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Description	



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Spectral Parameters and Hamaker Constants of Silicon Hydride Compounds and Organic Solvents

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Abstract

Cyclopentasilane (CPS) and polydihydrosilane, which consist of hydrogen and silicon only, are unique materials that can be used to produce intrinsic silicon film in a liquid process, such as spin coating or an inkjet method. Wettability and solubility of general organic solvents including the above can be estimated by Hamaker constants, which are calculated according to the Lifshitz theory. In order to calculate a Hamaker constant by Simple Spectral Method (SSM), it is necessary to obtain absorption frequency and function of oscillator strength in the ultraviolet region. In this report, these physical quantities were obtained by means of an optical method.

As a result of examination of the relation between molecular structures and ultraviolet absorption frequencies, which were obtained from various liquid materials, it was concluded that ultraviolet absorption frequencies became smaller as electrons were delocalized. In particular, the absorption frequencies were found to be very small for CPS and polydihydrosilane due to σ -conjugate of their electrons. The Hamaker constants of CPS and polydihydrosilane were successfully calculated based on the obtained absorption frequency and function of oscillator strength.

Introduction

A number of experiments have been conducted to produce electronic devices by means of the liquid process. The liquid process has advantages is cost reduction, low environmental load and shorter processing time, compared with conventional processes such as vapor deposition in vacuum and photolithography. In particular, the ink-jet method has already been used for mass production of color filters, since it has high material efficiency and patterning precision at the level of several tens of µm, and it enables printing in multiple colors. Research results for other liquid process methods including organic EL ^[1], organic TFT ^[2], and Si-TFT using liquid silicon ^[3] have also been reported. Thus, many researchers have been developing highly functional materials and practical liquid process methods.

Liquid silicon is a unique material that can produce silicon film of high quality by solution process. The liquid silicon can be made from cyclopentasilane (CPS), which was synthesized by Hengge et al. ^[4,5]. It was reported

that the electron field-effect mobilities of polysilicon TFTs that are applied with liquid silicon by means of spin coating method and ink-jet method are 108cm²/Vs and 6.5cm²/Vs, respectively. The experimental results for n-type silicon film ^[6], which is doped with phosphorus, and oxide silicon film ^[7], which is produced by baking liquid silicon in oxygen, have been reported as well.

For technological development of the liquid process, it is necessary to understand physical phenomena and various interactions in liquid, such as stability of colloid, wettability of liquid, solubility of polymer, and compatibility of solute and substrate. These factors are determined by various interactions including hydrogen bonding, hydrophobic interaction, van der Waals force and coulomb interaction, and the most influential interaction differs depending on the system. Among several interactions, the van der Waals (vdW) force is a very important interaction for understanding various physical phenomena, since it works ubiquitously. The influence of this force is particularly important in systems that consist mainly of nonpolar substances.

The vdW force between macroscopic bodies can be written with a Hamaker constant A according to the Lifshitz theory of continuum approximation. In order to calculate a Hamaker constant based on the Lifshitz theory, an accurate full spectrum of dielectric function is required. However, obtaining an accurate full spectrum is very complicated, so some approximation methods such as Tabor Winterton Approximation (TWA)^[8] and Simple Spectral Method (SSM)^[9,10,11] have been proposed.

In TWA, a Hamaker constant is obtained by using the three values of a material; namely, static permittivity, refractive index and ultraviolet absorption frequency. As for the absorption frequency, an approximate value of 1.88×10^{16} rad/s is sometimes used for all materials. This makes calculation easy and gives a relatively good result. Materials with different absorption frequencies, however, tend to produce errors in the results.

In contrast, in SSM, a Hamaker constant is obtained by the three values of resonant frequency (which features a spectrum of dielectric function), function of oscillator strength, and static permittivity. SSM gives a better result than TWA in the case of materials with different ultraviolet absorption frequencies. Consequently, SSM is effective in the evaluation of more materials than is TWA. Since many kinds of liquid materials are used in the liquid process, SSM is preferable to TWA in calculation of Hamaker constants for estimation of vdW energy between the materials.

In this report, we aimed to obtain resonant frequency, function of oscillator strength and static permittivity, which are required in calculation of SSM. Absorption frequency and function of oscillator strength in the ultraviolet region were measured by means of an optical measurement method. Static permittivity, absorption frequency and function of oscillator strength in the infrared region were mainly referred to in the data of the literature ^[12,13], and were measured for only some materials.

Since absorption frequency in the ultraviolet region is the most important factor in calculation of Hamaker constants, the relation between absorption frequency and molecular structure was examined.

We measured absorption frequency and function of oscillator strength in the ultraviolet region for silicon hydride compounds and organic solvents used in the liquid process. The values for some polymers and substrates were also measured. Based on the measured values, Hamaker constants in some systems were calculated. In particular, much attention was paid to CPS and polydihydrosilane, which are silicon hydride compounds used for the production of liquid silicon, since to know their Hamaker constant in any given situations is necessary for their

application in liquid process.

Theory

The free energy per unit area $W_{132}(L)$ acting between Plate 1 and Plate 2, which are positioned on both sides of Material 3 at a distance of (L), is represented as follows, according to the non-retarded Lifshitz theory ^[14,15]:

$$W_{132} = -\frac{A_{132}}{12\pi L^2} \quad (1)$$

In this equation, A is a Hamaker constant, which is represented as follows:

$$A_{132} = -\frac{3kT}{2} \sum_{n=0}^{\infty} \sum_{s=1}^{\infty} \frac{\left(\Delta_{13}\Delta_{23}\right)^s}{s^3}$$
(2)
$$\Delta_{kj} = \frac{\varepsilon_k(i\xi_n) - \varepsilon_j(i\xi_n)}{\varepsilon_k(i\xi_n) + \varepsilon_j(i\xi_n)}$$
(3)
$$\xi_n = n \left(\frac{2\pi kT}{\hbar}\right)$$
(4)

The prime for \sum means that the term for n=0 is multiplied by 1/2. (h) is the Planck constant, (T) is the absolute temperature, and (k) is the Boltzmann constant. The dielectric function of material $\mathcal{E}(\omega)$ is replaced by $\mathcal{E}(i\xi_n)$, which is obtained by mathematical consideration.

Thus, vdW energy is represented by Hamaker constant (A). The properties of material are correlated with Hamaker constant (A) through $\mathcal{E}(i\xi_n)$ value. In general, dielectric function is represented as follows:

$$\varepsilon(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$$
 (5)

 \mathcal{E}' is a real part, and \mathcal{E}'' is an imaginary part. \mathcal{E}'' represents dispersion of energy, which corresponds to the absorption spectrum of the material. Accordingly, when a material has no absorption, this term becomes zero, and when a material has no absorption in the visual light range, \mathcal{E} is related to refractive index (n) as follows:

$$\varepsilon(\omega_{vis}) = \varepsilon'(\omega_{vis}) = n^2 \qquad (6)$$

 ε " and $\varepsilon(i\xi)$ are linked by Kramers-Kronig relation as follows^[16]:

$$\mathcal{E}(i\xi) = 1 + \frac{2}{\pi} \int_0^\infty \frac{x\mathcal{E}''(x)}{x^2 + \xi^2} dx$$
(7)

It is necessary to obtain \mathcal{E}'' in all the frequency bands to determine an accurate value of the Hamaker constant. For that purpose, experimental data obtained by means of EELS and VUV are needed. Since it is difficult to obtain \mathcal{E}'' in all the frequency bands, however, an approximate model of $\mathcal{E}(i\xi)$ is represented by Parsegian and Ninham as follows: ^[17,18]

$$\varepsilon(i\xi) = 1 + \sum_{j} \frac{d_j}{1 + \xi\tau_j} + \sum_{i} \frac{f_i}{\omega_i^2 + g_i\xi + \xi^2} \qquad (8)$$

(ω) is natural frequency, (g) is spectrum width, and (d,f) is a function of strength. The first term (1) is permittivity in vacuum. The first Σ represents rotational relaxation of polar material (Debye oscillator). Though it is important in the case of a material with high polarity such as water, the term can be ignored in the case of nonpolar material. The second Σ represents absorption in the infrared region and in the bands with higher frequency (Lorentz oscillator). The absorption in the infrared region is caused mainly by molecular oscillation, and absorption in the ultraviolet region by electronic oscillation, respectively. In the case of a nonpolar material, equation (8) is represented as follows (by ignoring absorption in the microwave range).

$$\varepsilon(i\xi) = 1 + \sum_{i=1}^{N} \frac{C_i}{1 + \left(\xi/\omega_i\right)^2}$$
(9)
$$C_i = \frac{2}{\pi} \frac{f_i}{\omega_i}$$
(10)

Equation (9) is known as a Parsegian-Ninham representation. According to (9), static permittivity $\varepsilon(0)$ is represented as follows:

$$\varepsilon(0) = 1 + \sum_{i=1}^{N} C_i \quad (11)$$

Equation (9) is simplified by assigning absorption frequency (ω) and function of oscillator strength (C) for the infrared region and the ultraviolet region that specify $\mathcal{E}(i\xi)$ ^[19].

$$\varepsilon(i\xi) = 1 + \frac{C_{IR}}{1 + (\xi/\omega_{IR})^2} + \frac{C_{UV}}{1 + (\xi/\omega_{UV})^2}$$
(12)

According to equations (6), (11) and (12), nonpolar substance C_{IR} is roughly represented as follows:

$$C_{IR} = \varepsilon \left(0 \right) - C_{UV} - 1 \tag{13}$$

As shown in equation (4), the number of terms in the infrared region is one digit less than that in the ultraviolet region. In addition, C_{IR} is smaller than C_{UV} in the case of nonpolar substances. Accordingly, an appropriate result can be obtained even if equation (12) is simplified by ignoring the infrared region, as shown below ^[10,20].

$$\varepsilon(i\xi) = 1 + \frac{C_{UV}}{1 + \left(\xi/\omega_{UV}\right)^2} \quad (14)$$

For most liquids and oxides, the term for the ultraviolet region is significant, and ignoring the infrared region exerts little influence. The infrared term cannot be ignored, however, in cases of substances with strong molecular vibration, such as $BaTiO_3^{[19]}$. In this report, equation (12) is used, considering the importance of the infrared region.

Hough and White used the relation between refractive index and permittivity (6) in order to obtain the two parameters ω_{UV} and C_{UV} that characterize absorption spectra in the ultraviolet region^[9,10]. By applying $\xi = i\omega$, equation (14) is represented as follows:

$$n^{2} - 1 = (n^{2} - 1)\frac{\omega^{2}}{\omega_{UV}^{2}} + C_{UV}$$
(15)

In the case of transparent substances in the visible light range, in the plot with the vertical axis of $(n^2 - 1)$ and

the horizontal axis of $(n^2 - 1)\omega^2$, $(\omega_{UV})^2$ is obtained by its gradient, and C_{UV} is obtained by its y-intercept.

This is called the Cauchy plot.

Thus, as a parameter of the spectra in a wide range of energy, the method of describing dielectric function based on the Lorentz oscillatory model is called SSM. TWA is known as a similar method that uses refractive index as a function of the spectra of substances.

In this experiment, ω_{UV} and C_{UV} were obtained by equation (15), and C_{IR} was obtained by equation (13). The values used for ω_{IR} and $\epsilon(0)$ were referred to in the literature ^[12,13]. Finally, Hamaker constants were obtained according to equation (2) by applying these values.

Experimental Equipment

Refractive index was measured by means of multi-wavelength Abbe refractometers DR-M2 and DR-M4 manufactured by ATAGO. When the wavelength is 589mm, DR-M2 can measure a refractive index of 1.3000 to 1.7100, and DR-M4, an index of 1.4700 to 1.8700. The refractive index was measured at wavelengths of 450, 480, 520, 546, 589, 644, 720 and 1,000 mm at a temperature of 20°C. Static permittivity was measured by means of a surface acoustic wave (SAW) solution sensor that was jointly developed by Japan Radio Co., Ltd., Riso Kagaku Corporation and SAW&SPR-Tech ^[21]. Absorption spectra of IR were measured by ALPHA which is the product of Bruker Optics. Since some of the measured materials might ignite or hydrolyze in the air, they were measured in a glove box made by Miwa Seisakusho Co., Ltd. Oxygen concentration was 0.5ppm or lower, and the dew point was -70°C or lower.

Material

As shown in the Appendix, 75 kinds of solutions, three kinds of polymers, and two kinds of solid substrates were used. The materials were purchased from Kanto Chemical Co., Inc., except for the following:

CPS was synthesized according to the Kipping method ^[22]. Polydihydrosilane was synthesized by means of ring-opening polymerization induced by UV irradiation. As for polystyrene, the standard polymer A-500 (Mw=500) made by TOSOH Corporation was used. For polydimethylsiloxane, 200R (Mw=200) by SIGMA-ALDRICH was used. For the substrates, quartz substrate VIOSIL made by Shin-Etsu Chemical Co., Ltd. and OA-10 glass substrate made by Asahi Glass Co, Ltd. were used.

Experimental Procedure

Refractive index was measured by means of either DR-M2 or DR-M4, depending on the properties of the materials. Ten measurements were conducted for each wavelength to calculate the average values. Using the average values, ω_{UV} and C_{UV} for all the materials were obtained from the Cauchy plots that were drawn

according to equation (15).

In the measurement of static permittivity by means of the SAW solution sensor, materials whose permittivity had already been examined, such as water, ethanol and toluene, were measured for calibration of the sensor. Then, specimens of 40 μ l were placed on the electrode and their static permittivities were measured. The values for most of the materials were referred to in the literature^[12], and only the materials that could not be found in the literature^[12], such as CPS, polydihydrosilane and titanium complex, were actually measured.

Similarly, the values of ω_{IR} were found in the literature ^[13], and only CPS and polydihydrosilane were actually measured.

CPS, polydihydrosilane and titanium complex were measured in the glove box because in the air, CPS and polydihydrosilane might easily ignite, and titanium complex might easily hydrolyze.

Results

The results of measurement are indicated in the Appendix. Only the structures and ultraviolet absorption frequencies (ω_{UV}) of some of the materials are highlighted below.

1.Saturated Compounds

Ultraviolet absorption frequencies (ω_{UV}) of the solvents that had no double bond in their molecular structures were approximately 1.88×10^{16} rad/s in spite of the differences in their structures, as shown in Table 1. The value of Alkane conformed to the result obtained by Hough and White^[10].

1 1	
Name/structure	$\omega_{\rm UV}$ (rad/s)
Water H H	1.86×10 ¹⁶
Glycerin HO OH OH	1.89×10 ¹⁶
Hexane	1.88×10 ¹⁶
Octane	1.86×10 ¹⁶
Decane	1.85×10 ¹⁶
Tetrahydrofuran	1.88×10 ¹⁶
Cyclohexane	1.86×10 ¹⁶

Table 1 Structures and Ultraviolet Absorption Frequencies of Saturated Compounds

2.Unsaturated Compounds

In Table 2, ultraviolet absorption frequencies (ω_{UV}) of hexane and its analogs are shown, in order to identify the influence of the number of double bonds and their positions. 1-hexene, which had one double bond, showed a slightly smaller value than hexane. Hexadiene, which had two double bonds, showed an even smaller value. The values of the two nonconjugated dienes, 1,4-hexadiene and 1,5-hexadiene, were almost the same as each other. The conjugated diene, 1,3-hexadiene, showed an even smaller value than the nonconjugated dienes.

Name/structure	$\omega_{\rm UV}$ (rad/s)
Hexane	1.88×10 ¹⁶
1-hexene	1.72×10 ¹⁶
1,5-hexadiene	1.57×10 ¹⁶
1,4-hexadiene	1.53×10 ¹⁶
1.3-hexadiene	1.34×10 ¹⁶

Table 2 Structures and Ultraviolet Absorption Frequencies of Hexane and Its Analogs

3.Fluorine Compounds

In Table 3, ultraviolet absorption frequencies (ω_{UV}) of decalin and its analogs are given in order to show the influence of fluorine. The value of methylnaphthalene was found in the literature ^[12]. Perfluorodecalin showed a higher value than did saturated compounds. The value became smaller as the number of double bonds (aromatic rings) increased, in a way similar to the trend seen in the analogs of hexane, as shown in Table 2.

Table 3 Structures and Ultraviolet Absorption Frequencies of Perfluorodecalin and Its Analogs

Name/structure	$\omega_{\rm UV}$ (rad/s)
Perfluorodecalin F F_F F F F F F F FF F F F F F F F F F	2.55×10 ¹⁶
Decalin	1.84×10 ¹⁶
Tetralin	1.42×10 ¹⁶
Methylnaphthalene	1.12×10 ¹⁶

4.Acetylacetone

Table 4 shows the ultraviolet absorption frequency (ω_{UV}) of acetylacetone. Acetylacetone is known to be in equilibrium of keto form and enolic form in the solution state ^[23]. Its ultraviolet absorption frequency was smaller than those of saturated compounds and close to those of unsaturated compounds.

Name/structure	$\omega_{\rm UV}$ (rad/s)
Acetylacetone	
	1.27×10 ¹⁶

Table 4 Structure and Ultraviolet Absorption Frequency of Acetylacetone

5.Silicon Compounds

Table 5 shows the ultraviolet absorption frequencies (ω_{UV}) of silicon compounds. Polydimethylsiloxane showed a value close to those of saturated compounds. In contrast, CPS (cyclopentasilane) and polydihydrosilane showed smaller values than carbon compounds with the same structures.

Name/structure	$\omega_{\rm UV}$ (rad/s)
Polydimethylsiloxane	1.78×10^{16}
$\begin{array}{c} \text{CPS} \\ H_2 \\ Si \\ H_2 \\ Si \\ H_2 \\ H_2 \\ Si \\ Si \\ H_2 \\ Si \\ S$	1.13×10 ¹⁶
Polydihydrosilane H_2 Si H_2 H_2 n	9.93×10 ¹⁵

Table 5 Structures and Ultraviolet Absorption Frequencies of Silicon Compounds

Figure 1 shows the Cauchy plots of CPS and polydihydrosilane.



Fig. 1. Cauchy Plots of CPS and Polydihydrosilane

6.Calculation of Hamaker Constants

Table 6 indicates the non-retarded Hamaker constants (A₁₃₂) in some materials. These were calculated based on the measured values of $\omega_{UV_1} C_{UV_2} \omega_{IR_2} C_{IR_2}$ and $\epsilon(0)$.

Material1	Medium	Material2	A _{Hamaker}
Octane	Air	Octane	11.12
Decalin	Air	Decalin	15.13
CPS	Air	CPS	16.46
Polystyrene	Air	Polystyrene	14.91
Poly- dihydrosilane	Air	Poly- dihydrosilane	16.57
Polystyrene	Decalin	Polystyrene	0.25
Polystyrene	CPS	Polystyrene	0.18
Poly- dihydrosilane	Decalin	Poly- dihydrosilane	1.26
Poly- dihydrosilane	CPS	Poly- dihydrosilane	0.07
Polystyrene	Decalin	Quartz	-0.05
Polystyrene	CPS	Quartz	0.38
Poly- dihydrosilane	Decalin	Quartz	-0.07
Poly- dihydrosilane	CPS	Quartz	-0.21

Table 6 Calculated Non-retarded Hamaker Constants (Unit: kT, T=293)

Surface energy was calculated according to the equation below for octane, decalin, toluene and CPS.

$$\gamma = \frac{A_{101}}{24\pi D_0^2}$$
(16)

In this equation, $\gamma(mN/m)$ is surface tension, and $D_0(m)$ is cutoff distance. Israelachvili et al. proved that the calculated value and the measured value were in agreement when D_0 was set to 0.165nm in an experiment using carbon solvents ^[24]. Accordingly, this set value of 0.165nm was used in our calculation as well. Table 7 shows the calculated values when D_0 was 0.165nm, and the measured values of surface tension. The calculated values

and measured values also conformed in the case of a silicon compound, CPS.

	Calculated by (16)	Measured
Octane	21.9	21.4
Decalin	29.9	30.5
Toluene	23.1	27.3
CPS	32.5	31.6

Table 7 Comparison of Calculated/Measured Surface Tension (Unit: mN/m)

Discussion

1.Saturated Compounds

The London dispersion force is an electrostatic interaction caused by fluctuation of electrons. The ultraviolet absorption frequency (ω_{UV}) reflects the energetic status of the peripheral electrons, which form covalent bonds in compounds. In short, the covalent bond is the source of energy. It should be concluded that all saturated compounds show the same ultraviolet absorption frequency (ω_{UV}), since their covalent bonds are single, so they have equal energy. Consequently, it is possible to use a simple approximation such as TWA in dealing with saturated compounds.

2.Unsaturated Compounds

The energetic status of the peripheral electrons, namely, ω_{UV} , fluctuates due to the influence of the double bonds that delocalize electrons. Stabilization of energy due to conjugated structure is thought to be the reason why the conjugated diene, 1,3-hexadiene, showed a smaller value of ω_{UV} compared with 1,4-hexadiene and 1,5-hexadiene, which showed approximately the same values. It can be concluded that the longer the conjugated length, that is, the wider the delocalized field of the peripheral electrons, the more stable the electrons, energetic status, and ω_{UV} becomes smaller.

3.Fluorine Compounds

Fluorine is known to have a strong electron affinity, which localizes electrons. This property is contrary to energetic stabilization, which delocalizes electrons by means of double bonding. As Table 3 shows, ω_{UV} becomes higher when fluorine elements are introduced, because energy becomes destabilized due to localization of electrons.

4.Acetylacetone

Acetylacetone in keto form is a nonconjugated diene, and acetylacetone in enolic form is a conjugated diene. According to the discussion about unsaturated compounds, ω_{UV} of a nonconjugated diene is presumed to be close to 1.55×10^{16} rad/s. Acetylacetone in enolic form, however, is presumed to have a lower ω_{UV} . The fact that ω_{UV} of acetylacetone was a value as small as 1.27×10^{16} rad/s suggests that it does not exist in keto form in the solution state; it could be partly forming a big conjugate structure, such as that of the enolic form.

5.Silicon Compounds

The silicon compounds used in the experiment consist of Si-C, Si-O, Si-H and Si-Si bonds, while carbon compounds are made up of C-C, C-O and C-H bonds. The fact that the bonds of Si-C, Si-O and Si-H in polydimethylsiloxane are single bonds, as are C-C, C-O and C-H bonds, is considered to be the reason why polydimethylsiloxane showed a ω_{UV} value close to those of the saturated compounds shown in Table 1. The ω_{UV} values of CPS and polydihydrosilane were smaller than those of saturated compounds, and rather close to those of the unsaturated compounds shown in Table 2 and Table 3. Since Si-Si bonds are proven to be σ -conjugates ^[25], the reason that the ω_{UV} values of CPS and polydihydrosilane are relatively small can be explained by energetic stabilization due to σ -conjugates.

6.Calculation of Hamaker Constants

Equation (2) was used for calculation, since it was impossible to use a simple approximation such as TWA for substances that had inherent ω_{UV} values.

The Hamaker constants of the system of polydihydrosilane / decalin or CPS /quartz were negative values, as shown in Table 6. That illustrates repulsive force operates between the solute (polydihydrosilane) and the substrate (quartz). Therefore it is presumed that polymers don't tend to adhere to the substrate in this system. That means coating of polydihydrosilane film onto the quartz substrate is expected to be difficult. Since this system is similar to that used by Shimoda et al ^[3]., in which the coating of polydihydrosilane film was somehow achieved in spite of the existence of the assumed repulsive force, the influence of it over the coating property in a liquid process should be investigated furthermore. Table 7 indicates that the calculated values conform to the measured values of surface tension. It proves that ω_{UV} , C_{UV} , ω_{IR} , C_{IR} , and $\varepsilon(0)$ that were measured or referred to were proper. CPS and polydihydrosilane, which are σ -conjugates made up of Si-Si bonds, were properly calculated according to equation (2).

Conclusion

The values of ω_{UV} and C_{UV} of silicon hydride compounds and a series of organic materials were obtained by drawing Cauchy plots based on the wavelength dependence of refractive index in the visual light region. Furthermore, the values of ω_{IR} , C_{IR} , and $\varepsilon(0)$ of CPS, polydihydrosilane and titanium complex were measured.

In examination of the relation between ω_{UV} and molecular structure, ω_{UV} , which is a resonant frequency of the peripheral electron, varied depending on the bonding condition in molecules. In short, ω_{UV} tended to become smaller as electrons became delocalized, i.e. as conjugation lengths became longer. The ω_{UV} values of silicon compounds, which were composed of silicon and hydrogen only, and have not been preciously studied in detail, were first measured and found to be remarkably small. This is considered to be due to σ -conjugation of Si-Si bonds.

Hamaker constants of several systems were calculated by using SSM in order to deal with substances with different ω_{UV} values. The system of polydihydrosilane / decalin / quartz is similar to the system that is actually

used in the manufacture of electronic devices. Our calculation result shows that there is weak repulsion between polydihydrosilane and the quartz substrate in decalin. This means that affinity and adhesion between polymers and substrates are weak, which is not a preferable condition in film formation. The influence of Hamaker constants, which predicts forces between solutes and substrate, on the actual application process should be examined in the future. The attached Appendix is a list of experimental results for organic solvents. It also contains the values for solid substrates, which were previously used in an experiment and reported on by Bergstrom^[19]. Interaction between organic solvents and solids in many systems can be examined by comparing the results of their experiment and ours.

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Appendix

List of static permittivity: $\varepsilon(0)$, refractive index at 589nm: n, ultraviolet oscillator strength function: C_{UV} , ultraviolet absorption frequency: ω_{UV} , infrared oscillator strength function: C_{IR} , and infrared absorption frequency: ω_{IR} . The values of n, C_{UV} , and ω_{UV} were measured. The C_{IR} values were calculated according to equation (13). The values of $\varepsilon(0)$ and ω_{IR} were referred to in the literature ^[12,13], except for the measured values of CPS, polydihydrosilane, and titanium complex.

Non-aromatic hydrocarbon	3	n	C_{UV}	$\omega_{\rm UV}({\rm rad/s})$	C _{IR}	$\omega_{IR}(rad/s)$
Hexane	1.890	1.3756	0.8662	1.88E+16	0.0238	5.57E+14
Octane	1.948	1.3977	0.9251	1.86E+16	0.0229	5.51E+14
Decane	1.991	1.4116	0.9630	1.85E+16	0.0280	5.51E+14
Dodecane	2.016	1.4217	0.9916	1.88E+16	0.0244	5.52E+14
Tetradecane	2.042	1.4288	1.0097	1.85E+16	0.0323	5.51E+14
Hexadecane	2.050	1.4343	1.0244	1.84E+16	0.0256	5.51E+14
Cyclopentane	1.965	1.4057	0.9481	1.89E+16	0.0169	5.59E+14
Cyclohexane	2.030	1.4265	1.0045	1.86E+16	0.0255	5.52E+14
Cycloheptane	2.112	1.4446	1.0558	1.89E+16	0.0560	5.51E+14
Cyclooctane	2.152	1.4583	1.0946	1.90E+16	0.0571	5.50E+14
Cyclodecane	2.191	1.4716	1.1333	1.91E+16	0.0573	5.51E+14
Methylcyclohexane	2.020	1.4231	0.9956	1.88E+16	0.0244	5.51E+14
Ethylcyclohexane	2.054	1.4328	1.0219	1.86E+16	0.0321	5.50E+14
Dicyclohexyl	2.213	1.4791	1.1521	1.85E+16	0.0607	5.51E+14
Cyclohexene	2.220	1.4466	1.0545	1.71E+16	0.1655	5.51E+14
Cyclooctene	2.163	1.4706	1.1218	1.70E+16	0.0408	5.51E+14
1,3-Cyclohexadiene	2.179	1.4762	1.1184	1.41E+16	0.0606	1.26E+14
1,4-Cyclohexadiene	2.170	1.4733	1.1223	1.58E+16	0.0482	5.70E+14
Perhydrofluorene	2.281	1.5022	1.2202	1.88E+16	0.0613	5.51E+14
Dimethyladamantane	2.212	1.4787	1.1512	1.85E+16	0.0603	5.46E+14
Decahydronaphthalene	2.197	1.4761	1.1432	1.84E+16	0.0538	5.50E+14
1-Methyldecahydronaphthalene	2.197	1.4794	1.1529	1.85E+16	0.0441	5.50E+14
1,3-Hexadiene	2.108	1.4431	1.0208	1.34E+16	0.0867	1.89E+14
1,4-Hexadiene	2.014	1.4105	0.9462	1.53E+16	0.0682	1.87E+14
1,5-Hexadiene	1.997	1.4044	0.9320	1.57E+16	0.0655	1.72E+14
1-Hexene	2.060	1.3881	0.8945	1.72E+16	0.1655	5.51E+14
Aprotic	3	n	C_{UV}	$\omega_{\rm UV}(\text{rad/s})$	C _{IR}	$\omega_{\text{IR}}(\text{rad/s})$
Acetonitrile	37.5	1.3444	0.7840	1.89E+16	-	4.25E+14
Dimethyl sulfoxide	48.9	1.4788	1.1399	1.61E+16	-	1.98E+14
γ-Butyrolactone	39.1	1.4368	1.0336	1.88E+16	-	3.33E+14
N-Methylpyrrolidone	32.0	1.4707	1.1208	1.68E+16	-	3.18E+14
N,N-Dimethylformamide	36.7	1.4296	1.0029	1.62E+16	-	3.16E+14

Halogenide	з	n	$C_{\rm UV}$	$\omega_{\rm UV}({\rm rad/s})$	C _{IR}	$\omega_{IR}(rad/s)$
Dichloromethane	10.7	1.4235	0.9938	1.81E+16	-	1.39E+14
Chlorobenzene	5.621	1.5242	1.2498	1.36E+16	-	2.78E+14
Dichlorobenzene	9.93	1.5515	1.3298	1.36E+16	-	2.74E+14
Chloroform	4.8	1.4450	1.0514	1.75E+16	-	1.43E+14
Aromatic hydrocarbon	з	n	C_{UV}	$\omega_{\rm UV}(\rm rad/s)$	C _{IR}	$\omega_{IR}(rad/s)$
Toluene	2.24	1.4970	1.1731	1.38E+16	0.0669	1.37E+14
o-Xylene	2.27	1.5052	1.2000	1.40E+16	0.0660	1.40E+14
m-Xylene	2.37	1.4972	1.1765	1.40E+16	0.1975	1.45E+14
p-Xylene	2.27	1.4957	1.1705	1.38E+16	0.0995	1.50E+14
Mesitylene	2.28	1.4994	1.1841	1.41E+16	0.0949	1.58E+14
Pseudocumene	2.4	1.5049	1.1985	1.40E+16	0.2015	2.84E+14
Cyclohexylbenzene	2.33	1.5257	1.2663	1.49E+16	0.0615	5.51E+14
Tetrahydronaphthalene	2.73	1.5412	1.3056	1.42E+16	0.4274	5.52E+14
Ether	3	n	C_{UV}	$\omega_{\rm UV}(\rm rad/s)$	C _{IR}	$\omega_{\rm IR}(\rm rad/s)$
Tetrahydrofuran	8.2	1.4073	0.9518	1.88E+16	-	2.02E+14
Diethylether	4.42	1.3524	0.8054	1.90E+16	-	2.12E+14
1,4-Dioxane	2.23	1.4221	0.9937	1.92E+16	-	2.12E+14
Dibenzylether	4.0	1.5615	1.3594	1.37E+16	-	2.06E+14
1,2-Dimethoxyethane	5.5	1.3800	0.8790	1.90E+16	-	2.09E+14
1,8-Cineole	4.57	1.4594	1.0950	1.82E+16	-	5.59E+14
Anisole	4.33	1.5170	1.2294	1.35E+16	-	2.35E+14
Thioanisole	4.54	1.5872	1.4180	1.24E+16	-	2.79E+14
Methylanisole	3.99	1.5124	1.2162	1.36E+16	-	2.85E+14
Ester	3	n	$C_{\rm UV}$	$\omega_{\rm UV}({\rm rad/s})$	C _{IR}	$\omega_{IR}(rad/s)$
Buthylacetate	5.01	1.3943	0.9173	1.90E+16	-	3.28E+14
Ethylacetate	6.05	1.3725	0.8592	1.92E+16	-	3.28E+14
Diethylmalonate	7.87	1.4141	0.9692	1.86E+16	-	3.27E+14
Keton	з	n	C _{UV}	$\omega_{\rm UV}(\rm rad/s)$	C _{IR}	$\omega_{IR}(rad/s)$
Cyclohexanone	18.3	1.4504	1.0717	1.89E+16	-	3.23E+14
Acetylacetone	23.1	1.4523	1.0394	1.27E+16	-	3.06E+14
Acetone	21.0	1.3586	0.8199	1.82E+16	-	3.23E+14
Methylethylketone	15.5	1.3785	0.8744	1.88E+16	-	3.24E+14
2-Heptanone	12.5	1.4093	0.9562	1.84E+16	-	3.23E+14

Alcohol	3	n	$C_{\rm UV}$	$\omega_{\rm UV}(\rm rad/s)$	C _{IR}	$\omega_{IR}(rad/s)$
Isopropanol	18.62	1.3772	0.8709	1.90E+16	-	5.60E+14
Ethyleneglycol	38.66	1.4323	1.0190	1.84E+16	-	5.53E+14
Glycerin	47.0	1.4742	1.1396	1.89E+16	2.020[26]	3.28E+14
n-Butanol	17.1	1.3992	0.9306	1.88E+16	-	5.58E+14
Methanol	33.0	1.3291	0.7448	1.91E+16	3.955[26]	3.52E+14
Ethanol	25.0	1.3615	0.8292	1.90E+16	2.370[26]	2.59E+14
Diethyleneglycol	31.69	1.4473	1.0636	1.90E+16	-	6.35E+14

Others	3	n	$C_{\rm UV}$	$\omega_{\rm UV}(\rm rad/s)$	C _{IR}	$\omega_{IR}(rad/s)$
Perfluorodecalin	1.727	1.3141	0.7156	2.55E+16	0.0113	2.31E+14
Silicone oil	2.70	1.4012	0.9321	1.78E+16	0.7679	2.06E+14
Phenylsilane	2.284	1.5113	1.2104	1.34E+16	0.0736	1.70E+14
Diphenylsilane	2.50	1.5807	1.4038	1.27E+16	0.0947	1.59E+14
Titanium tetrachloride	2.47	1.6072	1.4321	1.04E+16	0.0379	8.84E+13
Titanium tetrabutoxide	2.25	1.4919	1.1693	1.51E+16	0.0807	5.57E+14
Titanium tetrapropoxide	3.5	1.4652	1.0936	1.49E+16	1.4064	5.58E+14
Cyclopentasilane	2.85	1.6951	1.7244	1.13E+16	0.1256	1.66E+14

Polymer	з	n	$C_{\rm UV}$	$\omega_{\rm UV}(rad/s)$	CIR	$\omega_{IR}(rad/s)$
Polystyrene	2.557	1.5603	1.3601	1.41E+16	0.1969	5.51E+14
Polyethylenglycol	40.0	1.4600	1.0985	1.87E+16	-	2.11E+14
Polydihydrosilane	2.7-3.5	1.7678	1.9049	9.93E+15	0.5951	1.66E+14
Solid	3	n	$C_{\rm UV}$	$\omega_{\rm UV}(\rm rad/s)$	C _{IR}	$\omega_{IR}(rad/s)$
SiO2(OA-10)	3.810	1.5165	1.2601	1.84E+16	1.5499	1.74E+14
SiO2(quartz)	3.810	1.4480	1.0980	2.02E+16	1.7120	1.86E+14
Reference	З	n	$C_{\rm UV}$	$\omega_{\rm UV}({\rm rad/s})$	C _{IR}	$\omega_{IR}(rad/s)$
Water[26]	80.3	1.33336	0.753	1.86E+16	3.4222	5.66E+14
1-Methylnaphthalene[12,13]	2.62	1.61755	1.49	1.12E+16	0.1312	1.49E+14
Diiodomethane[27]	5.32	1.76	2.1	1.44E+16	2.2200	2.09E+14
1-Bromonaphthalene[27]	5.12	1.66	1.75	1.23E+16	2.3700	1.44E+14

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