Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Excited-state hydrogen relay along a blended-alcohol chain as a model system of a proton wire: deuterium effect on the reaction dynamics

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Table S1 List of abbreviations

Symbol	Word	Symbol	Word
7HQ	7-Hydroxyquinoline	ESPT	Excited-state proton transfer
7DQ	Deuterated 7HQ	ESDT	Excited-state deuteron transfer
ROH	Normal alcohol	H bond	Hydrogen bond
ROD[a]	Deuterated alcohol	K	Association constant
N	Normal species of 7DQ	α	Proton-donating ability (acidity)
T	Tautomeric species of 7DQ	β	Proton-accepting ability (basicity)
Nc	Cyclic 7DQ·$(ROD)_2$ complex	k_{PT}	Rate constant of ESPT
S[b]	Relatively strong-acidic alcohol in **Nc**	k_{DT}	Rate constant of ESDT
W[b]	Relatively weak-acidic alcohol in **Nc**	KIE[c]	Kinetic isotope effect

[a] MeOD, EtOD, and BuOD are symbols for deuterated methanol, ethanol, and *tert*-butanol, respectively. [b] In a blended alcohol chain. [c] Calculated as k_{PT}/k_{DT}.

Table S2 Alcohol-dependent K and k_{DT} in *n*-heptane

Alcohol	α[a]	β[a]	K/M^{-2}	k_{DT}^{-1}/ps	KIE[b]
Methanol	0.93	0.62	8400[c] (9100)[d]	430	6.8
Ethanol	0.83	0.77	5200 (6800)	560	7.8
tert-Butanol	0.68	1.01	3400 (4200)	920	5.6

[a] Proton-donating (α) and -accepting abilities (β), which signify the acidity and the basicity, respectively, of ROH because the values of ROD are not available in literatures.[46–48] [b] Kinetic isotope effect calculated as k_{PT}/k_{DT}.[34] [c] For 7DQ·(ROD)$_2$.[33] [d] For 7HQ·(ROH)$_2$.[33]

Table S3 Fluorescence kinetic constants of 7DQ in ROD-added *n*-heptane[a]

	N* fluorescence decay		**T*** fluorescence	
Alcohol[b]	τ_{fast}[c]/ps	τ_{slow}/ps	τ_{rise}/ps	τ_{decay}/ps
MeOD	430	1800 (10%)[d]	430	4900
EtOD	560	1700 (13%)	560	5300
BuOD	920	1600 (13%)	920	5000

[a] **N*** and **T*** fluorescence were monitored at 420 nm and 550 nm, respectively, after excitation of **Nc** at 355 nm. [b] The concentration of each alcohol was kept at 30 mM in *n*-heptane. [c] ESDT time (k_{DT}^{-1}). [d] Initial amplitude percentage of the slow decay component.