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SUPPORTING INFORMATION

Facile and Fast Photosensing of Polarity by Stimuli-Responsive Materials Based on Spiropyran for Reusable Sensors: A Physico-Chemical Study on the Interactions

Amin Abdollahi, Zeinab Alinejad, Ali Reza Mahdavian*

Polymer Science Department, Iran Polymer & Petrochemical Institute, P.O. Box: 14965/115,

Tehran, Iran Tel: +9821 4478 7000, Fax: +9821 4478 7023

Email: a.mahdavian@ippi.ac.ir

* Corresponding author

Table 1S. Some properties of several alcohols as protic solvents

Protic solvent	V[a] cm³	ρ[b] (g.cm⁻³)	RP[c]	δ_d [d] (MPa)$^{1/2}$	δ_p [d] (MPa)$^{1/2}$	δ_h [d] (MPa)$^{1/2}$	δ_t [e] (MPa)$^{1/2}$	δ_{new} [f] (MPa)$^{1/2}$
Methanol	40.7	0.79	0.762	15.1	12.3	22.3	29.60	25.46
Ethanol	58.5	0.79	0.654	15.8	8.8	19.4	26.52	21.30
Propanol	75.2	0.80	0.617	15.9	3.3	11.8	20.07	12.25
Iso-propanol	76.8	0.78	0.546	15.8	6.1	16.4	23.57	17.50
Butanol	91.5	0.81	0.586	16.00	5.7	15.8	23.19	16.80
2-Butanol	92.00	0.81	0.500	15.8	5.7	14.5	22.18	16.80
Cyclohexanol	106.0	0.93	0.509	17.4	4.1	13.5	22.40	14.11

[a] Molar volume ; see reference 1
[b] Density ; see reference 1
[c] Relative polarity ; see reference 2
[d] Solubility parameters extracted from reference 3
[e] Calculated from: $\delta_t^2 = \delta_d^2 + \delta_p^2 + \delta_h^2$
[f] Calculated from: $\delta_{new}^2 = \delta_p^2 + \delta_h^2$, extracted from reference 4

Table 2S. Some properties of different aprotic solvents

Aprotic solvent	V[a] cm³	ρ[b] (g.cm⁻³)	RP[c]	δ_d [d] (MPa)$^{1/2}$	δ_p [d] (MPa)$^{1/2}$	δ_h [d] (MPa)$^{1/2}$	δ_t [e] (MPa)$^{1/2}$	δ_{new} [f] (MPa)$^{1/2}$
DMF	77.00	0.94	0.386	17.40	13.70	11.30	24.86	17.76
Acetone	74.00	0.79	0.355	15.50	10.40	7.00	19.94	12.53
Acetonitrile	52.60	0.79	0.460	15.30	18.00	6.10	14.40	19.00
DCM	63.90	1.33	0.309	18.20	6.30	6.10	20.20	8.77
MEK	90.10	0.81	0.327	16.00	9.00	5.10	19.05	18.36
THF	81.70	0.89	0.207	16.80	5.70	8.00	19.46	9.82
Toluene	106.80	0.87	0.099	18.00	11.40	2.00	18.16	11.57
Ethyl acetate	98.50	0.90	0.228	15.80	5.30	7.20	18.15	8.94

[a]Molar volume ; see reference 1
[b]Density ; see reference 1
[c] Relative polarity ; see reference 2
[d] Solubility parameters extracted from reference 3
[e] Calculated from: $\delta_t^2 = \delta_d^2 + \delta_p^2 + \delta_h^2$
[f] Calculated from: $\delta_{new}^2 = \delta_p^2 + \delta_h^2$, extracted from reference 4

Table 3S. Group contributions to partial solubility parameters of SPOH [a]

Functional group	number	$\Delta V.\delta^2_d$ (cal.mol^{-1})	$\Delta V.\delta^2_p$ (cal.mol^{-1})	$\Delta V.\delta^2_h$ (cal.mol^{-1})	ΔV (cm^3.mol^{-1})
-C-	2	350	0	0	-19.2
CH_3	2	1125	0	0	33.5
CH_3CH_2OH	1	1683.83	1083.26	5264.68	58.5
HC= , Vinylic	2	875±100	18±5	180±75	13.5
Phenyl	2	7530	50±25	50±50	71.4
NO_2	1	2550±125	1750±100	350±50	32
-N-	1	1050±450	600±350	1350±200	19.2
-O-	1	0	600±150	450±25	3.8

[a] See reference 3

Table 4S. Group contributions to partial solubility parameters of MCOH [a]

Functional group	number	$\Delta V.\delta^2_d$ (cal.mol^{-1})	$\Delta V.\delta^2_p$ (cal.mol^{-1})	$\Delta V.\delta^2_h$ (cal.mol^{-1})	ΔV (cm^3.mol^{-1})
-C-	1	350	0	0	-19.2
-CH-	2	820	0	0	-1
CH_3	2	1125	0	0	33.5
CH_3CH_2OH	1	1683.83	1083.26	5264.68	58.5
HC= , Aliphatic	2	875±100	18±5	180±75	13.5
HC= , Cycloaliphatic	3	875±100	18±5	180±75	13.5
Phenyl	1	7530	50±25	50±50	71.4
NO_2	1	2550±125	1750±100	350±50	32
C=O	1	2350±400	1000±300	400±125	10.8
$-N^+-$	1	1050±300	600±200	1350±200	19.2
C=	1	800±100	60±10	180±75	-5.5

[a] See reference 3

Table 5S. Flory-Huggins interaction parameter (χ_{12}) for different protic solvents and SPOH, MCOH and PMMA

Protic solvent	SPOH	MCOH	PMMA
Methanol	0.87	0.66	1.49
Ethanol	0.66	0.43	1.37
Propanol	0.33	0.23	0.90
Iso-propanol	0.50	0.29	1.33
Butanol	0.51	0.28	1.46
2-butanol	0.43	0.23	1.25
Cyclohexanol	0.37	0.17	1.23

Table 6S. Flory-Huggins interaction parameter (χ_{12}) for aprotic solvents and SPOH, MCOH and PMMA

Aprotic solvent	SPOH	MCOH	PMMA
DMF	0.34	0.29	0.49
Acetone	0.38	0.36	0.23
Acetonitrile	0.89	0.86	0.48
MEK	0.52	0.28	1.28
THF	0.14	0.17	0.32
Toluene	0.92	1.20	0.11
Ethyl acetate	0.39	0.39	0.53

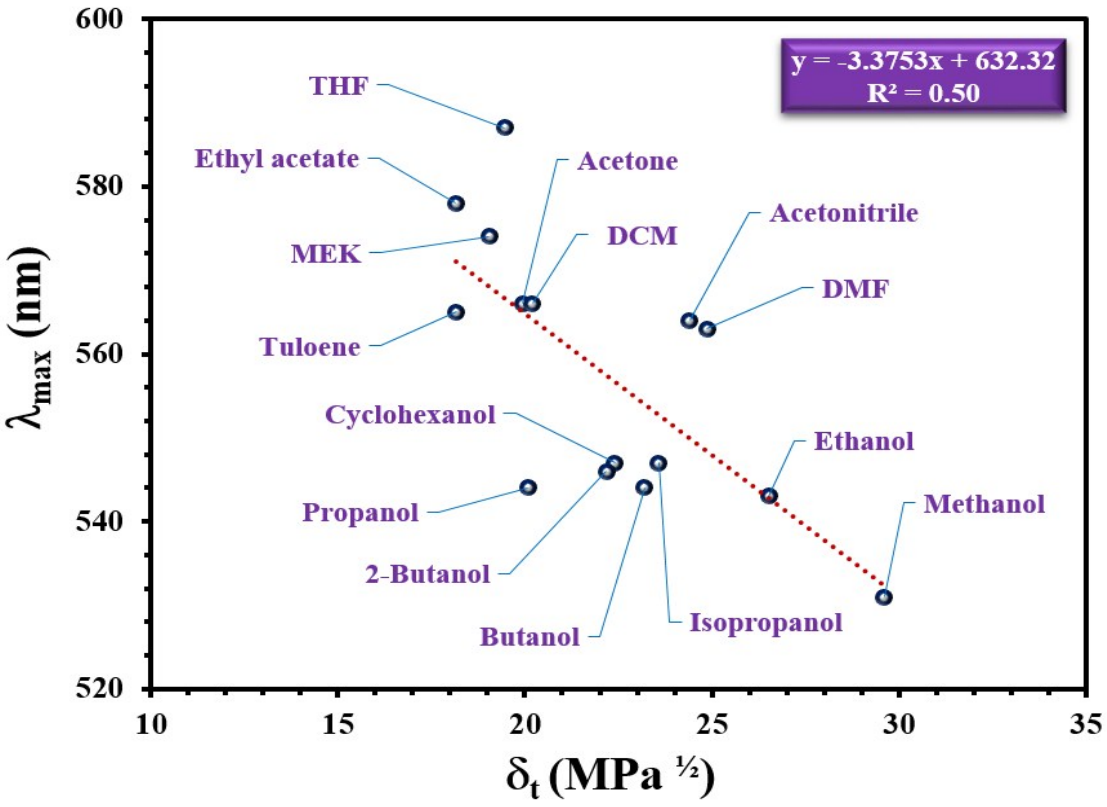

Figure 1S. Relationship between δ_t and λ_{max} for MCOH (after UV irradiation at 365 nm)

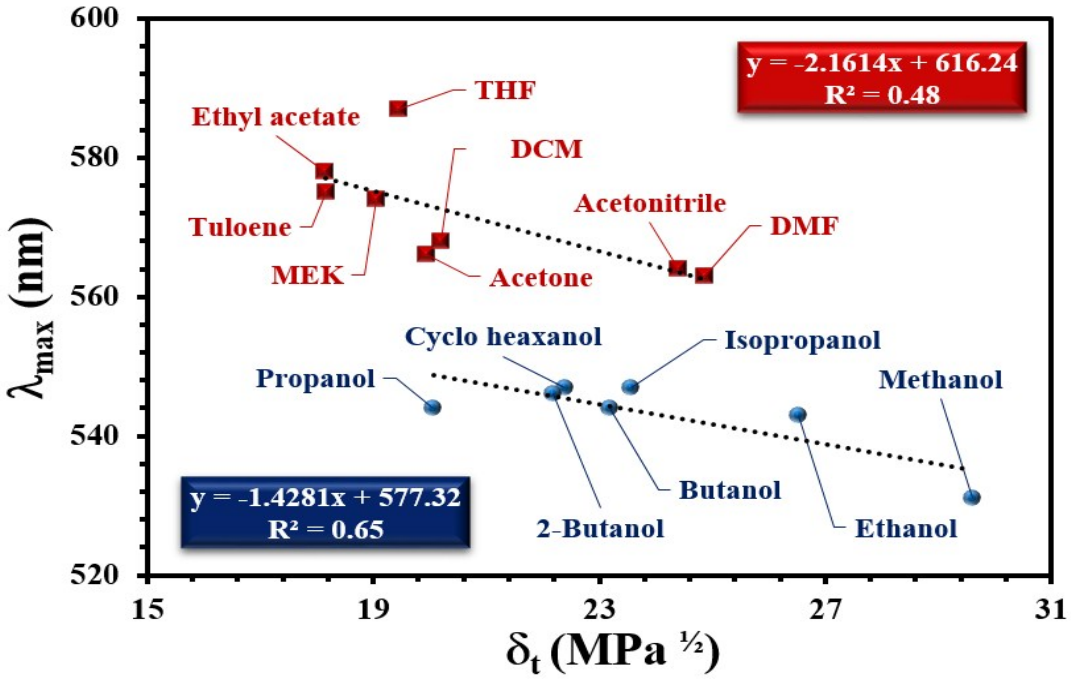

Figure 2S. Relationship between δ_t and λ_{max} for MCOH (after UV irradiation at 365 nm) for protic (blue dots) and aprotic solvents (red squares) separately

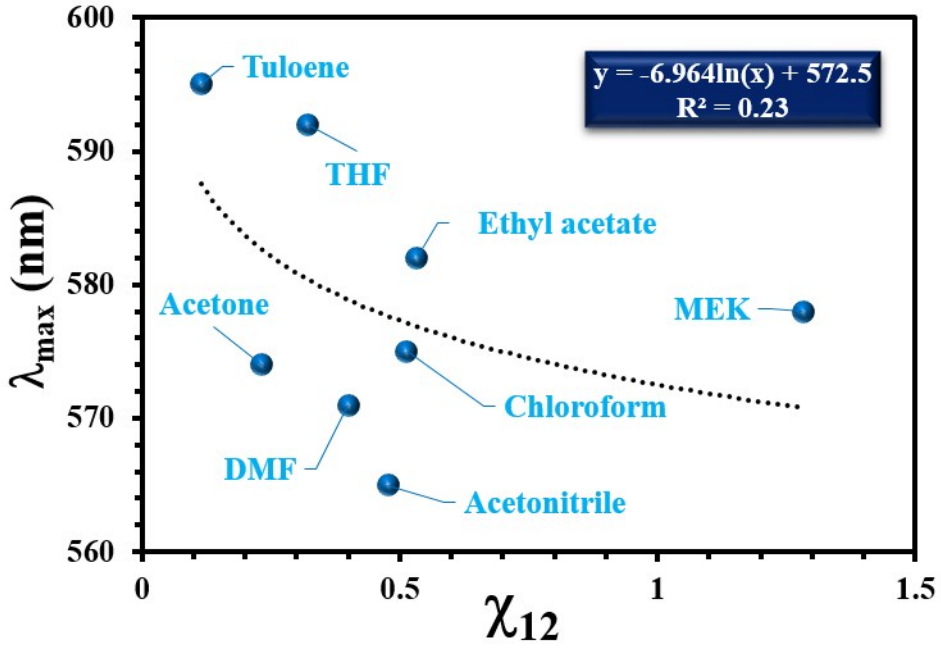

Figure 3S. The relationships between χ_{12} (interaction between solvent and PC with the λ_{max} in aprotic solution

References

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