

Supporting Information

Determining the Liquid Light Scattering Cross-section and Depolarization Spectra using Polarized Resonance Synchronous Spectroscopy

Sumudu A. Athukorale,[†] Yadong Zhou,[§] Shengli Zou,[§] and Dongmao Zhang^{†,✉,}*

[†]Department of Chemistry, Mississippi State University, Mississippi State, Mississippi, 39762, United States

[§]Department of Chemistry, University of Central Florida, Orlando, Florida 32816, United States

[✉]Department of Chemistry, Xihua University, Chengdu, 610039. China.

^{*}*Corresponding author: Email: Dongmao@chemistry.msstate.edu
dmzhang@mail.xhu.edu.cn
Fax: 662-325-1618*

Content	Page
S1. Purity and catalog number of the model solvents.....	S3
S2. Experimental quantification of light scattering depolarization and scattering cross-section for hexane and difluorobenzene isomers.....	S4
S3. Comparison of the experimental and computational light scattering depolarization and cross-section of the model solvents.....	S5
S4. Stokes-Shifted Fluorescence (SSF) spectra of fluorobenzene and 1,4-difluorobenzene.....	S6
S5. Experimental demonstration of methanol filtration-induced fluorescence impurities and the membrane dissolution	S7
S6. Comparison of the depolarization values in this work with literature values.....	S8
S7. Experimental quantification of light scattering depolarization and cross-section spectra for model solvents.....	S9
S8. References.....	S10

S1. Purity and catalog number of the model solvents used

Table S1: Purity and catalog number of the model solvents

solvent	purity	catalog number
Methanol	99.8%	BDH20864.400
Ethanol	200 proof	111ANH200
1-Propanol	99.7%	279544
1-Butanol	≥99%	B7906
Acetone	≥99.9%	650501
Hexane	95%	296090
3-methylpentane	≥99%	M66005
2,3-dimethylbutane	≥99.5%	39760
Carbondisulfide	≥99%	335266
Dimethylsulfoxide	≥99.5%	D4540
Chloroform	≥99%	288306
Dichloromethane	≥99.5%	D37-4
Acetonitrile	≥99.8%	AC268270025
Dimethylformamide	99.8%	227056
Carbontetrachloride	99.9%	319961
Tetrahydrofuran	≥99.9%	401757
Pyridine	99.8%	270970
Cyclohexane	≥99 %	C556-1
Benzene	≥99.9%	270709
Toluene	99.8%	244511
Fluorobenzene	≥99 %	F6001
1,2-Difluorobenzene	98%	126152
1,3-Difluorobenzene	≥99%	D102008
1,4-Difluorobenzene	≥99 %	D102202
Chlorobenzene	99.8%	284513
1,2-Dichlorobenzene	99%	240664
1,3-Dichlorobenzene	98%	113808
Nitrobenzene	≥99 %	252379

S2. Experimental quantification of light scattering depolarization and scattering cross-section for hexane and difluorobenzene isomers

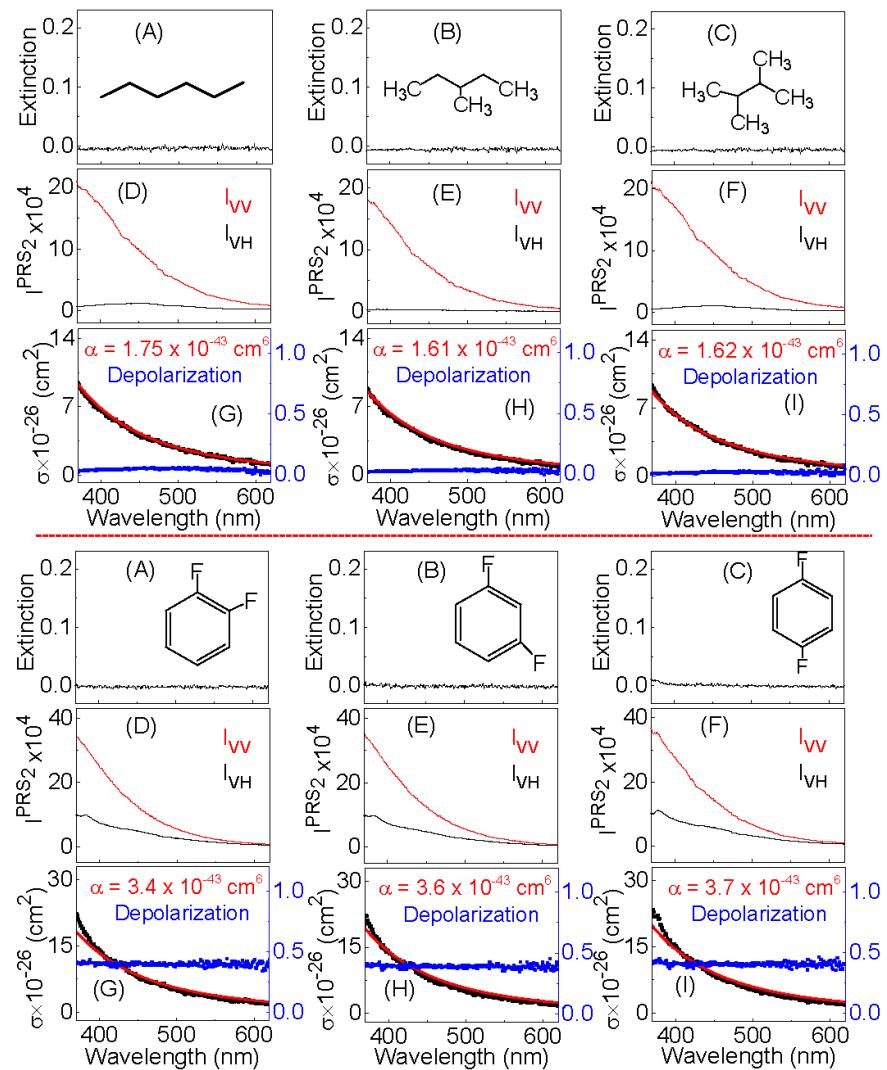


Figure S1: Experimental quantification of the scattering cross-section and depolarization for (top) hexane, 3-methylpentane, and 2,3-dimethylbutane, (bottom) 1,2-, 1,3-, and 1,4-difluorobenzene isomers. (A-C) UV-vis extinction spectra. (D-F) PRS2 spectra with excitation and detection polarization of (red) VV and (black) VH respectively. (G-I) depolarization spectrum and (black) scattering cross-section spectrum. The red line in the scattering cross-section spectra is obtained by curve fitting the scattering cross-section spectrum with the equation of $\sigma(\lambda) = \alpha\lambda^{-4}$.

S3. Comparison of the experimental and computational light scattering depolarization and cross-section for model solvents

Table S2: Comparison of the experimental and computational light scattering depolarization and cross-section for model solvents

solvent	depolarization		cross-section 10^{-26} cm^2	
	experimental	computational	experimental	computational
Water	0.026 ± 0.017	0.009	0.28 ± 0.01	0.005
Methanol	0.025 ± 0.009	0.006	1.77 ± 0.10	0.031
Ethanol	0.031 ± 0.016	0.007	1.70 ± 0.12	0.091
1-Propanol	0.026 ± 0.017	0.017	3.13 ± 0.22	0.177
1-Butanol	0.044 ± 0.016	0.024	2.64 ± 0.03	0.293
Acetone	0.065 ± 0.009	0.055	7.65 ± 0.16	0.153
Hexane	0.036 ± 0.012	0.0356	6.72 ± 0.15	0.550
3-methylpentane	0.027 ± 0.012	NA	6.17 ± 0.08	NA
2,3-dimethylbutane	0.023 ± 0.011	NA	6.46 ± 0.09	NA
*Carbondisulfide	0.473 ± 0.017	0.449	18.37 ± 1.78	0.328
Dimethylsulfoxide	0.085 ± 0.016	0.030	2.29 ± 0.04	0.258
Chloroform	0.119 ± 0.016	0.075	4.06 ± 0.06	0.238
Dichloromethane	0.148 ± 0.013	0.162	3.56 ± 0.11	0.125
Acetonitrile	0.150 ± 0.019	0.112	2.39 ± 0.06	0.068
*Dimethylformamide	0.280 ± 0.021	0.112	2.39 ± 0.26	0.244
Carbontetrachloride	0.023 ± 0.011	0.000	4.45 ± 0.09	0.38
Tetrahydrofuran	0.036 ± 0.018	0.014	2.56 ± 0.05	0.240
Pyridine	0.338 ± 0.018	0.125	9.05 ± 0.32	0.428
Cyclohexane	0.026 ± 0.013	0.005	4.90 ± 0.05	0.480
Benzene	0.269 ± 0.019	0.119	10.40 ± 1.14	0.511
Toluene	0.333 ± 0.021	0.127	14.50 ± 1.28	0.740
Fluorobenzene	0.315 ± 0.016	0.125	11.60 ± 0.71	0.490
1,2-Difluorobenzene	0.398 ± 0.016	0.125	14.10 ± 0.49	0.376
1,3-Difluorobenzene	0.389 ± 0.016	0.126	14.20 ± 0.06	0.375
1,4-Difluorobenzene	0.406 ± 0.017	0.127	15.30 ± 0.06	0.373
Chlorobenzene	0.404 ± 0.017	0.173	18.30 ± 1.63	0.737
1,2-Dichlorobenzene	0.491 ± 0.017	0.156	19.80 ± 1.51	1.00
1,3-Dichlorobenzene	0.513 ± 0.019	0.179	14.20 ± 1.18	1.03
*Nitrobenzene	0.619 ± 0.022	0.228	18.20 ± 1.40	1.05

The depolarization and cross-sections were calculated for the photon scattering at 400 nm.

The experimental values are either directly measured experimentally for all the solvents with the only exception of solvents labelled with *. The cross-sections for those solvents at 400 nm are calculated by curve-fitting the experimental cross-sections at the longer wavelengths with the equation of $\sigma(\lambda) = \alpha\lambda^{-4}$.

S4. Stokes-Shifted Fluorescence (SSF) spectra of fluorobenzene and 1,4-difluorobenzene.

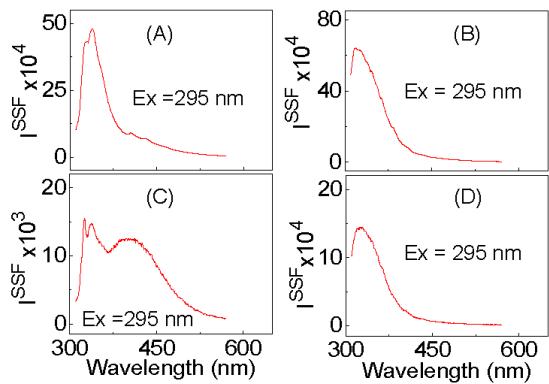


Figure S2: Stokes-Shifted Fluorescence (SSF) spectra for as-received and double-distilled fluorobenzene and 1,4-difluorobenzene. (A-B) As-received and (C-D) Double-distilled (top) fluorobenzene and (bottom) 1,4-difluorobenzene respectively.

S5. Experimental demonstration that the methanol filtration-induced fluorescent impurities and the membrane dissolution

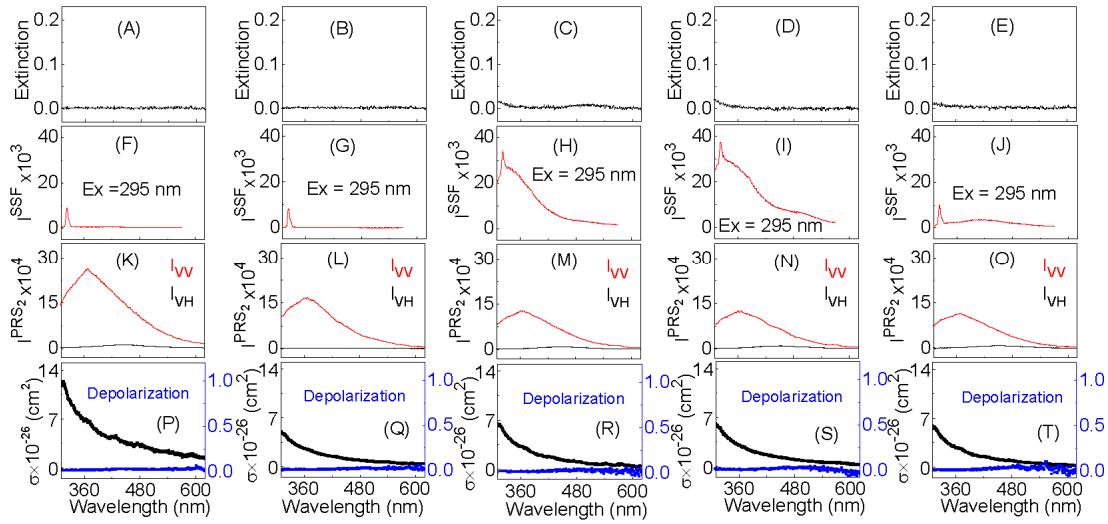


Figure S3: Experimental demonstration that the effect of filtration-induced fluorescence impurities and the membrane dissolution for as-received, double distilled and filtered methanol. Experimental data obtained with methanol; (1st column) as-received,(2nd column) double-distilled, (3rd column) filtered with PP membrane, (4th column) filtered with PES membrane, (5th column) filtered with anopore inorganic membrane. (A-E) UV-vis extinction spectrum, (F-J) SSF spectra. (K-O) Solvent PRS2 spectra with excitation and detection polarization of (red) VV and (black) VH respectively. (P-T) Depolarization spectrum and (black) scattering cross-section spectrum.

S6. Comparison of the depolarization values in this work with literature values

Table S3: Comparison of the depolarization values in this work with literature values

solvent	experimental depolarization	literature reported depolarization
Water	0.026±0.017	0.025 (632.8 nm) ¹
Methanol	0.025±0.009	0.025 (632.8 nm) ^{1,2,3}
Carbondisulfide	0.473±0.017	0.485 (632.8 nm), ¹ 0.483 (632.8 nm), ⁴ 0.41 (632.8 nm) ⁵
Acetone	0.065±0.009	0.084 (632.8 nm), ¹ 0.089 (632.8 nm) ⁴
Chloroform	0.119±0.016	0.118 (632.8 nm), ¹ 0.120 (632.8 nm) ⁴
Carbontetrachloride	0.023±0.011	0.018 (632.8 nm), ¹ 0.023 (632.8 nm), ² 0.021 (633 nm) ³
Cyclohexane	0.026±0.013	0.024 (632.8 nm), ¹ 0.024 (632.8 nm) ⁵
Benzene	0.269±0.019	0.265 (632.8 nm), ¹ 0.268 (632.8 nm), ⁴ 0.245 (633 nm) ³
Toluene	0.333±0.021	0.325 (632.8 nm), ¹ 0.327 (632.8 nm), ⁴ 0.31 (633 nm) ³
Acetonitrile	0.150±0.019	0.186 (632.8 nm), ⁴ 0.17 (632.8 nm) ⁵
Nitrobenzene	0.619±0.022	0.52 (632.8 nm), ² 0.604 (632.8 nm), ⁴ 0.5 (632.8 nm) ⁵

S7. Experimental light scattering depolarization and cross-section spectra for model solvents

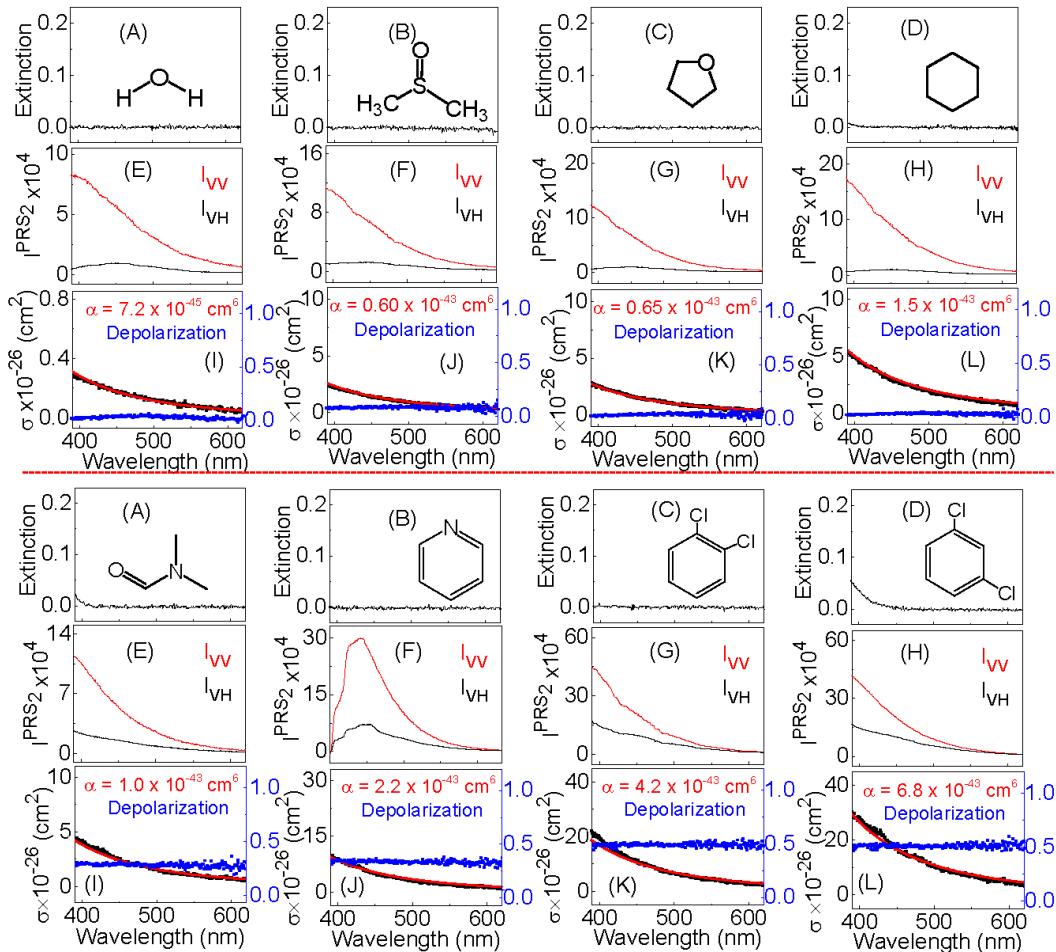


Figure S4: Experimental scattering and depolarization spectra for (top) water, dimethylsulfoxide, tetrahydrofuran, cyclohexane, (bottom) dimethylformamide, pyridine, 1,2-dichlorobenzene, and 1,3-dichlorobenzene. (A-D) UV-vis extinction spectra. (E-H) solvent PRS2 spectra with excitation and detection polarization of (red) VV and (black) VH respectively. (I-L) Depolarization spectrum and (black) scattering cross-section spectrum. The red line in the scattering cross-section spectra is obtained by curve fitting the scattering cross-section spectrum with the equation of $\sigma(\lambda) = \alpha\lambda^{-4}$.

S8. References

- (1) Kaye, W.; McDaniel, J. B. *Appl. Opt.* **1974**, 13, 1934-1937.
- (2) Cardamone, M. J.; Hunt, J. L.; Stevens, J. R. *Chem. Phys. Lett.* **1972**, 12, 628-630.
- (3) Pike, E. R.; Pomeroy, W. R. M.; Vaughan, J. M. *J. Chem. Phys.* **1975**, 62, 3188-3192.
- (4) Burnham, A. K.; Gierke, T. D. *J. Chem. Phys.* **1980**, 73, 4822-4831.
- (5) Malmberg, M. S.; Lippincott, E. R. *J. Colloid Interface Sci.* **1968**, 27, 591-607.