Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting information

–Revised Version–

Aminobenzodione-based polymers with low band gap and solvatochromic behavior

Haichang Zhang[a], Saman Ghasimi[a], Bernd Tieke*[a] Alexander Schade[b] and Stefan Spange[b]

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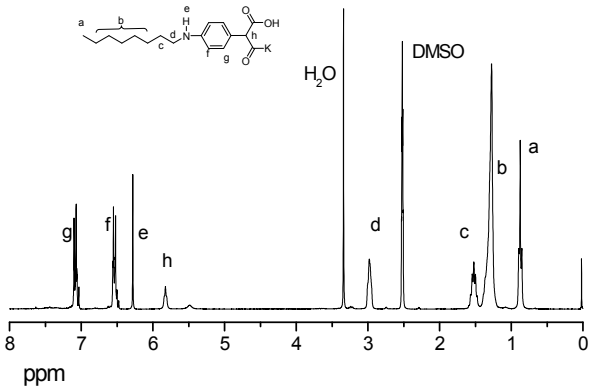

Figure S1. ^{1}H NMR spectrum of 4-(octylamino)phenyltartronic acid.

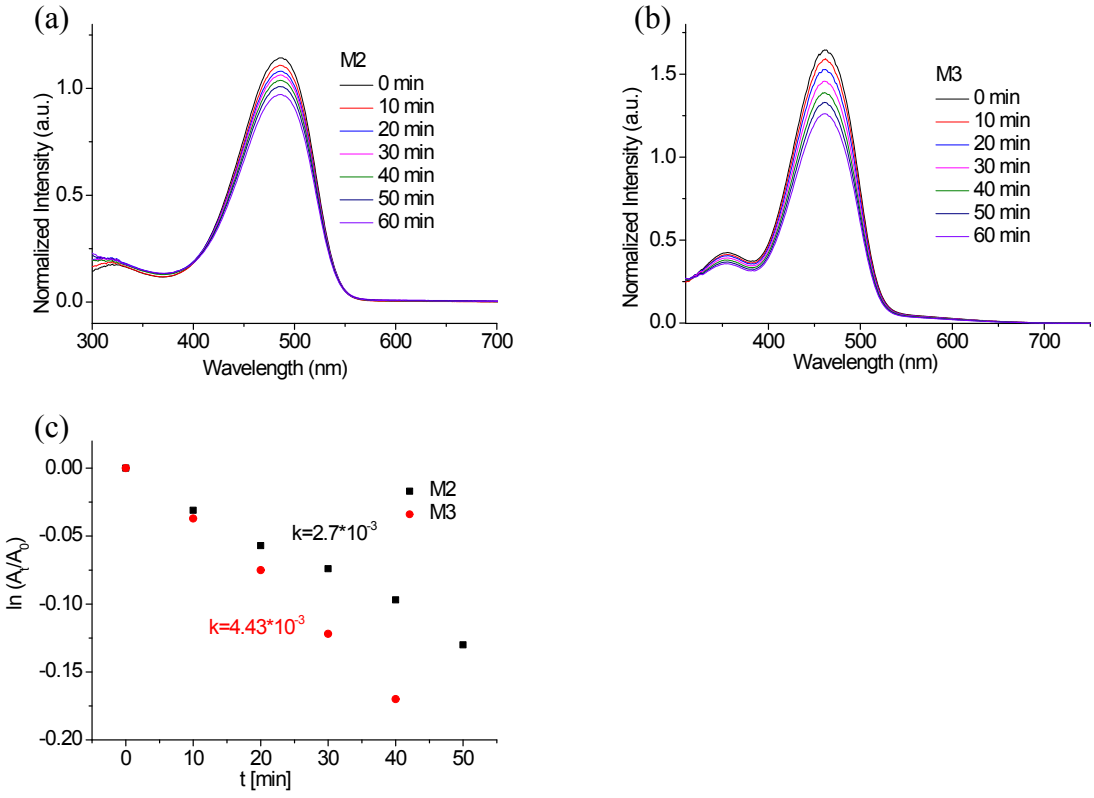

Figure S2. UV/vis absorption spectra of **M2** (a) and **M3** (b) before and after irradiation in toluene and ln(A_t/A_0) *vs*. time for determination of rate constants *k* (c).

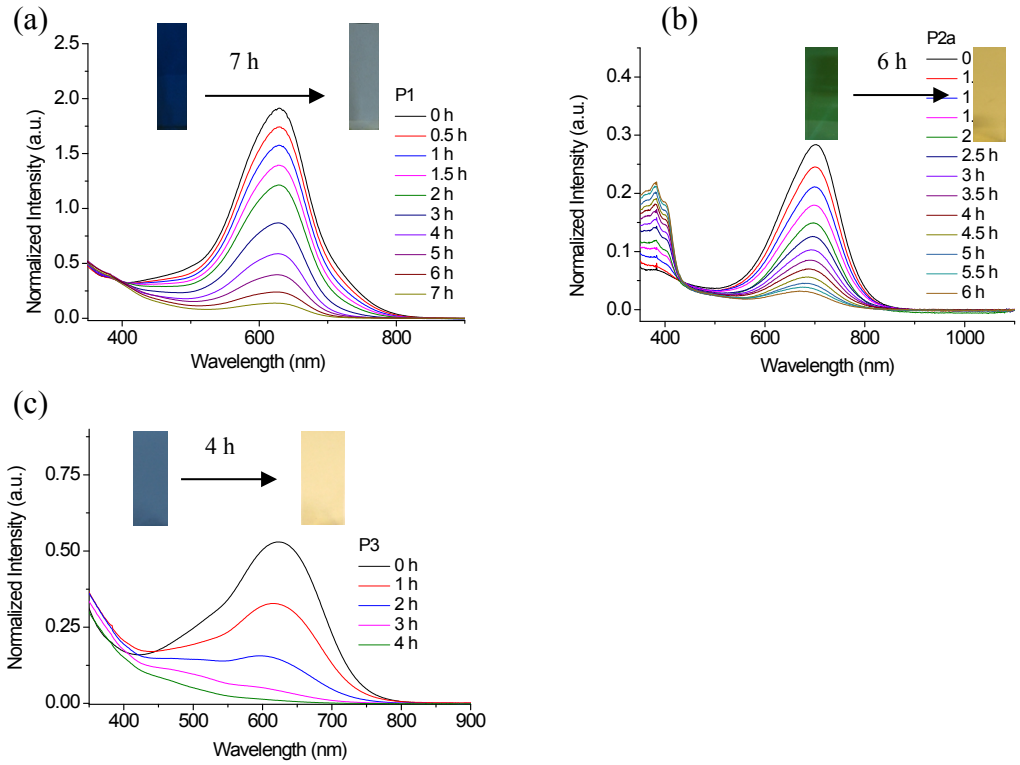

Figure S3: UV/vis absorption spectra of **P1**, **P2a** and **P3** before and after irradiation in toluene.

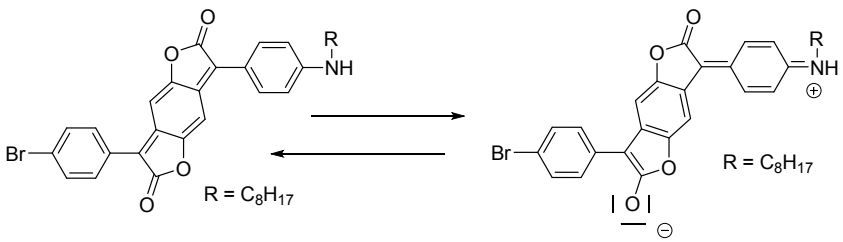

Figure S4: Suggested mechanism of electronic polarization of **M1**.

Table S1: Kamlet–Taft and Catalán parameter sets and UV/vis absoption maxima of **M1**, **P1** and **P2a** in different solvents.

Solvents	Catalán–Parameters[1]				Kamlett– Taft–Parameters[2]			λ_{max} **M1**	λ_{max} **P1**	λ_{max} **P2a**
	SA	*SB*	*SP*	*SdP*	*α*	*β*	*π**	[nm]	[nm]	[nm]
1,1,2,2-tetraclorethane	0	0.017	0.845	0.792	0	0	0.95	640	682	722
1-butanol	0.341	0.809	0.674	0.655	0.84	0.84	0.47	662	659	705
1-propanol	0.367	0.782	0.658	0.748	0.84	0.9	0.52	660	661	708
1-decyl alcohol	0.259	0.912	0.722	0.383	0.7	0.82	0.45	-- a)	-- a)	-- a)
2,2,2,-trifluoroethanol	0.893	0.107	0.543	0.922	1.51	0	0.73	-- a)	-- a)	-- a)
acetone	0	0.475	0.651	0.907	0.08	0.43	0.71	638	664	691
acetonitrile	0.044	0.286	0.645	0.974	0.19	0.4	0.75	626	627	693
anisole	0.084	0.299	0.82	0.543	0	0.32	0.73	630	640	696
benzene	0	0.124	0.793	0.27	0	0.1	0.59	621	634	689
benzonitrile	0.047	0.281	0.851	0.852	0	0.37	0.9	649	685	714
butyrolactone	0.057	0.399	0.775	0.945	0	0.49	0.87	631	662	705
chloroform	0.047	0.071	0.783	0.614	0.2	0.1	0.58	622	661	703
cyclohexane	0	0.073	0.683	0	0	0	0	608	602	678
1,2-dichlorethane	0.030	0.126	0.771	0.742	0	0.1	0.81	625	641	705
dichloromethane	0.04	0.178	0.761	0.769	0.13	0.1	0.82	628	645	709
dioxane	0	0.444	0.737	0.312	0	0.37	0.55	616	630	674
1,2-dimethoxyethane	0	0.636	0.68	0.636	0	0.41	0.53	639	662	689
dimethyl sulfoxide	0.072	0.647	0.83	1	0	0.76	1	670	690	730
diethyl ether	0	0.562	0.617	0.385	0	0.47	0.27	625	614	682
ethanol	0.4	0.658	0.633	0.783	0.86	0.75	0.54	655	650	698
ethyl acetate	0	0.542	0.656	0.603	0	0.45	0.55	632	633	691
ethylene glycol	0.717	0.534	0.777	0.91	0.9	0.52	0.92	-- a)	-- a)	-- a)
formamide	0.549	0.414	0.814	1.006	0.71	0.48	0.97	-- a)	-- a)	-- a)
hexane	0	0.056	0.616	0	0	0	-0.04	602	592	672
hexafluorisoproporol	1.011	0.014	--	--	1.96	0	0.65	656	683	711
HMPA	0	0.813	0.744	1.1	0	1.05	0.87	706 b)	727	731
methanol	0.605	0.545	0.608	0.904	0.98	0.66	0.6	644	640	675
N,N-dimethylacetamide	0.028	0.65	0.763	0.987	0	0.76	0.88	669	703	717
N,N-dimethylformamide	0.031	0.613	0.759	0.977	0	0.69	0.88	665	689	721
nitromethane	0.078	0.236	0.71	0.954	0.22	0.06	0.85	630	634	694
N-methylformamide	--	--	--	--	0.62	0.8	0.9	662	679	712
pyridine	0.033	0.581	0.842	0.761	0	0.64	0.87	664	690	713
triethylamine	0	0.885	0.66	0.108	0	0.71	0.14	631	619	684
tetramethylurea	0	0.624	0.778	0.878	0	0.8	0.83	669	693	721
corbontetrachloride	0	0.044	0.768	0	0	0.1	0.28	618	611	674
tetrahydrofuran	0	0.591	0.714	0.634	0	0.55	0.58	644	671	692
toluene	0	0.128	0.782	0.284	0	0.11	0.54	621	639	689
water	1.062	0.025	0.681	0.997	1.17	0.47	1.09	-- a)	-- a)	-- a)
p-xylene	0	0.16	0.778	0.175	0	0.12	0.43	620	620	692

Table S2: Solvent-independent correlation coefficients a, b and s of the Kamlet–Taft parameters α, β and π^*, solute property of the reference system $\nu_{max,0}$ cyclohexane, number of solvents (n), correlation coefficient (r), standard deviation (sd), and significance (f) of the calculated solvatochromism of the model compounds **M1**, **P1** and **P2a**.

Compound	Kamlet-Taft-equation				Correlation Data			
	$\tilde{\nu}_{max,0}$	a	b	s	n	r	sd	f
M1	16.623	–0.295	–0.951	–0.843	34	0.93	0.185	<0.0001
P1	16.912	–0.143	–0.756	–1.949	35	0.86	0.393	<0.0001
P2b	14.985	–0.058	–0.290	–0.858	35	0.80	0.207	<0.0001

References

1 J. Catalán, *J. Phys. Chem B* 2009, **113**, 5951–5960.

2 Y. Marcus, *Chem. Soc. Rev.* 1993, **22**, 409–416.