Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Excited-state Proton Transfer in *N*-methyl-6-hydroxyquinolinium Salts: Solvent and Temperature Effects

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Supporting Information

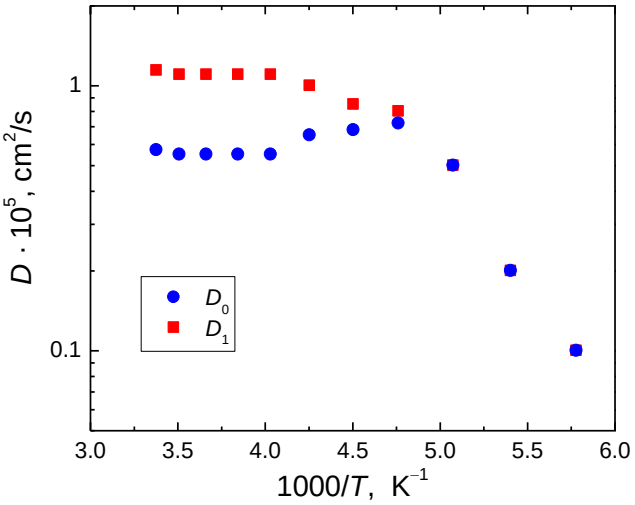


Figure S.1. Mutual diffusion coefficients of a proton-zwitterion pair at different temperatures in BuOH. Both D_0 (circles) and D_1 (squares) are shown.

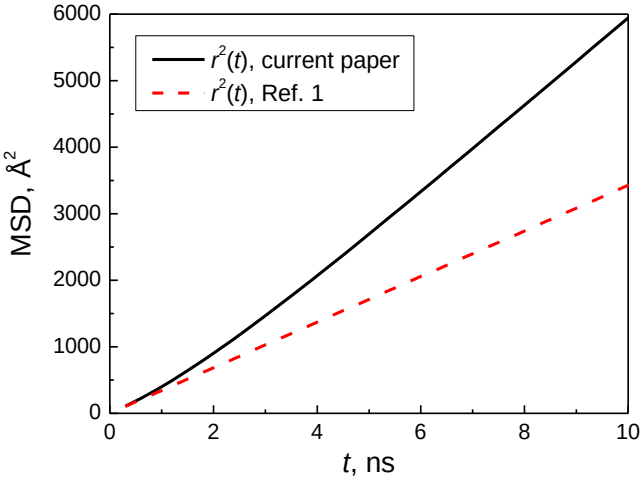


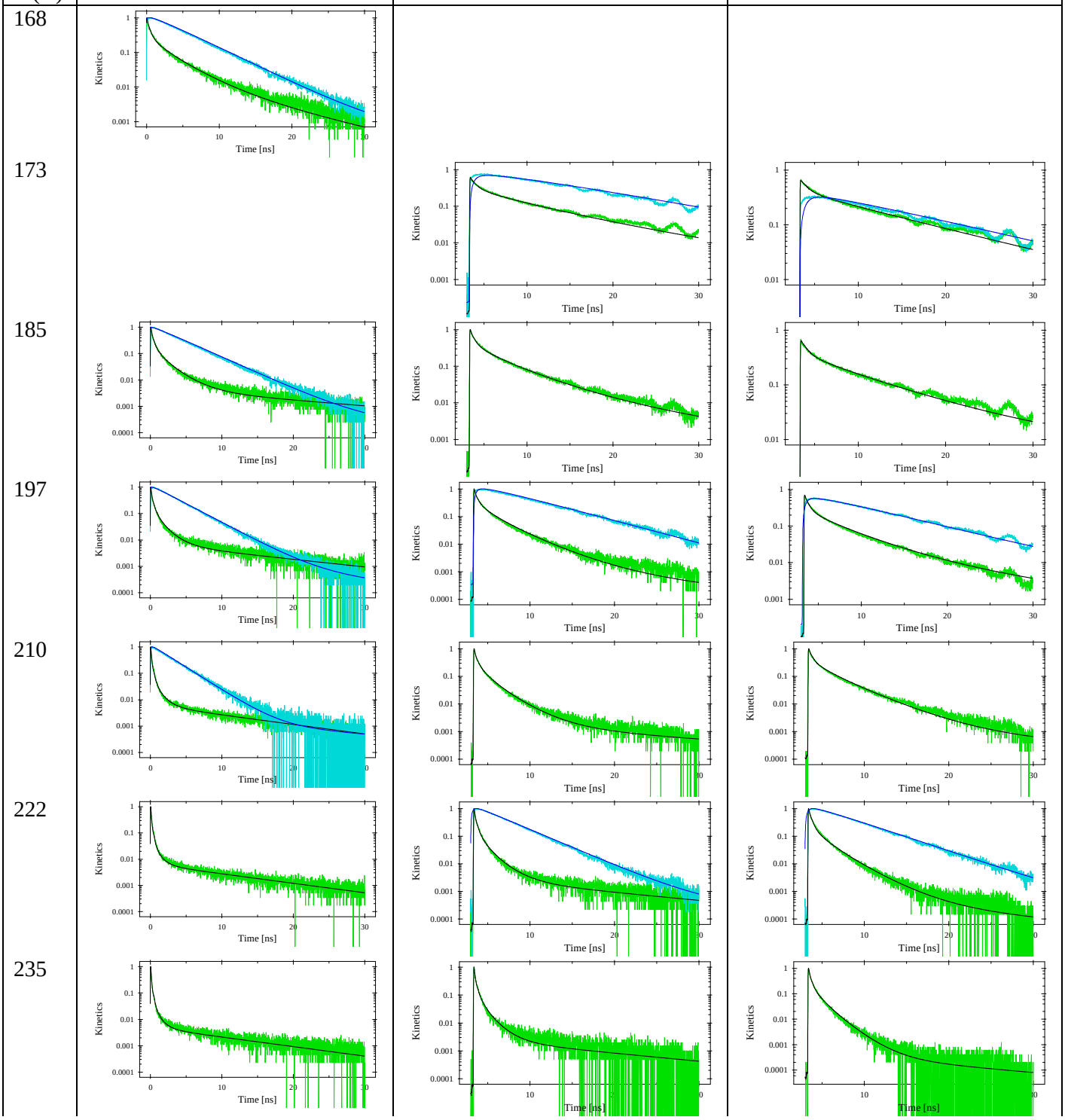
Figure S.2. The mean square displacement of a proton-zwitterion pair at T=293 K in BuOH. Solid line: according to Eq. 7. Dashed line: MSD from Ref. 1.

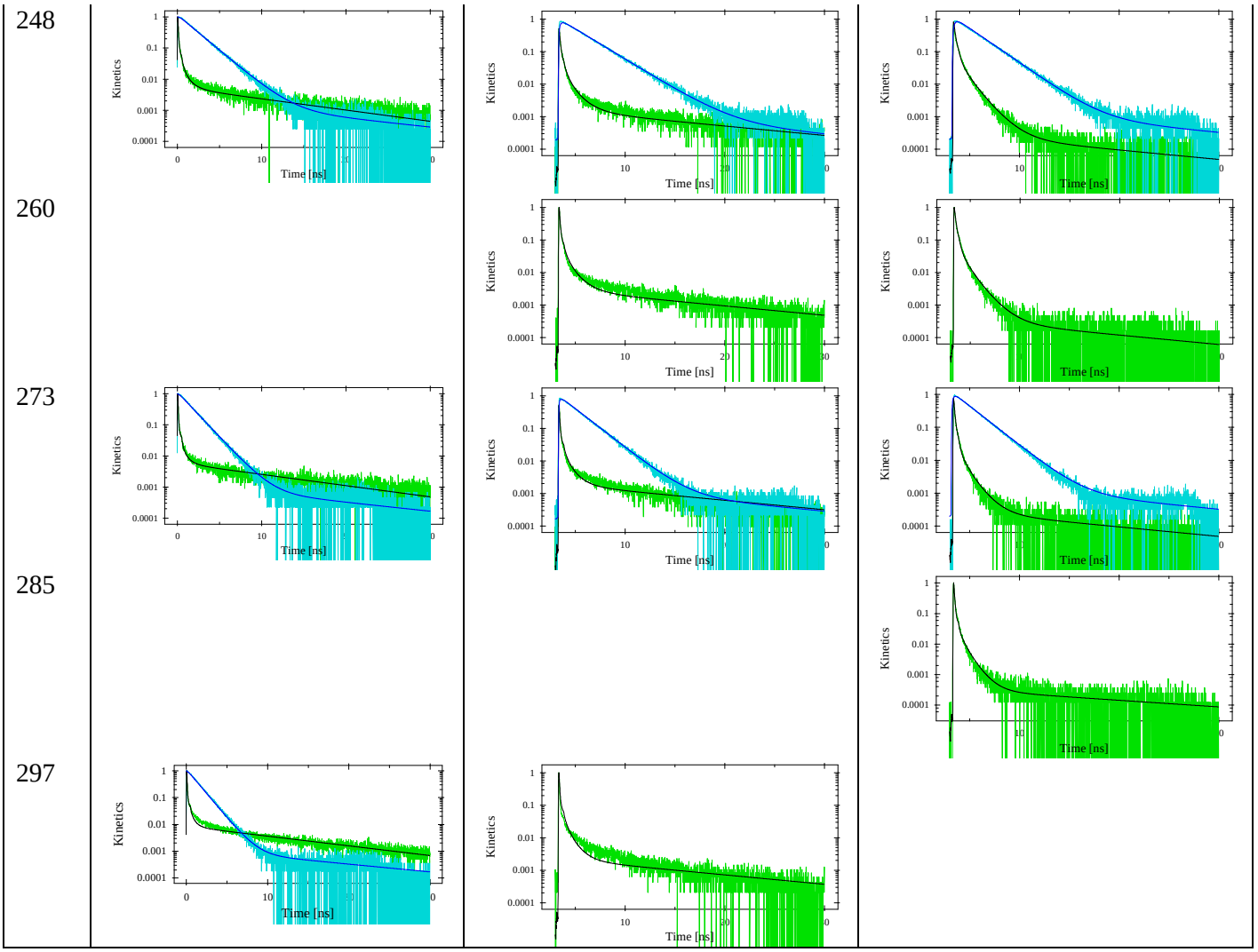
Table S.1. SSDP fit parameters for MHQ in alcohols . Values of τ_{RO^*} are obtained from the experiment while those which are in parentheses are found during SSDP-fitting. When two diffusion coefficients are presented, the first one (in parentheses) denotes the initial diffusion coefficient, D_0, and the second one denotes the final diffusion coefficient, D_1 (see the text).

Solvent	T (K)	k_d (ns^{-1})	k_r (Å/ns)	R_D (Å)[a]	a (Å)	τ_{ROH^*}(ns)	τ_{RO^*}(ns)	D (cm^2/s)	τ (ns)
BuOH	173	0.7	0.08	54.8	5.5	18	8.8	1.0e-6	--
	185	0.9	0.13	51.2	5.5	18	(7.494)	2.0e-6	--
	197	2.0	0.22	48.1	5.5	18	6.5	5.0e-6	--
	210	2.5	0.42	45.1	5.6	18	(5.5)	(7.2e-6) 8.0e-6	3
	222	3.3	0.42	42.7	5.7	18	4.2	(6.8e-6) 8.5e-6	2.5
	235	4.6	0.6	40.3	5.7	18	(2.805)	(6.5e-6) 10.0e-6	2
	248	6	0.4	38.2	5.7	18	2.0	(5.5e-6) 11.0e-6	2
	260	7	0.6	36.4	6	18	(1.978)	(5.5e-6) 11.0e-6	2
	273	9	0.43	34.7	5.9	18	1.8	(5.5e-6) 11.0e-6	2
	285	13	0.6	33.2	5.8	18	(1.482)	(5.5e-6) 11.0e-6	2
	293[b]	13	0.4	35.8	5.7	20	1.25	**5.71e-6**	--
PrOH	173	1.3	0.45	44.7	5.7	18	9.5	1.5e-6	--
	185	2.2	0.7	41.8	5.7	18	(6.953)	3.5e-6	--
	197	3.3	1	39.3	5.7	18	5.2	6.0e-6	--
	210	4.2	1.7	36.8	5.8	18	(4.107)	9.0e-6	--
	222	6	2.1	34.9	6	18	3.3	12.0e-6	--
	235	8	2.9	32.9	6	18	(2.713)	14.0e-6	--
	248	10	3	31.2	6.3	18	2.3	15.0e-6	--
	260	14	3.5	29.8	6.2	18	(2.2)	15.0e-6	--
	273	18	4	28.3	6.2	18	1.8	15.0e-6	--
	297	20	6	27.1	6.3	18	(1.6)	15.0e-6	--
EtOH	168	3	1	41.3	6.3	18	4.0	1.5e-6	--
	185	4.5	1.6	37.5	6.3	18	3.5	5.0e-6	--
	197	6.5	3	35.2	6.3	18	3.0	11e-6	--
	210	10	3.2	33.1	6.3	18	2.5	19e-6	--
	222	11.5	3.4	31.3	6.3	18	(2.203)	20e-6	--
	235	13	4.8	29.5	6.4	18	(1.96)	23e-6	--
	248	18	5.5	28.0	6.4	18	1.9	25e-6	--
	273	24	6	25.4	6.5	18	1.5	25e-6	--
	297	28	11	23.4	6.4	18	1.2	25e-6	--

[a]From the temperature dependent formula: $R_D = 168668/\varepsilon T$ (A˚) [b] From Ref. 1 of the main text.

Figure S.3. SSDP Fits of C* (green) and Z* (cyan) decays on MHQ in various alcohols at different temperatures.




248
260
273
285
297
Kinetics
Time [ns]

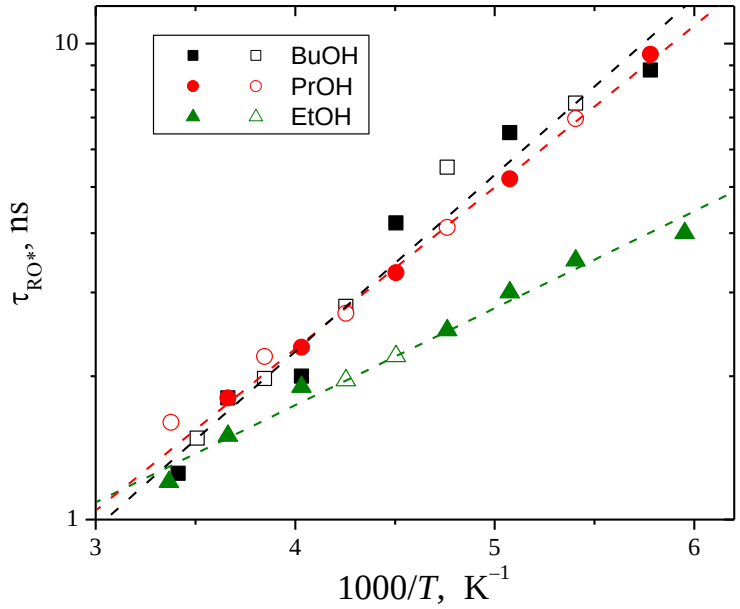


Figure S.4. The lifetime τ_{RO^*} of a proton-zwitterion pair at different temperatures in BuOH (black squares), PrOH (red circles) and EtOH (green triangles). Filled symbols correspond to the values obtained from the experiment while open ones are found by SSDP-fitting. Slopes of straight lines indicate the activation energies which are 7.1, 6.5 and 3.9 kJ/mol for BuOH, PrOH and EtOH, respectively.