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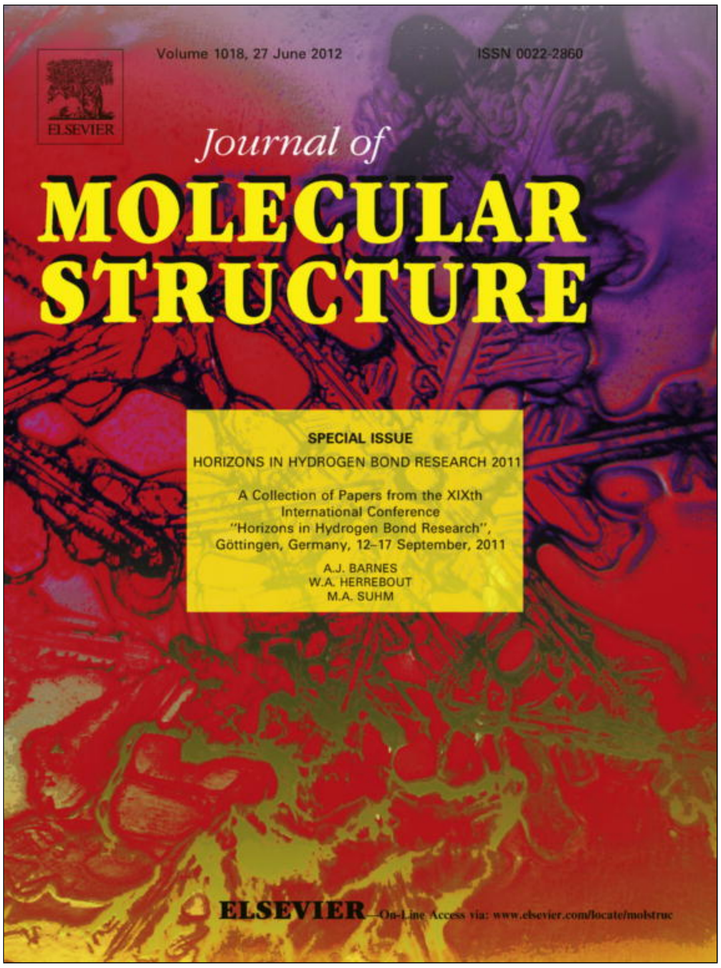

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The dielectric constant dependence of absorption intensities and wavenumbers of the fundamental and overtone transitions of stretching vibration of the hydrogen fluoride studied by quantum chemistry calculations

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ABSTRACT

Vibrational potentials and dipole moment functions of HF molecule in solutions have been calculated as a function of dielectric constant by using the self-consistent reaction field (SCRF)/isodensity surface polarized continuum model (IPCM) calculation. We have selected HF molecule as the simplest polar molecule. The wavenumbers and absorption intensities of the fundamental and the first, second and third overtones of H–F stretching mode have been calculated as a function of dielectric constant. The SCRF/IPCM model calculations have revealed that the vibrational potential and dipole moment function of HF molecule vary continuously with a change in the dielectric constant of the solvent. The calculations were carried out at B3LYP/6-311++G(3df,3pd) and CCSD/aug-cc-pVQZ levels. It has also been found that the absorption intensities of the fundamental increase with the increase of the dielectric constant smoothly but those of the first, second and third overtones do not increase continuously. Moreover, the B3LYP and CCSD levels yielded significantly different results in the dependence of absorption intensities on the dielectric constant.

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1. Introduction

Recently, many basic and application studies using overtones of molecular vibrational modes have been developed partly because of the advances in near-infrared (NIR) instruments and partly because of the development of quantum chemical calculations. It has been well known that absorption bands due to overtones are forbidden in harmonic oscillator approximation [1–5]. An appearance of a band due to an overtone is explained by anharmonicity of a molecular vibration. An IR absorption intensity is described by a transition dipole moment function, and its transition dipole moment function is given by an integral of dipole moment function and wave function. Moreover, the wave function is yielded by molecular vibrational potential. Therefore, as is well known, an IR absorption intensity reflects very well molecular structure and molecular interactions. For example, symmetry of a molecular vibration determines selection rules of IR absorption; a symmetric stretching mode gives, in general, a forbidden transition (or a weak band) while an asymmetric and an asymmetric stretching modes show an allowed transition. Moreover, the formation of a hydrogen bonding, which is a strong molecular interaction, increases the absorption intensity of fundamental vibration by several hundred times in some cases [6].

Galabov et al. [7–9] carried out a number of studies on the relations between IR absorption intensity and molecular structure as well as intramolecular charge distribution. Recent development of quantum chemical calculations enables one to reproduce very well the relation between molecular structure and frequencies and absorption intensities of vibrational modes [10–13]. Theoretical calculations of molecular structure and IR spectra have been recognized as effective tools even for the identification of interstellar molecules [14,15].

Molecular vibration analyses by quantum chemistry calculations are, in general, based on a harmonic oscillator model. However, actual vibrations are anharmonic, and thus, one cannot

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reproduce experimental data with sufficient precision by a harmonic oscillator model [16,17]. The reason why quantum chemical calculations considering anharmonicity have not been popularized is that the amounts of calculations are enormous. Thus, even now, development of quantum chemical calculations including anharmonicity is in progress [18,19].

It is well known that an IR absorption intensity of a fundamental increases with the formation of a hydrogen bonding, but intensity changes of overtones due to the formation of a hydrogen bonding have not been studied well. Kjaergaard et al. [20,21] studied the effects of hydrogen bondings in water dimer and trimer, and methanol-trimethylamine complex on their overtone bands by comparing their NIR spectra in the gas phases with quantum chemical calculations including the anharmonicities. They found that the absorption intensities of the first overtones of these molecules decrease dramatically upon the formations of hydrogen bondings. Moreover, they investigated wavenumbers and absorption intensities of higher order overtones of basic molecules and explored methods of quantum chemical calculations that can reproduce experimental data more accurately [22]. Gonjo et al. [23] found in the research on inter- and intramolecular hydrogen bondings of phenol and 2,6-dihalogenated phenols that the absorption intensity changes of overtones of OH stretching mode upon the formation of inter- and intramolecular hydrogen bondings show “parity” in vibrational quantum numbers.

Recently the number of reports on the quantum chemical calculations involving solvent effects have increased significantly. Preat et al. [24] investigated dependences of dielectric constant on the wavenumber and IR absorption intensity of CO stretching mode and electronic excitation energy of coumarin by using a polarized continuum model (PCM). According to their calculation results together with IR measurement, the frequency of CO stretching mode decreases while its intensity increases with the increase in the dielectric constant up to $\varepsilon = \sim 25$, and that remain almost constant above $\varepsilon = \sim 25$. Polovkova et al. [25] reached similar conclusion that the frequency and the intensity of a NH stretching band change little above $\varepsilon = \sim 25$ for 3-dimethylamino-2-acetyl propenenitrile and 3-dimethylamino-2-methylsulfonyl propenenitrile by the use of PCM and a static isodensity surface polarized continuum model (IPCM).

However, one can find only a few studies on effects of weak intermolecular interactions such as solvent effects on absorption intensities of overtones [23–28]. Takahashi et al. calculated the absorption intensities of the fundamental and the first overtone of CH stretching mode of 1,2-dichloroethylene in gas and solution states by using Onsager model of self-consistent reaction field (SCRF) [26]. Futami et al. [27,28] carried out quantum chemical calculation investigations of effects of hydrogen bondings and solvent effects on absorption intensities of the fundamental and the first overtone of NH stretching mode of pyrrole. According to them, upon the formation of hydrogen bonding between pyrrole and pyridine the absorption intensity of the fundamental of NH stretching mode of pyrrole increases while that of the first overtone decreases markedly. This result is in good agreement with that of OH stretching mode of water dimer and methanol-trimethylamine complex by Kjaergaard et al. [20,21]. In contrast, the study of pyrrole by using CCl_4, $CHCH_3$, and CH_2Cl_2 as solvents showed that both the fundamental and the first overtone of NH stretching mode of pyrrole increase with the increase of the dielectric constant. In this way, Futami et al. [27,28] showed that so called “hydrogen bonding effects” and “solvent effects” should be calculated by using different modes.

Calculations of continuous variations of vibrational potential and dipole moment function as a function of dielectric constant by using IPCM model can explain systematic relations among anharmonicity of a molecular vibration, its wavenumber, and absorption intensity.

In the present study, we have calculated vibrational potential and dipole moment functions of H–F stretching mode of hydrogen fluoride and then, absorption intensities of its fundamental and overtones by using SCRF/IPCM model. The calculations were carried out at B3LYP/6-311++G(3df,3pd) and CCSD/aug-cc-pVQZ levels. SCRF calculations cannot estimate local strong interactions such as a hydrogen bonding but can estimate extensive electrostatic interactions induced by a dielectric field. The increase in the dielectric constant produces the increase in the potential energy with bond length and the increase in the slope of dipole moment function. We discuss the relations between absorption intensities, wavenumbers and dielectric constant for the fundamental, the first, second and third overtones.

2. Calculation method

The SCRF/IPCM//DFT calculations were carried out by the Gaussian 09 program [29] with 6-311++G(3df,3pd) basis set. Becke’s three-parameter hybrid density function in combination with the Lee–Yang–Parr correlation functional (B3LYP) was used for the optimization of geometrical structures and the calculations of vibrational potential curves, and dipole moment functions [30,31]. The quantum chemical calculation based on a SCRF/IPCM model was carried out with chemical structures in gas phase. Moreover, similar calculation was performed at CCSD/aug-cc-pVQZ level, and the results were compared.

In the present study, we solved the Schrödinger equation of one-dimensional H–F stretching vibration

$$H\psi_v(q) = \left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}q^2} + V(q)\right]\psi_v(q) = E_v\psi_v(q) \tag{1}$$

where q, μ and $V(q)$ are the interatomic distance, the reduced mass and the potential energy function, respectively.We calculated the oscillator strength f_{v0} for each H–F stretching transition by

$$f_{v0} = \frac{4m_e\pi}{3e^2\hbar}\left|\vec{\mu}_{v0}\right|^2\tilde{\nu}_{v0} = 4.702\times10^{-7}\left|\vec{\mu}_{v0}\right|^2\tilde{\nu}_{v0} \tag{2}$$

where $\tilde{\nu}_{v0}$ is the transition energy in cm^{-1}, and $|\vec{\mu}_{v0}|^2$ is the sum of the squared transition dipole moments of the x, y, and z components in $(\mathrm{debye})^2$ unit [20,32]. $|\vec{\mu}_{v0}|^2$ is given by

$$\begin{aligned}\left|\vec{\mu}_{v0}\right|^2 &= \left|\vec{\mu}^x_{v0}\right|^2 + \left|\vec{\mu}^y_{v0}\right|^2 + \left|\vec{\mu}^z_{v0}\right|^2\\ &= \left|\int\psi_v(q)\vec{\mu}^x\psi_0(q)\mathrm{d}q\right|^2 + \left|\int\psi_v(q)\vec{\mu}^y\psi_0(q)\mathrm{d}q\right|^2\\ &\quad + \left|\int\psi_v(q)\vec{\mu}^z\psi_0(q)\mathrm{d}q\right|^2\end{aligned} \tag{3}$$

Here, $|\vec{\mu}^x_{v0}|^2 = 0$ and $|\vec{\mu}^y_{v0}|^2 = 0$, because this is diatomic molecule (i.e. spherical symmetry)

We obtained the numerical results for the energy levels and the wave functions using the method given by Johnson [33]. The potential energy curves used for the calculations cover the range from 0.5 to 2.0 Å in 0.02 Å steps around the equilibrium position.

The number of calculation points is sufficient for the numerical calculations without such assumption as the Morse function. This ensures converged energy levels with precision higher than 0.001 cm^{-1}. The calculation conditions of Gaussian09 were tight convergence in the SCF, standard grid in DFT.

3. Results and discussion

Fig. 1 shows the stabilization energy ΔE of HF molecule versus dielectric constant calculated by both B3LYP/6-311++G(3df,3pd) and CCSD/aug-cc-pVQZ levels. The results of calculations reveal that the molecule becomes stable as the ΔE increases. HF molecule is a molecule of strong polarity, and thus it is stabilized with the increase in the dielectric constant. It is noted that the change in the stability is remarkable when the dielectric constant varies from 1 to 10. This tendency is similar between the B3LYP and CCSD calculations.

Fig. 2a and b displays vibrational potentials and dipole moment functions calculated by the B3LYP/6-311++G(3df,3pd) and CCSD/aug-cc-pVQZ levels, respectively, for various dielectric constants ($\varepsilon = 1$–80) together with wave functions calculated for $v = 0$–4. Anharmonicity of vibrational potential increases with the dielectric constant. The degree of its increase is larger for B3LYP level than for CCSD level. The slope of dipole moment function also increases depending on the dielectric constant. The variation in the anharmonicity of vibrational potential and that in the slope of dipole moment function are significant when the dielectric constant changes from 1 to 10. These tendencies are very similar to that for the change in the stabilization energy.

By using the calculated vibrational potentials and dipole moment functions, we calculated the wavenumber and absorption intensities of the fundamental, and the first, second and third overtones. Table 1 compares the calculation results for $\varepsilon = 1$ (gas phase) with the observed results by Kirkpatrick and Salant [34] and Naude and Verleger [35]. Moreover, reference values by Kjaergaard et al. [22,36] are shown in Table 1.

The calculated frequencies do not always reproduce the observed frequencies, however, the ratios between the calculated wavenumbers of the fundamental, and the first, second, and third overtones of H–F stretching mode and the corresponding observed ones are nearly constant. The calculated frequencies at the B3LYP level are smaller by ca. 1% while those at the CCSD level are larger by ca. 1% compared with the experimental data. Thus, the differences between the observed and calculated wavenumbers can be calibrated by multiplying with one scale factor. The CCSD(T) calculation, its calculated wavenumbers agree with experiment to within 0.1%.

The calculated absoption intensity ratios are in good agreement with the experimental ones for the fundamental and the first, second, and third overtones (Table 1). The B3LYP and CCDS levels calculations have reproduced very well the experimental data in terms of both vibrational frequencies and absorption intensities. The CCSD calculation gives better intensities compared to the B3LYP calculation, thus likely much better dipole [37].

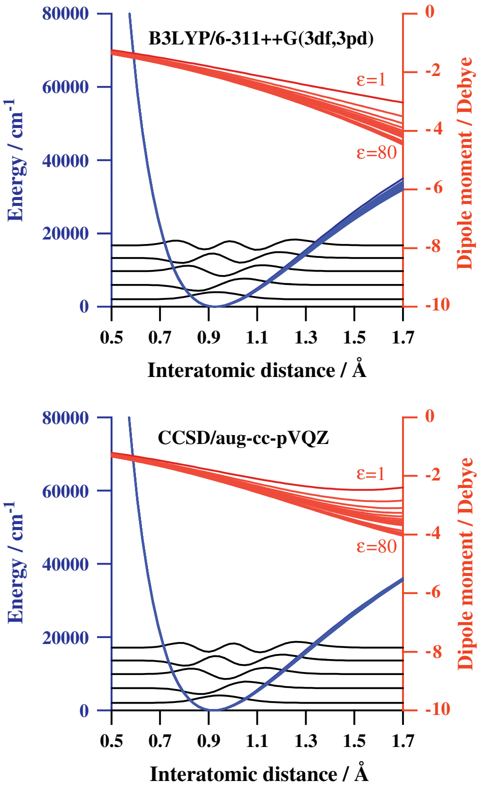

Fig. 2. Dependences on the dielectric constant of the potential energy curve, dipole moment function ($\varepsilon = 1$–80) and wave function ($\varepsilon = 1$) of HF stretching mode calculated at the IPCM//DFT/B3LYP/6-311++G(3df,3pd) and IPCM//CCSD/aug-cc-pVQT level.

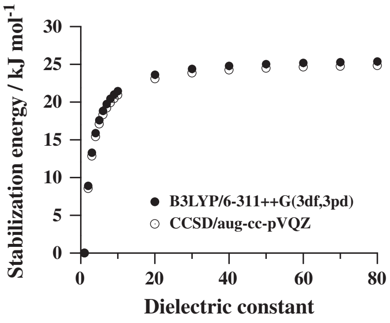

Fig. 1. Dielectric constant and Stabilization energy of hydrogen fluoride.

Fig. 3a–d illustrates dependences of the wavenumber and absoption intensity of the H–F stretching mode on the dielectric constant for the fundamental, the first, second, and third overtones, respectively, calculated at the B3LYP level and CCSD level. The calculated wavenumbers of the fundamental, and the first, second, and third overtones all show a small wavenumber shift with the increase in the dielectric constant. These are derived from the anharmonicities of vibrational potentials which vary depending upon the dielectric constant. In the calculation results at the B3LYP level, the absorption intensity changes of the fundamental, and the first, second, and third overtones of the H–F stretching mode as a function of the dielectric constant are very similar to those of the N–H stretching vibrations of pyrrole [28] and the O–H stretching vibration of phenol derivatives [23].

It can be seen from Fig. 3 that both B3LYP and CCSD levels give similar tendencies for the dependence of vibrational frequencies on the dielectric constant. However, the B3LYP and CCSD levels yield different results for the absorption intensities. For the absorption intensity of the fundamental, both levels provide the results of similar tendency. On the other hand, both methods give different results for the absorption intensity of the first overtone; the absorption intensity increases with the increase in the dielectric constant in the calculation at the B3LYP level while it increases with the increases in the dielectric constant from 1 to 5 but decreases from 6 to 8 at the CCSD level.

Moreover, the rate of absorption intensity change versus the increase in the dielectric constant is about twice larger for the B3LYP level than the CCSD level. Similar results for the rate of absorption intensity variation were obtained for the second and third overtones. For the second and third overtones the variations in the absorption intensities with the increase in the dielectric constant show undulations in the calculations at both levels.

If overtones arise from the anharmonicity of a molecular vibration, it is very likely that the intensity increases with the increase

Table 1
Calculated and experimental wavenumbers (cm^{-1}) and absorption intensities (int.) of the fundamental and the first, second, and third overtones of H–F stretching vibration of hydrogen fluoride. The dielectric constant used for the calculations was 1 ($\varepsilon = 1$).

v	B3LYP/6-311++G(3df,3pd)		CCSD/aug-cc-pVQZ		CCSD(T)/aug-cc-pVQZ[a]		Obs.[b]	Obs.[c]	Obs.[d]	
	v	Int.	v	Int.	v	Int.	v	Int.	v	Int.
1	3921.38	1.96E-05	4015.13	2.02E-05	3965	1.9E-05	3962.56	3962.96	3961.4	1.78E-05
2	7678.51	3.89E-07	7861.11	5.69E-07	7759	5.7E-07	7751.69	7751.77	7750.8	5.61E-07
3	11277.30	1.54E-08	11542.74	1.60E-08	11,387	1.6E-08	11372.88	11372.57	11372.8	1.39E-08
4	14723.40	1.08E-09	15064.67	7.69E-10	14,851	8.2E-10	14831.68	14831.55	14831.7	

[a] Ref. [22].
[b] Ref. [34].
[c] Ref. [35].
[d] Ref. [36].

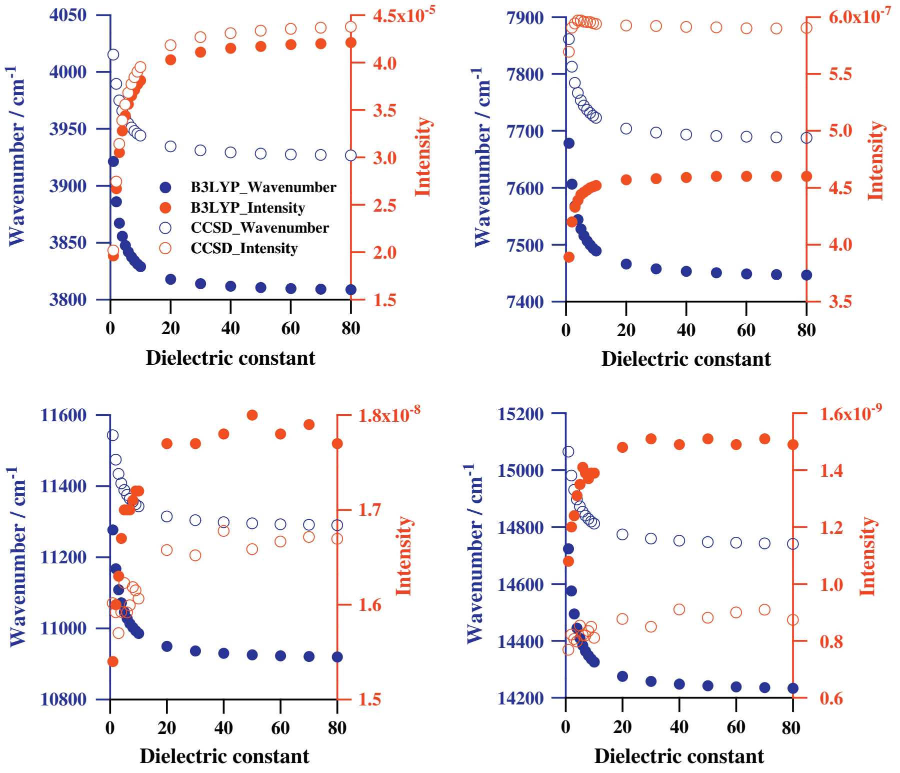

Fig. 3. Dependence on dielectric constant of the wavenumber and intensity ratio of: (a) the fundamental, (b) the first overtone, (b) the second overtone, (b) the third overtone of the HF stretching mode calculated at the IPCM//DFT/B3LYP/6-311++G(3df,3pd) and IPCM//CCSD/aug-cc-pVQT level.

in the dielectric constant are more marked for the overtones than the fundamental. In contrast to this anticipation, the absorption intensity of the fundamental increases even twice at $\varepsilon = 80$ compared with case of $\varepsilon = 1$ while those of the overtones vary at most one point two times compared with case of $\varepsilon = 1$. The intensity increase of the third overtone with increasing dielectric constant is significantly larger than those of the first and second overtones for the calculation of B3LYP level. The absorption intensity of the fundamental increases by about twice with the increase in the dielectric constant. This happens probably because the slope of dipole moment function increases by about twice. On the other hand, in the case of the first and second overtones it is very likely that a change of overlapping integral of wave function cancels a change in the dipole moment function.

The absorption intensities of second and third overtones do not always increase smoothly; for example, the absorption intensities for $\varepsilon = 7$ are weaker than those for $\varepsilon = 6$ by the B3LYP level. Upon going from the second to the third overtone, the variations in the intensities become more complicated. Thus, it may be concluded that the variations in the wavenumbers can be examined in terms of the effect of dielectric constant but those in the absorption intensities may not be examined simply in terms of the effect of dielectric constant.

With the increase in the vibrational quantum number the number of node of wave functions increases. This number of node complicates the changes in the values of transition dipole moment. Moreover, variations in the shapes of wave functions induced by variations in vibrational potential become more marked with the increase in the number of vibrational quantum number. Furthermore, dipole moment functions vary with the increase in the dielectric constant. Absorption intensity, which results from the combinations of several factor mentioned above, shows more complicated changes for higher overtones even if the vibrational potential and dipole moment functions vary continuously as a function of dielectric constant.

In this study we did not consider the hydrogen bonding of HF molecule. It is rather hard to carry out quantum chemical calculations including hydrogen bonding effects because for the calculations we must consider HF cluster structure that is not easy to be determined. Thus, the hydrogen bonding was not included in the present study, but this study has provided a significantly interesting example for the quantum chemical calculations of the frequencies and absorption intensities of overtones.

4. Conclusions

We have calculated the dependences of the vibrational potentials and dipole moment functions of HF molecule on the dielectric constant by using SCRF/IPCM model. It has been found that the calculated vibrational potentials and dipole moment functions vary extensively as the dipole moment increases from $\varepsilon = 1$ to $\varepsilon = 10$. Based on the calculated vibrational potential and dipole moment function, we have calculated the wavenumbers and absorption intensities of the fundamental, and the first, second, and third overtones.

For the fundamental both B3LYP and CCSD levels gave the results that the absorption intensity and frequency increase with the increase in the dielectric constant. However, as for the first overtone, the B3LYP and CCSD levels provided different results; according to the B3LYP level, the absorption intensity increases with the increase in the dielectric constant whereas CCSD level becomes the maximum at $\varepsilon = 5$ and decreases above $\varepsilon = 5$. The absorption intensity versus the dielectric constant waves for the second and third overtones.

Even if vibrational potential and dipole moment functions change continuously with a change in the dielectric constant, absorption intensity, which comes from the complicated combination of potential and dipole moment functions as mentioned above, does not show a smooth variation but shows a complicated change for higher overtones. A possibility that the complicated change arises from uncertainty in the calculations still has not be ruled out in the present study.

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