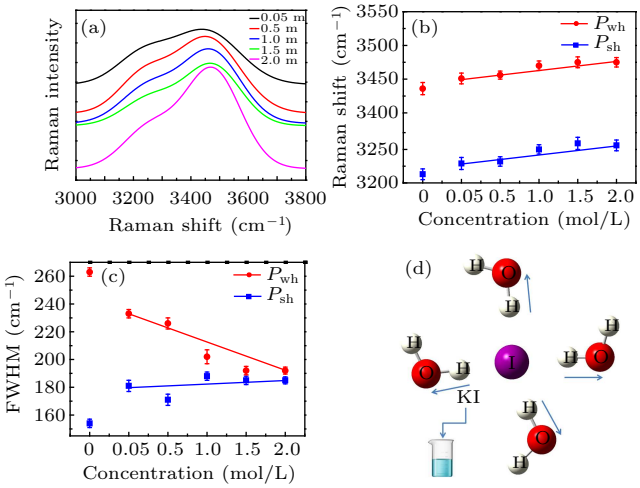


Fig. 6. (a) The spectrum of I^- aqueous solution at different concentrations and (b) the corresponding frequency shift trend, (c) the change trend of FWHM, (d) schematic molecular interaction.

As shown in Fig. 7, the results of IO_3^- are relatively similar to I^-. Since the solubility of IO_3^- was 0.38 mol/L at room temperature, a narrower concentration interval was chosen, which was 0.01, 0.05, 0.1, 0.3, and 0.5 mol/L, respectively. The peak position basically remains unchanged both before and after exceeding the saturation concentration. The results show that the number of hydration layers remains unchanged due to the limitation of solubility after the change of its concentration. The Raman shift and FWHM all change little from the spectra. On the other hand, the radius of IO_3^- is larger than that of I^-, leading to the interaction between ions and water molecules weaker, and the number of bounded water molecules is small, so the number of hydration layers is less than that of I^-.

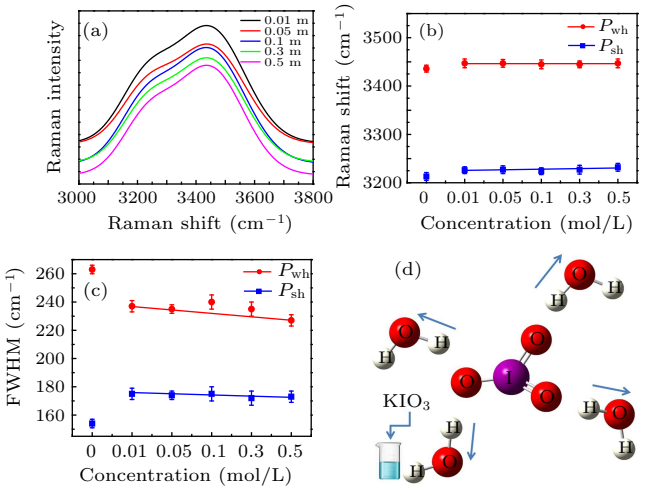


Fig. 7. (a) The spectrum of IO_3^- aqueous solution at different concentrations and (b) the corresponding frequency shift trend, (c) the change trend of FWHM, (d) schematic molecular interaction.

4. Conclusion

Through the separate analysis of I^- and IO_3^- aqueous solution with different concentrations, the H bond in water is weakened after adding I^- or IO_3^-, which is caused by the addition of ions forming a hydration layer, resulting in the weakening of the H bond. Moreover, the H-down structure can be inferred from the special change of FWHM, which makes it easy for ions to exist on the surface and increases the risk of ozone layer destruction. Compared with IO_3^-, I^- demonstrates a larger frequency shift and broadening degree, which shows that the hydration layer formed by I^- is larger, the H bond is weaker, and the corresponding OH vibration is stronger. The main reason is that the radius of IO_3^- is larger than that of I^-. As two acid ions containing iodine, they play a significant part in the process of ozone destruction. The effect of I^- on water molecules is similar to that of IO_3^- at the same concentration; when the concentration changes, IO_3^- exhibits a smaller effect than I^- due to its small solubility. This study is helpful for the differential treatment of I^- and IO_3^- in seawater, accordingly alleviating their damage to atmospheric ozone and protecting the ecological environment.

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