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DFT Calculations on Refractive Index Dispersion of Fluoro-compounds in the DUV-UV-Visible Region

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Density functional theory (DFT) calculations using the B3LYP hybrid functional have been performed to predict the refractive indices and their dispersion for fluoring-containing compounds which are expected to show high transparency in the vacuum UV (VUV) and the deep UV (DUV) region. The linear polarizabilities at wavelengths of 157, 193, 248, 300, 350, 434, 486, 540, 589, 656, 730 and 800 nm were calculated, and the corresponding refractive indices were estimated by assuming the molecular packing coefficient (K_p) as 0.56. The refractive indices at 193 nm are linearly proportitional to those at 589 nm for most of the compounds. In addition, the calclulated Abbe numbers representing the refractive index dispersion in the visible region are in linear relationships with the calculated refractive indices at 589 nm. The DFT calculations predict that alicyclic compounds, lactones, siloxanes, nitriles, sulfonylfluorides, and SO_3-esters exbihit relatively high refractive indices and good transparency in the DUV region.
Keywords / Density functional theory / Refractive Index / Dispersion / Abbe number / Fluoro-compounds / DUV region / Immersion fluid /

1. Introduction

The wavelength dispersion of refractive indices is an important property of optical materials. In particular, high refractive index and high transparency at wavelengths of 157 and 193 nm are required for fluids used for immersion lithography. This lithographic method uses transparent fluids to fill the lens-to-wafer gap. Although a convenient and transparent fluid at 193 nm is water [1], the development of an inexpensive, transparent fluid exhibiting higher refractive indices is required for the next-generation immersion lithography. Kunz et al.[2] have measured the transparencies of more than 50 fluorocarbon liquids over the wavelength range of 150–200 nm for use in the 157 nm immersion lithography. Very recently, Kaplan *et al.*[3] have measured the values of the refractive index, thermo-optic coefficient, and absorption coefficient of a number of organic solvents and aqueous inorganic solutions that may be used as immersion fluids at 193 or 248 nm.

We have reported that the time-dependent density functional theory (TD-DFT) calculations can reproduce the observed absorption spectra of model compounds for optical polymers without incorporation of empirical corrections [4-8]. In this study, we calculated wavelengh-dependent linear polarizabilities for more than 100 organic compounds which are expected to show high transparency, and we predicted the refractive indices and their wavelength dispersions in the deep UV (DUV)-UV-visible region using the DFT.

2. Theory and Methods

The DFT level of theory with the three-parameter Becke-style hybrid functional (B3LYP), which employs the Becke exchange and LYP correlation functionals, was adopted in conjunction. The Gaussian basis set of 6-311G(d) was used for geometry optimizations under no constraints, and the 6-311++G(d,p) was used for calculations of wavelength-dependent linear polarizabilities. All the calculations were performed using the software package of Gaussian-03 (Rev.C02 and D01)[9] installed on a Compaq Alpha server of the computer center of Tokyo Inst. Tech.

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Refractive index and its temperature dependence (thermo-optical (TO) coefficients) of molecular materials can be calculated using the Lorentz-Lorenz equation :

$$\frac{n_\lambda^2 - 1}{n_\lambda^2 + 2} = \frac{4\pi}{3}\frac{\rho \cdot N_A}{M_w}\alpha_\lambda = \frac{4\pi}{3}\frac{\alpha_\lambda}{V_{mol}} \quad (1)$$

$$\frac{dn_\lambda}{dT} = -\frac{(n_\lambda^2 - 1)(n_\lambda^2 + 2)}{6n_\lambda}\beta \quad (2)$$

where n is the refractive index, ρ the density, N_A the Abogadoro number, M_w the molecular weight, α_λ the linear molecular polarizability, V_{mol} the molecular volume, and β the volume expansion coefficient. The wavelength dependence of α_λ is the origin of the dispersion of refractive indices and TO-coefficients. The α_λ can be calculated by solving the coupled perturbed Hartree-Fock equations, and this procedure was recently implemented in Gaussian-03 with "POLAR" and "CPHF= Rdfreq" keywords. In this study, the polarizability (α_λ) of each molecule were calculated at wavelengths of 157, 193, 248, 300, 350, 434, 486, 540, 589, 656, 730, and 800 nm.

Moreover, either molecular volume or density is required to calculate the refractive index. However, such parameters are not easy to predict because of the difficulty in estimating the degrees of molecular packing. In addition, the high sensitivity of density to temperature makes the estimation complicated. In contrast, van der Waals volumes (V_{vdw}) can be easily calculated from the optimized geometries using the Slonimski's method [10,11] with the van der Waals radii of atoms.[12] The molecular packing constant K_p, which is used as a measure of molecular packing, is defined as

$$K_p = \frac{V_{vdw}}{V_{mol}} = \frac{\rho \cdot N_A}{M_w}V_{vdw} \quad (3)$$

The V_{mol} of a certain molecule is the summation of V_{vdw} and intermolecular free spaces. For instance, dense molecular packing caused by intermolecular hydrogen bondings or charge transfer interactions increases K_p due to the decrease in free space.

Abbe number, ν, has been used as a measure of the wavelength dispersion of refractive indices in the visible region. This value is defined as

$$\nu = \frac{n_D - 1}{n_F - n_C} \quad (4)$$

where n_D, n_F and n_C are the refractive indices at the wavelengths of Fraunhofer D-, F- and C-spectral lines (589.2 nm, 486.1 nm and 656.3 nm respectively). Note that low dispersion materials have high values of ν. We have recently calculated the linear polarizabilities for 86 fundamental organic compounds using DFT, and demonstrated that the calculated Abbe numbers are linearly proportional to the experimental values as shown in Fig.1 when we assume K_p as 0.60. Fig.1 clearly indicates that the experimental dispersions in the

Table 1. Molecular weight, Van der Waals volumes (A^3), density, and packing coefficients of fluorocompounds.

Compounds	M_w	V_{vdw}	ρ	K_p
$C_2F_5COOCH_3$	178.1	114.3	1.393	0.547
$C_2F_5COOC_2H_5$	192.1	131.1	1.299	0.534
$C_2F_5CHFCHFCF_3$	252.1	144.0	1.600	0.550
$C_2F_5COOCOC_2F_5$	310.1	174.5	1.571	0.532
$C_3F_7COOCH_3$	228.1	141.0	1.472	0.548
$C_3F_7COOC_2H_5$	242.1	157.9	1.396	0.548
$C_4F_9OCH_3$	250.1	148.1	1.520	0.542
$C_4F_9OC_2H_5$	264.1	165.0	1.430	0.538
$C_4F_9SO_3CH_3$	314.1	188.1	1.688	0.609
$C_4F_9SO_3CH2CF_3$	342.1	219.1	1.636	0.565
n-C_5F_{12}	288.1	153.6	1.620	0.520
n-C_6F_{14}	338.1	180.3	1.669	0.536
n-C_7F_{16}	388.1	207.0	1.745	0.560
cyc(C_2F_4-CO-O-CO-)	172.0	100.7	1.609	0.567
cyc(C_3F_6-CO-O-CO-)	222.1	127.3	1.654	0.571
cyc($CF_2CF_2CF(CF_3)CF(CF_3)$)	300.1	159.4	1.670	0.534
cyc((CF_2)$_5$$CF(CF_3)$)	350.1	186.4	1.787	0.573
cyc((CF_2)$_4$($CF(CF_3)$)$_2$)	400.1	213.4	1.861	0.598
cyc((CF_2)$_3$$CF(CF_3)CF_2CF(CF_3)$)	400.1	213.1	1.828	0.586
average	-	-	-	0.556

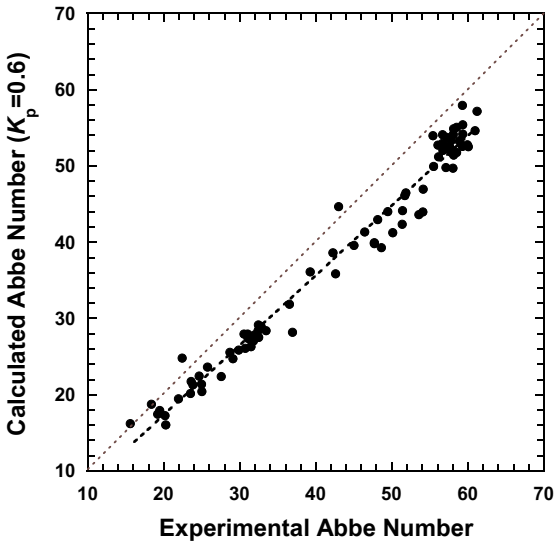


Figure 1. Calcuated Abbe numbers assuming K_p=0.6 *vs.* Experimental Abbe numbers for 86 fundamental organic compounds.[13]

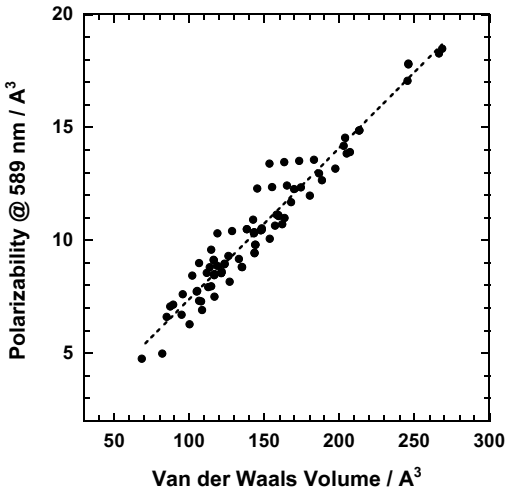


Figure 2. Calculated linear polarizability *vs.* van der Waals volumes with the optimized geometries for fundamental fluoro-compounds (Group I).

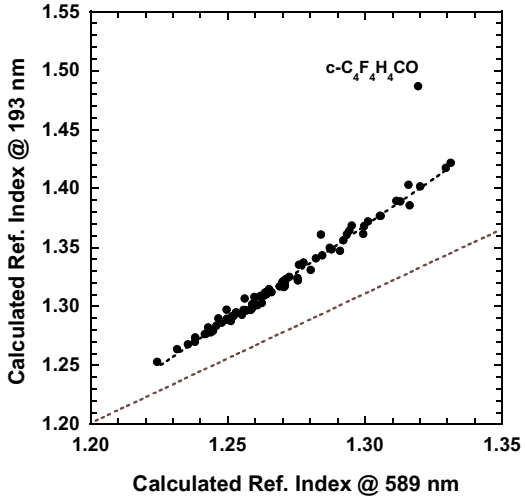


Figure 3. Calculated refractive indices at 589 nm *vs.* those at 193 nm. Most of the points are located on the correlation : n_{193}=1.588·n_{589} –0.696.

visible region can be well reproduced by the DFT calculations. In addition, we tentatively define the second Abbe number which expresses the dispersion in the DUV-UV region as follows.

$$\nu_2 = \frac{n_{248} - 1}{n_{193} - n_{300}} \qquad (5)$$

where n_{248}, n_{193} and n_{300} are the refractive indices at wavelengths of 248. 193, and 300 nm, respectively.

The objectives of this study is to calculate the wavelength-dependent linear polarizabilities and predict the refractive indices and their dispersions for fluorine-containing compounds which are expected to show high refractive indices and high transparency in the DUV region. The systematic examination of calculated refractive indices and their dispersions will be useful for screening immersion fluids for next generation lithography.

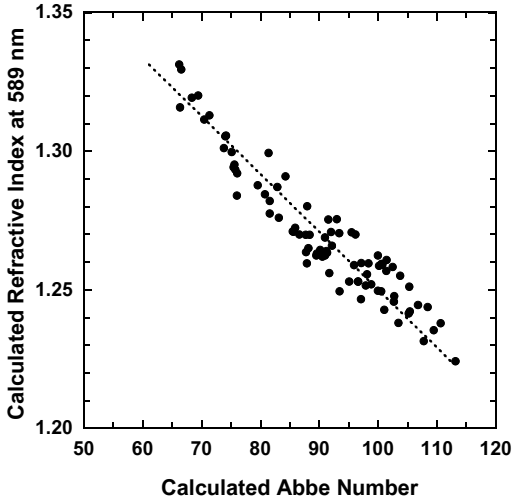


Figure 4. Calculated refractive indices at 589 nm *vs.* calculated Abbe numbers for fundamental fluoro-compounds (Group I).

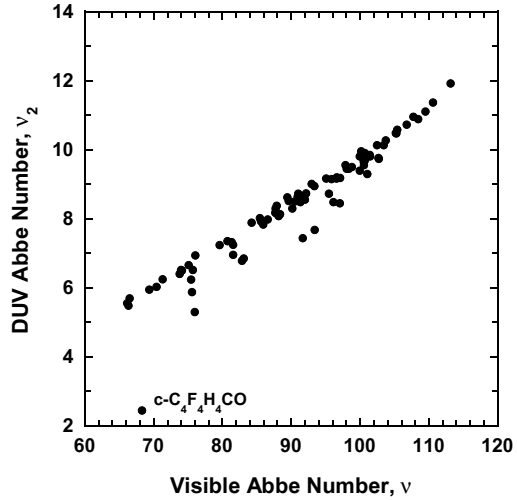


Figure 5. Calculated Abbe number in the visible region (ν) *vs.* calculated Abbe numbers in the DUV region (ν_2).

3. Results & Discussion

3.1 *Packing coefficients of fluoro-compounds.*

At first, we need to determine the molecular packing constant using experimental densities because experimental data for the wavelength dispersion of refractive indices for fluoro-compounds are very limited. Table 1 shows the values of molecular weight, van der Waals volumes, experimental density together with the packing coefficients (K_p) estimated using Eq.(2). The average value of K_p is ~0.56, which is slightly smaller than that for non-fluorinated compounds (~0.60).[12] This is due to the low polarizability of fluorines which significantly reduces the inter-molecular attracting interactions. We used this value (K_p=0.56) throughout this study. Table 2 lists the values of molecular weight, van der Waals volume, calculated polarizability, refractive index

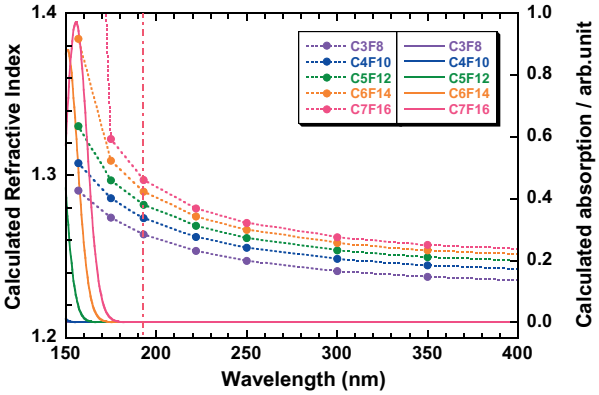


Figure 6. Calculated absorption spectra and refractive index dispersions for perfluoroalkanes in the VUV-DUV region.

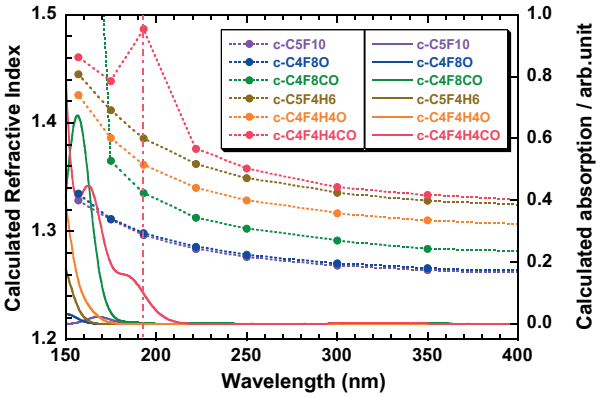
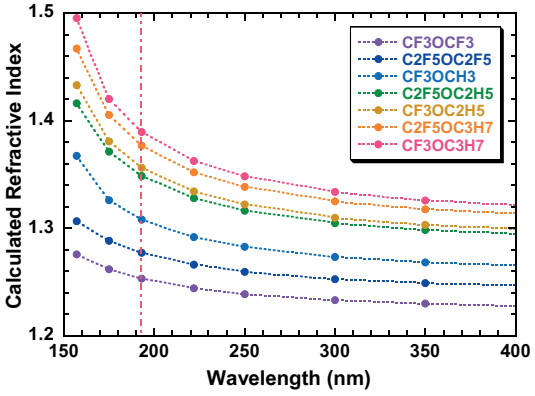


Figure 7. Calculated absorption spectra and refractive index dispersions for fluoroalkylethers and fluorocycloalkanones.

(n_λ) at five wavelengths, and Abbe parameter for the fundamental fluorocarbons called Group I. This group does not contain neither aromatic rings nor polar structures, such as -CN, -COO-, -SO_2F, and -SO_3-. As shown in Fig. 3, the values of α at 589 nm are linearity proportional to V_{vdw}. Since n is determined by the ratio of $\alpha\lambda/V_{mol}$ as expressed in Eq.(1), the variations in n are caused by the distributions in K_p and $\alpha\lambda/V_{vdw}$. As seen in Table 1, the refractive indices of Group I fall in a small range (1.224–1.319). Note that the calculated values of n at 193 nm are in linear relationships with those at 589 nm except for c-$C_4F_4H_4CO$. The relation is expressed as n_{193}=1.5879 n_{589} –0.69584, which means that the wavelength dispersion disappears at n_{193}=n_{589}=1.184. Figure 4 shows that the values of n_{589} are also in linear relationships with the estimated Abbe numbers (ν) despite the scatter of points. The estimated ν at n_{589}=1.184 goes beyond 130, which can be regarded as almost no dispersion. The linear relationships observed in Figs.3–5 indicate that the dispersion curves for Group I compounds can be well expressed by a common equation; the Cauchy's formula



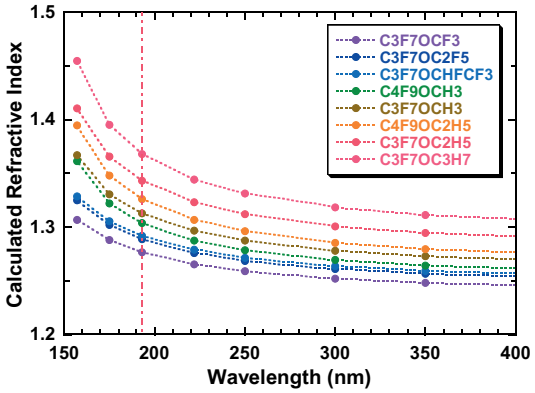


Figure 8. Calculated dispersions of refractive indices for fluoroalkylethers. The smaller fluorine contents, the higher refractive indices.

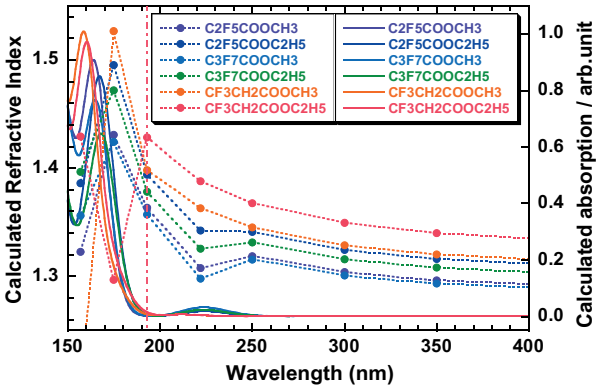


Figure 9. Calculated absorption spectra and refractive index dispersions of fluorocarbonylester compounds.

$$n_\lambda = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} \qquad (6)$$

where A, B and C are intrinsic coefficients for each material (C is generally very small).

Figures 6–8 show the wavelength dispersion of refractive indices for perfluoroalkanes, cyclicfluoroethers, cyclicfluoroalkanones, and fluoroalkylethers which are included in Group I. Fig. 6 shows that perfluoroalkanes exhibit the lowest n and the smallest dispersion with the largest ν and ν_2 in all the compounds. Note that the values of n increase as the molecular size

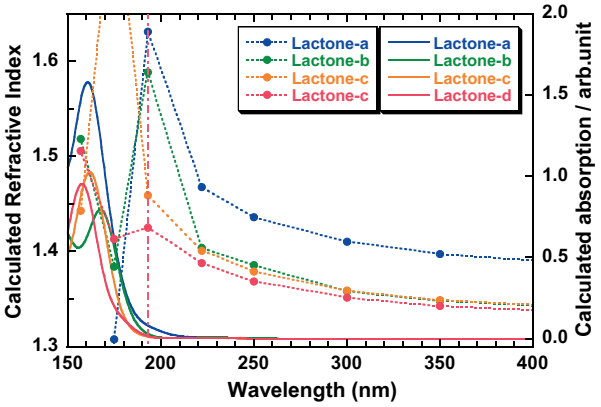


Figure 10. Calculated absorption spectra and refractive index dispersions of lactones.

and/or M_w increases. This trend is also observed for other types compounds and agrees well with the experimental results for hydrocarbons.[14] Fig. 7 shows that fluorocycloalkanones show characteristic absorptions in the VUV region, which should cause anomalous dispersion at longer wavelengths. These absorptions are assigned to the transitions from the lone-pair (*n*-) orbitals at the carbonyl oxygen to spacially spreading Rydberg orbitals. The deviations from the liearity of *c*-$C_4F_4H_4CO$ in Figs. 3 and 5 are attributable to the anomalous dispersion at 193 nm as seen in Fig. 7. Fig. 8 shows the calculated dispersion for fluoroalkylethers. Since there are no absorption peaks over 150 nm, these dispersion curves are well fitted by the Cauchy's formula. The dispersion behaviors are similar to those of perfluorocarbons and can be expressed as 1) the higher fluorine content, the lower *n*, and 2) the larger molecular size and/or M_w, the higher *n*.

Table 3 lists the calculated parameters for fluorocarbons having polar groups, which are included in Group II. In addition, Figs. 9–11 show the dispersions of fluorocarbonylesters, sulfonylfluorides, and sulfonylesters, which are expected to show good transparency in the VUV region.[5,7] Fluoro-carbonylesters show complicated shapes of dispersion as seen in Fig. 9. These are due to the characteristic absorptions appearing at 220–230 nm, and these peaks can be assigned to the $n \rightarrow \pi^*$ transitions at the carbonyl group. These esters are not suitable for immersion fluids because of the lower refractive indices and significant absorption. On the other hand, the lactones containing C=O group show characteristic absorptions at 165–175 nm as shown in Fig. 10, which are originated both from $n \rightarrow$Rydberg* and $\pi \rightarrow \pi^*$ transitions. Since the oscillator strenghs of $n \rightarrow \pi^*$ absorptions are much smaller than those

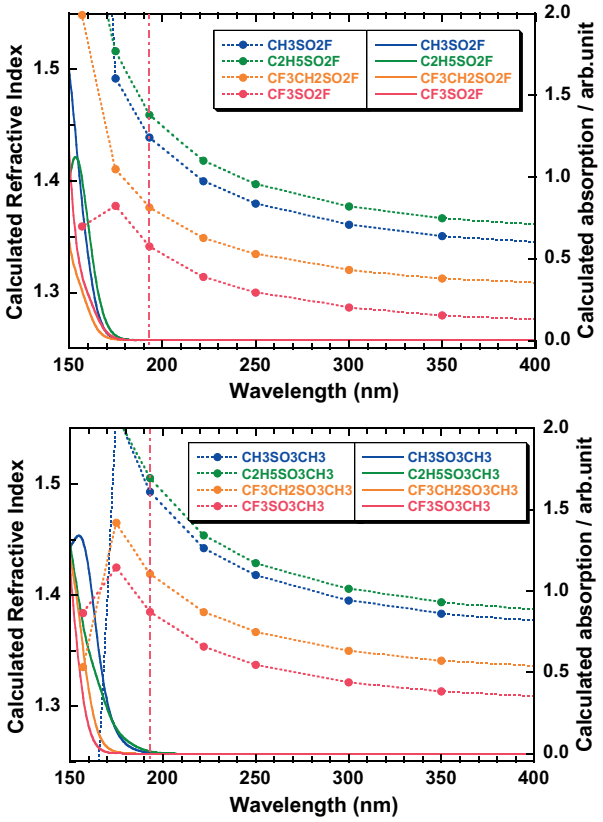


Figure 11. Calculated dispersions of sulfonylfluorides and sulfonylesters which were firstly reported as highly ransparent maerials at 157 nm by the authors.

for the esters in Fig. 9, these lactones can be candidates for immersion fluids. Fig. 11 show the dispersions of sulfonylfluorides and sulfonylesters which were firstly proposed by the authors as novel resist platforms for 157 nm lithography. Due to the appropriate absorptions in VUV region and the sulfur atoms possesing high atomic polarizability, these compounds show high refractive indices and good transparency at 193 nm. In particular,

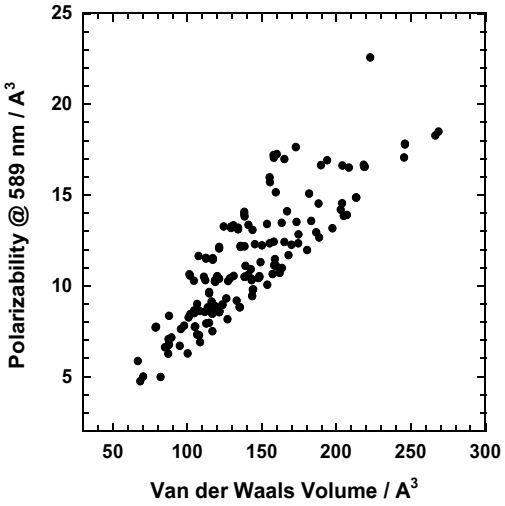


Figure 12. Calculated linear polarizability *vs.* van der Waals volumes with the optimized geometries for fundamental fluoro-compounds (Group I & II).

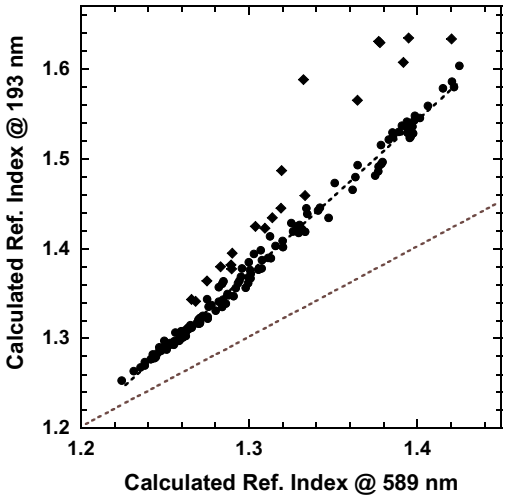


Figure 13. Calculated refractive indices at 589 nm *vs.* those at 193 nm. Most of the points are located on the correlation : $n_{193} = -0.690 + 1.5833 * n_{589}$.

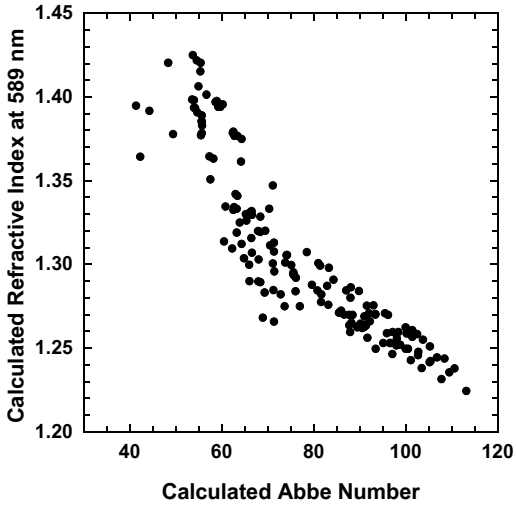


Figure 14. Calculated refractive indices at 589 nm *vs.* calculated Abbe numbers for fundamental fluoro-compounds (Group I & II).

sulfonylfluorides can be promising as 157 nm immersion fluids having refractive indices higher than 1.6. In addition, higher refractive indices can be expected for siloxanes, nitriles, and alicyclic compounds such as norbornaes and bicyclo[2,2,2]octanes as listed in Table 3.

Figures 12-15 show the relationships among the calculated parameters for all compounds (Groups I and II). Linear relationships are observed between α and V_{vdw} (Fig. 12), n_{589} and n_{193} (Fig. 13), n_{589} and ν (Fig. 14), and ν and ν_2 (Fig. 15) as well as in Figs. 2–5, though points are much more scattered. The wider distributions in the calculated parameters should be originated by the anomalous dispersion caused by absorptions in the VUV-DUV region. However, these relationships will be useful to infer and predict the optical properties of fluorocompounds in the VUV-DUV region from the data measured in the visible region. In addition, if we carefully choose compounds exhibiting high refractive indices and high transparency with the aid of DFT and TD-DFT calculations, wider range of fluoro-compounds can be taken as candidates for immersion fluids for the next-generation lithography.

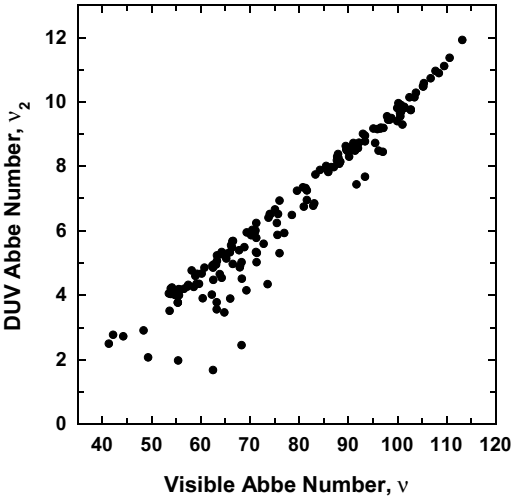


Figure 15. Calculated Abbe numbers in the visible region *vs.* calculated Abbe numbers in the DUV region (Group I & II).

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Table 2. Molecular weights, van der Waals volumes (angstrom^3), calculated polarizability (angstrom^3) and refractive indices at the five wavelengths (nm), and calculated Abbe numbers for Group I compounds.

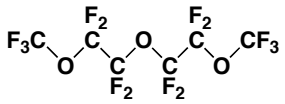
Compound	M_w	V_{vdw} / A^3	Polarizability / A^3					Refractive Index					Abbe	
			α(157)	α(193)	α(486)	α(589)	α(656)	*n*(157)	*n*(193)	*n*(486)	*n*(589)	*n*(656)	ν	ν_2
CF_3OCF_3	154.0	81.9	6.04	5.57	5.00	4.97	4.96	1.276	1.253	1.226	1.224	1.224	113.1	11.9
C_3F_8	188.0	100.2	7.76	7.09	6.31	6.28	6.26	1.291	1.264	1.233	1.231	1.231	107.7	11.0
$C_2F_5OCF_3$	204.0	108.5	8.50	7.79	6.95	6.90	6.89	1.294	1.268	1.237	1.235	1.235	109.5	11.1
$CF_3OCF_2OCF_3$	220.0	116.8	9.18	8.44	7.55	7.50	7.48	1.296	1.270	1.239	1.238	1.237	110.6	11.4
C_4F_{10}	238.0	126.9	10.35	9.30	8.21	8.16	8.14	1.307	1.274	1.240	1.238	1.237	103.4	10.1
$C_2F_5OC_2F_5$	254.0	135.1	10.99	10.01	8.88	8.83	8.81	1.307	1.277	1.244	1.242	1.242	105.4	10.6
$C_3F_7OCF_3$	254.0	135.1	11.00	10.00	8.86	8.81	8.79	1.307	1.277	1.243	1.242	1.241	105.2	10.5
$C_2F_5OCF_2OCF_3$	270.0	143.4	11.64	10.66	9.49	9.43	9.40	1.306	1.278	1.245	1.244	1.243	108.4	10.9
$CF_3OC_2F_4OCF_3$	270.0	143.4	11.72	10.71	9.51	9.46	9.43	1.308	1.279	1.246	1.245	1.244	106.8	10.7
C_5F_{12}	288.1	153.6	13.38	11.57	10.13	10.06	10.04	1.330	1.282	1.245	1.243	1.242	101.0	9.3
$C_4F_9OCF_3$	304.1	161.8	13.73	12.26	10.79	10.72	10.69	1.321	1.284	1.247	1.246	1.245	102.7	9.8
$N(C_2F_5)_3$	371.1	197.3	16.96	15.07	13.26	13.17	13.14	1.326	1.286	1.249	1.248	1.247	102.7	9.7
PF-diglyme	386.1	204.9	17.25	15.71	13.93	13.85	13.81	1.318	1.288	1.253	1.251	1.250	105.2	10.5
$C_3F_7OC_2F_5$	304.1	163.5	14.03	12.58	11.06	10.98	10.95	1.325	1.289	1.251	1.250	1.249	100.5	9.7
C_6F_{14}	338.1	180.3	17.98	13.93	12.06	11.98	11.95	1.384	1.290	1.248	1.247	1.246	97.1	8.5
$C_4F_9OC_2F_5$	354.1	188.4	16.43	14.55	12.75	12.67	12.63	1.331	1.290	1.251	1.250	1.249	100.0	9.4
$CF_3OCH_2OCF_3$	184.1	107.7	9.32	8.37	7.34	7.29	7.27	1.328	1.292	1.253	1.252	1.251	97.9	9.6
$C_3F_7OCHFCF_3$	286.1	157.1	13.61	12.22	10.72	10.65	10.62	1.329	1.292	1.254	1.252	1.251	98.8	9.5
PF-triglyme	502.1	266.4	22.86	20.78	18.39	18.27	18.23	1.325	1.293	1.257	1.255	1.254	103.7	10.3
$C_2F_5CHFCHFCF_3$	252.1	144.0	12.84	11.30	9.87	9.80	9.78	1.339	1.295	1.255	1.253	1.252	96.6	9.2
$C_5F_{10}H_2$	252.1	144.0	12.84	11.30	9.87	9.80	9.77	1.339	1.295	1.255	1.253	1.252	95.1	9.2
$C_2F_5CHFCHFCF_3$	252.1	144.0	12.84	11.30	9.87	9.80	9.78	1.339	1.295	1.255	1.253	1.252	96.6	9.2
c-C_5F_{10}	250.1	133.0	11.52	10.48	9.24	9.18	9.15	1.328	1.296	1.259	1.257	1.256	101.4	9.9
c-C_4F_8	200.0	106.5	9.37	8.41	7.37	7.32	7.30	1.334	1.297	1.258	1.256	1.255	98.1	9.5
c-C_6F_{12}	300.1	159.6	13.95	12.61	11.14	11.07	11.04	1.332	1.297	1.260	1.258	1.258	102.5	10.1
C_7F_{16}	388.1	207.0	38.46	16.37	14.01	13.91	13.87	1.821	1.297	1.251	1.250	1.249	93.4	7.7
c-C_4F_8O	216.0	114.5	10.09	9.08	8.01	7.96	7.94	1.335	1.298	1.260	1.259	1.258	100.2	10.0
c-$C_6F_{11}CF_3$	350.1	186.4	16.42	14.79	13.04	12.96	12.92	1.335	1.299	1.261	1.259	1.258	100.7	9.9
Cytop	316.1	167.9	15.23	13.37	11.76	11.69	11.66	1.346	1.300	1.261	1.259	1.258	100.7	9.7
Teflon-AF	382.1	202.8	18.06	16.22	14.29	14.19	14.16	1.339	1.301	1.263	1.261	1.260	101.4	9.8
c-$C_6F_{10}(CF_3)_2$-a	400.1	213.4	19.13	17.04	14.96	14.87	14.83	1.341	1.301	1.261	1.259	1.259	100.6	9.6
c-$C_6F_{10}(CF_3)_2$-b	400.1	213.1	21.39	17.05	14.96	14.86	14.82	1.387	1.301	1.261	1.260	1.259	98.4	9.5
c-$C_4F_6(CF_3)_2$	300.1	159.4	13.78	12.80	11.19	11.12	11.08	1.328	1.302	1.262	1.260	1.259	97.1	9.2
HFE-X	452.1	245.4	22.11	19.68	17.19	17.07	17.02	1.343	1.302	1.261	1.259	1.258	95.9	9.2
PF-MeMorpholine	299.1	158.1	14.15	12.72	11.20	11.13	11.10	1.341	1.303	1.264	1.262	1.262	100.0	9.8
$C_7F_{15}OC_2F_5$	504.1	268.6	–	21.84	18.62	18.49	18.43	–	1.307	1.258	1.256	1.255	91.7	7.4
CF_3OCH_3	100.0	68.2	6.53	5.57	4.79	4.75	4.74	1.367	1.308	1.262	1.260	1.259	87.9	8.2
$C_3F_7CH_3$	184.1	112.6	10.48	9.22	7.98	7.92	7.89	1.356	1.309	1.264	1.262	1.261	90.5	8.5
HFE-347-pc-f	200.1	121.2	11.25	9.92	8.60	8.54	8.51	1.354	1.309	1.265	1.262	1.262	91.0	8.6
HFE-347mcf	200.1	121.3	11.23	9.93	8.60	8.54	8.51	1.354	1.309	1.264	1.262	1.262	89.5	8.6
HFE-449mec-f	250.1	147.7	13.71	12.10	10.51	10.43	10.40	1.355	1.309	1.265	1.263	1.262	91.0	8.7
$CF_3CH_2OCF_2CF_2H$	200.1	121.2	11.33	9.96	8.62	8.56	8.53	1.357	1.310	1.265	1.263	1.262	89.6	8.5
$CF(CF_3)_2CF_2OCH_3$	250.1	148.1	14.12	12.18	10.54	10.47	10.44	1.365	1.310	1.265	1.263	1.263	91.3	8.5
HFE-54-11mec-f	300.1	174.3	16.32	14.33	12.43	12.34	12.30	1.358	1.310	1.266	1.264	1.263	91.2	8.7
$C_2F_5OCH_3$	150.1	94.8	9.05	7.83	6.75	6.70	6.68	1.366	1.312	1.266	1.264	1.263	87.7	8.3
PF-Triglyme	366.1	203.9	19.13	16.85	14.64	14.54	14.50	1.359	1.312	1.268	1.266	1.265	92.2	8.7
$C_3F_7OCH_3$	200.1	121.4	11.63	10.06	8.68	8.62	8.59	1.367	1.313	1.267	1.264	1.264	90.2	8.3
$C_4F_9OCH_3$	250.1	148.1	14.45	12.34	10.61	10.53	10.50	1.375	1.315	1.267	1.265	1.264	88.2	8.1
c-$C_5F_8H_2$-b	214.1	123.4	11.24	10.33	9.00	8.94	8.91	1.347	1.316	1.272	1.270	1.270	93.4	9.0
HFE-458mmzc	232.1	143.0	13.71	11.99	10.38	10.30	10.28	1.368	1.317	1.271	1.269	1.268	91.0	8.5
cis-PF-decaline	462.1	246.1	22.57	20.66	17.92	17.79	17.74	1.350	1.317	1.272	1.270	1.269	96.1	8.5
trans-PF-decaline	462.1	245.9	23.31	20.64	17.95	17.83	17.78	1.363	1.317	1.273	1.271	1.270	95.5	8.7
c-$C_5F_8H_2$-a	214.1	123.5	11.61	10.41	9.02	8.96	8.93	1.360	1.319	1.273	1.271	1.270	92.0	8.6
HFE-458-mecf	232.1	143.2	13.91	12.12	10.43	10.35	10.32	1.373	1.320	1.272	1.270	1.269	87.7	8.2
HFE-55-10mec-fc	282.1	169.7	16.59	14.36	12.36	12.27	12.23	1.376	1.320	1.272	1.270	1.269	88.4	8.1
HFE-458-pcf-c	232.1	143.3	14.07	12.17	10.44	10.36	10.33	1.378	1.321	1.272	1.270	1.269	86.6	8.0
c-$C_4F_6H_2$-b	180.1	104.9	9.99	8.93	7.78	7.73	7.70	1.365	1.322	1.278	1.275	1.275	93.0	9.0
HFE-356mf-c	182.1	116.5	11.43	9.93	8.52	8.46	8.43	1.377	1.323	1.273	1.271	1.270	85.5	8.0

Table 2. *(continued)*

Compound	M_w	V_{vdw} / A^3	Polarizability / A^3					Refractive Index					Abbe	
			α(157)	α(193)	α(486)	α(589)	α(656)	*n*(157)	*n*(193)	*n*(486)	*n*(589)	*n*(656)	ν	ν_2
HFE-356pcf	182.1	116.8	11.51	9.96	8.54	8.47	8.45	1.379	1.323	1.273	1.271	1.270	85.6	7.9
c-$C_4F_6H_2$-a	180.1	105.3	10.32	9.01	7.81	7.75	7.73	1.377	1.324	1.277	1.275	1.274	91.5	8.6
HFE-356mec	182.1	116.7	11.83	10.01	8.57	8.51	8.48	1.392	1.325	1.275	1.272	1.271	85.9	7.8
c-$C_5F_7H_3$	196.1	118.5	11.67	10.34	8.94	8.87	8.84	1.379	1.331	1.282	1.280	1.279	87.9	8.4
c-C_4F_8CO	228.1	126.1	–	11.13	9.38	9.30	9.27	–	1.335	1.278	1.276	1.275	83.1	6.8
$C_5F_{11}C_2H_5$	298.1	182.9	21.47	16.23	13.68	13.57	13.53	1.463	1.337	1.280	1.278	1.277	81.6	7.0
$C_4F_9OC_2H_5$	264.1	165.0	17.54	14.78	12.52	12.42	12.38	1.413	1.341	1.284	1.282	1.281	81.6	7.2
$C_3F_7OC_2H_5$	214.1	138.3	14.62	12.46	10.58	10.49	10.46	1.411	1.343	1.287	1.284	1.283	80.8	7.3
c-$C_5F_6H_4$	178.1	113.6	11.40	10.35	8.87	8.81	8.78	1.387	1.347	1.293	1.291	1.290	84.3	7.9
$C_2F_5OC_2H_5$	164.1	111.6	11.94	10.20	8.63	8.56	8.53	1.416	1.348	1.290	1.288	1.287	79.6	7.2
c-C_5F_9Cl	266.5	142.5	14.69	13.06	11.00	10.91	10.87	1.399	1.350	1.290	1.287	1.286	82.9	6.8
$CF_3OC_2H_5$	114.1	85.0	9.41	7.92	6.66	6.61	6.58	1.433	1.356	1.295	1.292	1.291	76.0	6.9
c-$C_4F_4H_4O$	144.1	95.7	10.44	9.03	7.67	7.61	7.59	1.426	1.361	1.302	1.299	1.298	81.4	7.3
HFE-449mcf-c	214.1	138.3	–	13.04	10.57	10.48	10.45	–	1.361	1.287	1.284	1.283	76.0	5.3
$C_4F_9C_3H_7$	262.1	173.1	20.19	16.34	13.64	13.52	13.47	1.459	1.361	1.296	1.293	1.292	75.7	6.5
c-$C_4F_6H_2CO$-b	192.1	116.3	–	11.06	9.19	9.11	9.08	–	1.364	1.297	1.294	1.293	75.4	6.2
$C_3F_7OC_3H_7$	228.1	155.1	17.93	14.89	12.46	12.35	12.31	1.455	1.368	1.303	1.300	1.299	75.1	6.7
c-$C_4F_6H_2CO$-a	192.1	116.2	9.40	11.17	9.21	9.13	9.10	1.305	1.369	1.298	1.295	1.294	75.6	5.9
$CH_3OCF_2OCH_3$	112.1	89.3	7.36	8.66	7.21	7.15	7.12	1.311	1.372	1.304	1.301	1.300	73.8	6.4
c-$C_4F_4H_4$	128.1	87.2	10.88	8.55	7.13	7.07	7.04	1.497	1.377	1.309	1.306	1.305	74.1	6.5
$C_2F_5OC_3H_7$	178.1	128.5	15.20	12.59	10.50	10.41	10.37	1.467	1.377	1.308	1.305	1.304	74.0	6.5
c-$C_5F_4H_6$	142.1	103.9	11.79	10.40	8.77	8.70	8.67	1.445	1.386	1.319	1.316	1.315	76.5	7.0
$CF_3OC_3H_7$	128.1	101.8	12.67	10.28	8.52	8.44	8.41	1.495	1.389	1.316	1.313	1.312	71.3	6.2
$C_3F_7C_4H_9$	226.1	163.3	20.49	16.49	13.59	13.47	13.42	1.500	1.390	1.315	1.311	1.310	70.4	6.0
$C_2F_5OC_4H_9$	192.1	145.4	18.72	15.09	12.41	12.30	12.25	1.516	1.402	1.323	1.320	1.319	69.4	6.0
$CF_3OC_4H_9$	142.1	118.7	16.11	12.75	10.41	10.31	10.27	1.550	1.418	1.333	1.329	1.328	66.5	5.7
$C_2F_5C_5H_{11}$	190.2	153.5	21.49	16.63	13.53	13.40	13.34	1.571	1.422	1.335	1.331	1.330	66.2	5.5
c-$C_4F_4H_4CO$	156.1	106.6	12.46	13.06	9.08	9.00	8.96	1.461	1.487	1.323	1.319	1.318	68.3	2.5

* abbreviations : c- : cyclo-, C_3F_7- : $CF_3CF_2CF_2$-, C_4F_9- : $CF_3CF_2CF_2CF_2$-, C_5F_{11}- : $CF_3CF_2CF_2CF_2CF_2$-, PF : perfluoro

HFE-347mcf : $CF_3CF_2CH_2OCHF_2$
HFE-347-pc-f : $CHF_2CF_2OCH_2CF_3$
HFE-356mec : $CF_3CHFCF_2OCH_3$
HFE-356mf-c : $CF_3CH_2OCF_2CH_2F$
HFE-356pcf : $CHF_2CF_2CH_2OCHF_2$
HFE-449mcf-c : $CF_2CF_2CH_2OCH_2CHF_2$
HFE-449mec-f : $CF_3CHFCF_2OCH_2CF_3$
HFE-458-mecf : $CF_3CHFCF_2CH_2OCHF_2$
HFE-458mmzc : $(CF_3)_2CHCF_2OCH_3$
HFE-458-pcf-c : $CHF_2CF_2CH_2OCF_2CHF_2$
HFE-54-11mec-f : $CF_3CHFCF_2OCH_2CF_2CF_3$
HFE-55-10mec-fc : $CF_3CHFCF_2OCH_2CF_2CHF_2$
HFE-X : $C_3F_7OCF(CF_3)_2CF_2OCFHCF_3$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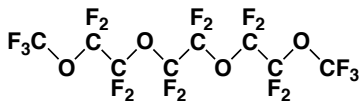
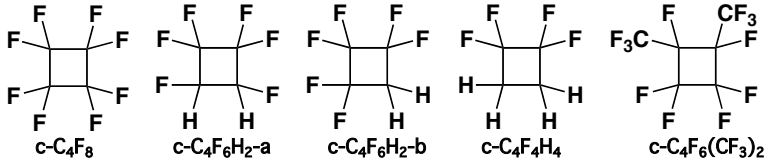

PF-triglyme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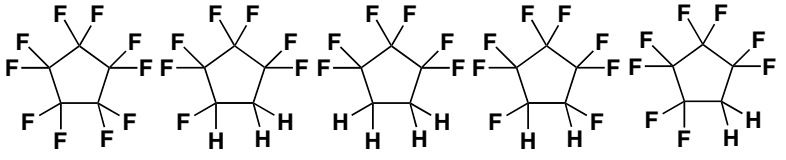
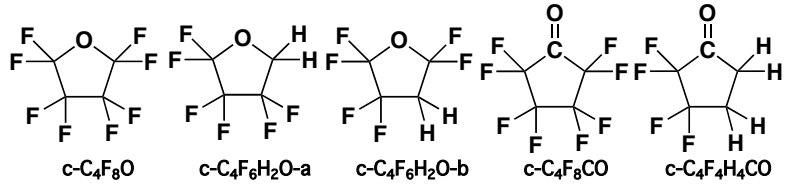

c-C_5F_{10} c-$C_5F_7H_3$ c-$C_5F_6H_4$ c-$C_5F_8H_2$-a c-$C_5F_8H_2$-b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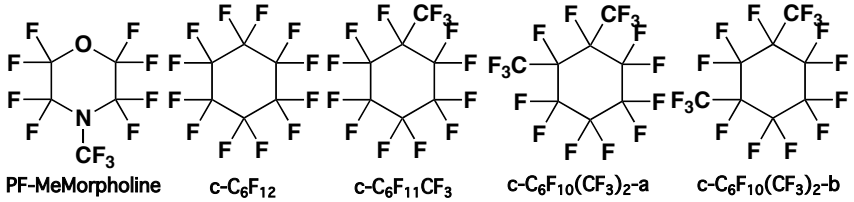
PF-MeMorpholine c-C_6F_{12} c-$C_6F_{11}CF_3$ c-$C_6F_{10}(CF_3)_2$-a c-$C_6F_{10}(CF_3)_2$-b

Table 3. Molecular weights, van der Waals volumes (angstrom^3), calculated polarizability (angstrom^3) and refractive indices at the five wavelengths (nm), and calculated Abbe numbers for Group II compounds.

Compound	M_w	V_{vdw} / A^3	Polarizability / A^3					Refractive Index					Abbe	
			α(157)	α(193)	α(486)	α(589)	α(656)	*n*(157)	*n*(193)	*n*(486)	*n*(589)	*n*(656)	ν	ν_2
Cytop-H_2	280.1	158.6	14.50	13.28	11.55	11.47	11.44	1.349	1.317	1.272	1.270	1.269	93.4	8.8
Safari-b	358.1	218.5	21.57	19.26	16.68	16.56	16.51	1.380	1.335	1.286	1.284	1.283	89.8	8.5
Safari-a	358.1	218.3	21.73	19.45	16.79	16.67	16.62	1.383	1.339	1.289	1.286	1.285	88.0	8.3
Cytop-H_4	244.1	148.9	11.49	13.26	11.39	11.31	11.27	1.290	1.339	1.287	1.285	1.284	87.0	8.0
CF_3SO_2F	152.1	87.1	8.18	7.81	6.32	6.26	6.24	1.359	1.341	1.271	1.268	1.267	68.9	5.5
CF_3COOH	114.0	70.2	8.34	6.33	5.05	5.00	4.98	1.469	1.343	1.268	1.266	1.265	71.3	5.0
$CF_3COOCH_2CF_3$	196.1	118.7	10.07	10.71	8.81	8.73	8.70	1.321	1.344	1.278	1.275	1.274	76.9	5.9
Safari-c	322.1	208.4	22.08	19.44	16.64	16.51	16.46	1.411	1.356	1.301	1.298	1.297	83.3	7.8
$C_3F_7COOCH_3$	228.1	141.0	13.13	13.17	10.71	10.62	10.58	1.356	1.357	1.285	1.282	1.281	72.8	5.6
$C_2F_5COOCH_3$	178.1	114.3	9.74	10.85	8.76	8.68	8.65	1.323	1.364	1.288	1.285	1.284	71.2	5.3
$C_2F_5COOCOC_2F_5$	310.1	174.5	16.48	16.58	12.95	12.83	12.78	1.362	1.364	1.278	1.275	1.274	73.6	4.3
Cytop-H_6	208.1	139.0	17.08	13.30	11.19	11.10	11.07	1.488	1.367	1.303	1.301	1.300	81.0	6.8
$CF_3CH_2SO_2F$	166.1	97.7	13.24	9.56	7.87	7.80	7.77	1.549	1.376	1.303	1.300	1.299	71.1	6.0
CF_3COOCH_3	128.1	87.7	6.46	8.61	6.83	6.77	6.74	1.276	1.377	1.293	1.290	1.288	67.9	4.9
$C_3F_7COOC_2H_5$	242.1	157.9	16.20	15.52	12.54	12.42	12.38	1.397	1.378	1.299	1.296	1.295	71.4	5.3
Safari-d	304.2	204.0	26.33	20.06	16.77	16.63	16.58	1.517	1.378	1.310	1.307	1.306	78.5	6.5
$C_4F_9SO_3CH_2CF_3$	382.1	219.1	21.01	21.63	16.72	16.56	16.50	1.368	1.380	1.286	1.283	1.282	69.3	4.2
CF_3CH_2COOH	128.1	86.9	9.92	8.62	6.77	6.70	6.68	1.448	1.382	1.292	1.289	1.288	68.4	4.5
$CF_3SO_3CH_3$	164.1	108.2	10.78	10.80	8.70	8.62	8.58	1.384	1.385	1.303	1.300	1.299	65.9	5.3
$CH_3SO_3CH(CF_3)_2$	246.1	149.9	–	15.06	12.34	12.23	12.18	–	1.387	1.311	1.308	1.306	71.3	5.8
$C_2F_5COOC_2H_5$	192.1	131.1	13.13	13.37	10.65	10.54	10.50	1.386	1.394	1.306	1.303	1.302	68.0	4.9
$CF_3CH_2COOCH_3$	142.1	104.4	5.73	10.75	8.58	8.50	8.47	1.201	1.398	1.310	1.307	1.306	66.5	5.0
$CClF_2CF_2CHClF$	202.9	114.7	14.81	11.94	9.68	9.59	9.55	1.518	1.403	1.319	1.316	1.314	66.3	5.5
$C_2H_5SO_3CH(CF_3)_2$	260.2	166.9	–	17.57	14.24	14.11	14.05	–	1.409	1.323	1.320	1.319	67.8	5.4
$CF_3COOC_2H_5$	142.1	104.5	10.31	11.12	8.73	8.64	8.61	1.380	1.414	1.316	1.312	1.311	64.2	4.6
$CF_3CH_2SO_3CH_3$	178.1	118.8	10.47	12.79	10.32	10.22	10.18	1.335	1.419	1.330	1.326	1.325	65.3	5.3
c-hexane-F_6	250.2	189.7	30.07	20.42	16.80	16.64	16.58	1.666	1.419	1.337	1.333	1.332	70.2	5.9
Nitrile-CF_3	258.2	193.7	3.58	20.94	17.09	16.93	16.86	1.066	1.421	1.335	1.332	1.330	66.4	5.7
c-(C_2F_4CO-O-CO)	172.0	100.7	8.04	10.93	8.35	8.26	8.23	1.301	1.423	1.313	1.310	1.308	62.2	4.0
Lactone-d	170.1	118.3	14.98	12.90	10.35	10.25	10.21	1.506	1.425	1.332	1.329	1.327	68.3	5.0
c-(C_3F_6CO-O-CO)	222.1	127.3	11.12	13.87	10.36	10.26	10.22	1.332	1.425	1.307	1.304	1.302	64.8	3.5
$CH_3SO_3CH_2CF_3$	178.1	118.6	20.73	12.98	10.42	10.32	10.28	1.756	1.427	1.334	1.330	1.329	65.2	5.1
$CF_3CH_2COOC_2H_5$	156.1	121.2	13.33	13.31	10.51	10.40	10.36	1.429	1.429	1.329	1.325	1.324	63.8	4.7
$CH_3OCOC_2F_6COO($	268.1	181.7	16.45	20.18	15.25	15.09	15.03	1.345	1.434	1.318	1.314	1.312	60.4	3.9
BCO-F_4	182.2	143.6	18.76	15.96	13.20	13.08	13.03	1.525	1.435	1.351	1.347	1.346	71.1	6.0
CH_3SO_2F	98.1	66.5	14.90	7.46	5.92	5.86	5.83	2.078	1.439	1.338	1.335	1.333	60.8	4.9
$CF_3CH_2SO_3C_2H_5$	192.2	135.6	22.39	15.31	12.27	12.14	12.10	1.702	1.443	1.345	1.341	1.339	63.3	5.1
$C_2F_5CHCl_2$	202.9	114.5	18.58	12.99	9.76	9.66	9.62	1.686	1.445	1.323	1.319	1.318	63.2	3.6
$CF_3COOC_4H_9$	170.1	138.4	20.52	15.70	12.30	12.18	12.13	1.612	1.445	1.338	1.334	1.333	62.6	4.5
$C_2H_5SO_3CH_2CF_3$	192.2	135.6	10.13	15.41	12.31	12.18	12.13	1.280	1.446	1.346	1.342	1.340	63.0	5.0
$C_2H_5SO_2F$	112.1	83.5	13.00	9.74	7.73	7.65	7.62	1.651	1.459	1.354	1.350	1.348	60.4	4.8
Lactone-c	170.1	120.0	13.56	13.99	10.64	10.54	10.49	1.443	1.459	1.337	1.333	1.332	63.2	3.8
c-hexane-F_2	120.1	111.0	18.01	13.10	10.59	10.48	10.44	1.686	1.466	1.365	1.362	1.360	64.1	5.3
$CF(CH_3)_2COOCH_3$	120.1	112.1	25.87	13.41	10.42	10.31	10.26	2.130	1.473	1.355	1.351	1.349	57.5	4.3
Nitrile-F	158.2	140.9	22.27	17.06	13.50	13.36	13.30	1.664	1.480	1.368	1.363	1.361	58.1	4.8
Norb-F_2-b	132.1	117.1	17.52	14.22	11.54	11.43	11.38	1.619	1.482	1.379	1.375	1.373	64.3	5.3
Norb-F_2-a	132.1	117.1	20.86	14.33	11.59	11.47	11.43	1.776	1.486	1.381	1.377	1.375	63.3	5.2
BCO-F_2-a	146.2	133.9	17.12	16.54	13.26	13.12	13.07	1.512	1.491	1.381	1.377	1.375	63.1	5.0
$CH_3SO_3CH_3$	110.1	87.6	–	10.85	8.43	8.34	8.30	–	1.493	1.369	1.365	1.363	57.2	4.3
Norb-F_2-c	132.1	117.1	–	14.54	11.64	11.52	11.47	–	1.494	1.383	1.378	1.377	62.4	4.9
BCO-F_2-b	146.2	134.0	3.36	16.70	13.34	13.21	13.15	1.090	1.497	1.384	1.379	1.378	62.5	4.9
$C_2H_5SO_3CH_3$	124.1	104.6	17.40	13.23	10.29	10.18	10.13	1.709	1.505	1.379	1.374	1.372	56.7	4.3
$CH_3SO_3C_2H_5$	124.1	104.4	–	13.43	10.39	10.27	10.22	–	1.516	1.383	1.378	1.376	55.6	4.2
$CH_3SO_3CH(CH_3)_2$	138.2	121.3	12.34	15.76	12.19	12.06	12.00	1.393	1.522	1.388	1.383	1.381	55.6	4.2
Norb-F_1-b	114.2	112.4	17.10	14.64	11.62	11.50	11.45	1.633	1.523	1.400	1.395	1.394	60.2	4.7
$C_2H_5SO_3C_2H_5$	138.2	121.3	22.59	15.85	12.27	12.14	12.08	1.823	1.525	1.390	1.385	1.383	55.5	4.2

Table 3. *(continued)*

Compound	M_w	V_{vdw} / A^3	Polarizability / A^3					Refractive Index					Abbe	
			α(157)	α(193)	α(486)	α(589)	α(656)	*n*(157)	*n*(193)	*n*(486)	*n*(589)	*n*(656)	ν	ν_2
Norb-F_1-c	114.2	112.4	19.05	14.67	11.63	11.51	11.46	1.726	1.525	1.401	1.396	1.394	59.2	4.7
Norb-F_1-a	114.2	112.4	13.63	14.76	11.67	11.55	11.50	1.481	1.529	1.402	1.397	1.396	58.9	4.6
BCO-F-a	128.2	129.2	19.83	16.99	13.32	13.18	13.12	1.640	1.529	1.399	1.394	1.392	59.2	4.4
$CH_3SO_3C(CH_3)_3$	152.2	138.3	29.23	18.20	13.98	13.82	13.76	1.987	1.530	1.390	1.385	1.383	55.6	4.0
$C_2H_5SO_3$ $CH(CH_3)_2$	152.2	138.2	27.20	18.21	14.10	13.94	13.88	1.890	1.530	1.394	1.389	1.387	55.6	4.2
Nitrile-H	122.2	130.9	20.87	17.39	13.48	13.33	13.26	1.671	1.536	1.399	1.393	1.391	54.2	4.2
BCO-F-b	128.2	129.1	17.89	17.17	13.40	13.26	13.20	1.564	1.536	1.402	1.397	1.395	58.6	4.3
$C_2H_5SO_3$ $C(CH_3)_3$	166.2	155.2	23.18	20.67	15.90	15.72	15.64	1.618	1.537	1.396	1.391	1.389	54.6	4.0
$CH_3SO_3C_4H_9$	152.2	138.2	15.61	18.53	14.24	14.08	14.01	1.443	1.542	1.399	1.394	1.392	53.9	4.0
Nitrile-CH_3	150.2	165.1	17.87	22.18	17.19	16.99	16.91	1.422	1.543	1.403	1.398	1.396	53.9	4.2
c-hexane (boat)	84.2	101.8	13.59	13.73	10.67	10.55	10.50	1.539	1.546	1.407	1.401	1.399	56.6	4.2
$C_2H_5SO_3$ C_4H_9	166.2	155.1	27.97	21.00	16.17	15.98	15.90	1.789	1.548	1.404	1.398	1.396	53.5	4.1
c-hexane (chair)	84.2	101.4	24.43	13.96	10.74	10.62	10.57	2.214	1.559	1.412	1.406	1.404	54.9	4.0
Siloxane-b	184.4	159.4	28.73	22.14	15.39	15.16	15.07	1.788	1.565	1.371	1.364	1.362	42.2	2.8
BCO	110.2	124.2	18.75	17.60	13.42	13.27	13.21	1.626	1.579	1.421	1.415	1.413	55.3	3.8
Norbornane	96.2	107.4	7.73	15.24	11.77	11.63	11.58	1.269	1.580	1.427	1.422	1.420	54.5	4.0
Di-c-hexane-b	138.2	157.9	12.33	22.61	17.25	17.06	16.98	1.293	1.586	1.426	1.421	1.418	55.4	3.8
Lactone-b	170.1	120.0	15.52	17.23	10.62	10.51	10.47	1.519	1.588	1.336	1.332	1.331	62.5	1.7
Di-c-hexane-a	138.2	157.8	33.15	23.13	17.40	17.20	17.12	1.979	1.604	1.431	1.425	1.423	53.7	3.5
Siloxane-c	240.5	222.6	37.58	32.80	22.90	22.58	22.45	1.722	1.608	1.398	1.392	1.389	44.2	2.7
$CFCl_2CH_3$	116.9	78.5	16.46	11.90	7.81	7.71	7.67	1.976	1.630	1.383	1.378	1.376	49.3	2.1
Lactone-a	86.1	78.9	–	11.98	7.83	7.74	7.70	–	1.631	1.382	1.377	1.375	55.4	2.0
Nitrile-Cl	191.0	159.9	15.36	24.37	17.49	17.26	17.17	1.368	1.634	1.427	1.420	1.418	48.3	2.9
Siloxane-a	166.4	172.7	63.32	26.35	17.91	17.64	17.54	4.412	1.635	1.402	1.395	1.392	41.3	2.5

* abbreviations : c- : cyclo-, C_3F_7- : $CF_3CF_2CF_2$-, C_4F_9- : $CF_3CF_2CF_2CF_2$-, C_5F_{11}- : $CF_3CF_2CF_2CF_2CF_2$-,

Nitrile-H : $CH_3CH(CN)CH_2CH(CN)CH_3$
Nitrile-CH_3 : $CH_3C(CH_3)(CN)CH_2C(CH_3)(CN)CH_3$
Nitrile-CF_3 : $CH_3C(CF_3)(CN)CH_2C(CF_3)(CN)CH_3$
Nitrile-F : $CH_3CF(CN)CH_2CF(CN)CH_3$
Nitrile-Cl : $CH_3CCl(CN)CH_2CCl(CN)CH_3$